Nanotechnology Research Centre

AFMD 2026

SRM INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)

2nd INTERNATIONAL CONFERENCE ON ADVANCED FUNCTIONAL MATERIALS AND DEVICES (AFMD-2026)

March 19 - 24, 2026

PROCEEDINGS

Supported by

Anusandhan National Research Foundation

CSIR-INDIA
सीएसआईआर
CSIR
भारत का नवाचार इंजन
The Innovation Engine of India

DRDO
DEFENCE R&D ORGANISATION
MINISTRY OF DEFENCE

Co-Supported by

International Society of Electrochemistry
ISE

The Japan Society of Applied Physics

The Ceramic Society of Japan

Organized by

NANOTECHNOLOGY RESEARCH CENTRE (NRC)
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY
Kattankulathur - 603 203, Chennai, Tamil Nadu, India



Conference Chair
Prof. M. Navaneethan

2nd International Conference on Advanced Functional Materials and Devices (AFMD - 2026)

19-24 March, 2026

PROCEEDINGS

Organized by

Nanotechnology Research Center (NRC)
SRM Institute of Science and Technology
Kattankulathur, Chennai,
Tamilnadu, India.

Edited by

Prof. M. Navaneethan

Supported by

Anusandhan National Research Foundation (ANRF), Department of Science and Technology, Government of India

Council of Scientific & Industrial Research (CSIR), Ministry of Science and Technology, Government of India

Defence Research and Development Organisation (DRDO) Ministry of Defence, Government of India

Co-Supported by

- The International Society of Electrochemistry (ISE)
- The Japan Society of Applied Physics, Japan
- The Ceramic Society of Japan, Japan
- Netweb Technologies, India
- Syinco Technologies, India
- Advance Riko, Japan
- GMS Elegant builders, India
- Solaris Computers, India
- Lab India Instruments, India
- Greatify AI, India
- Delta Electronics, India
- NETZSCH, Germany
- VT Vaccum Technologies Private Limited, India
- Icon Analytical, India
- Southern India Scientific Corporation, India
- Swans Enterprises, India
- Printography Systems, India
- Firstline Infotech, India
- Institute of Physics (IOP)
- Nanotech Instruments, India
- Codetantra, India
- Unicard Technologies Pvt. Ltd., India
- Jeol, India
- IR Tech, india

In Association with























SRM Institute of Science and Technology



Dr. Ravi Pachamuthu
Pro-Chancellor (Administration)
SRMIST

MESSAGE

Greetings from SRMIST!!

The 2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026), organized by the Nanotechnology Research Centre at the SRM Institute of Science and Technology, Kattankulathur, Chennai, to be held from March 19–24, 2026.

AFMD 2026 brings together distinguished scientists, academicians, industry experts, and young researchers from across the globe to deliberate on emerging advancements in advanced functional materials and device technologies. The conference provides a significant platform for interdisciplinary engagement, fostering scientific exchange and strengthening collaborative networks across nations. With its comprehensive technical sessions covering nanotechnology, energy and sustainable materials, electronic and photonic devices, thin films, computational materials science, and biomaterials, AFMD 2026 reflects the dynamic evolution of modern materials research. Such initiatives play a vital role in translating scientific discoveries into transformative technologies that address global challenges.

This international forum is expected to stimulate meaningful discussions, inspire innovative research directions, and encourage young scholars to pursue excellence in materials science and nanotechnology.

I wish the AFMD-2024 a great success.

Pro Chancellor (Administration)



Dr. P. Sathyanarayanan
Pro Chancellor (Academics)

09 – Mar - 2026

MESSAGE

It gives me great pleasure to learn that the Nanotechnology Research Centre at SRM Institute of Science and Technology is organizing the **2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026)** from March 19th – 24th, 2026.

Building on the success of its inaugural edition, AFMD 2026 brings together leading scientists, academicians, industry experts, and young researchers from across the world to deliberate on emerging advancements in functional materials and device technologies.

Research in advanced materials continues to play a transformative role in addressing critical global challenges. Developments in areas such as quantum materials, sustainable energy systems, biomaterials, environmental monitoring, and next-generation electronic and photonic devices are redefining technological possibilities and shaping the future of science and engineering.

Conferences such as AFMD 2026 are vital in promoting interdisciplinary dialogue, enabling global collaboration, and nurturing the next generation of researchers. By bringing together diverse scientific perspectives, the conference will serve as an important platform for knowledge exchange and the development of impactful research partnerships.

I congratulate the organizing committee for their efforts in hosting this international gathering and extend my best wishes for the grand success of AFMD 2026. I am confident that the discussions and outcomes of this conference will contribute significantly to advancing research and innovation in materials science.

Pro Chancellor (Academics)

Prof. C. Muthamizhchelvan, Ph.D
Vice Chancellor

SRM
INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be **University** *u/s 3 of UGC Act, 1956)*

4th March 2026



Message

The second International Conference on **Advanced Functional Materials and Devices (AFMD-2026)** is being organized by the Nanotechnology Research Centre, SRM Institute of Science and Technology during March 19-24, 2026. I am delighted to welcome the speakers and participants from a diverse spectrum of countries, including India, Japan, Malaysia, Australia, Malaysia, United Kingdom, and many more.

This conference is not merely a meeting of minds it is a celebration of human ingenuity and the limitless possibilities of science. With participants from across the globe India, Japan, Malaysia, Australia, the United Kingdom, and many more AFMD-2026 embodies the spirit of collaboration that transcends borders and cultures.

Material science and nanotechnology are at the heart of tomorrow's breakthroughs. They hold the power to reshape industries, revolutionize healthcare, and unlock sustainable solutions for our planet. The symposia and deliberations at this conference will illuminate pathways to innovations that can transform lives, inspire hope, and address the most pressing challenges of our time.

AFMD-2026 is more than a scientific forum; it is a beacon for young researchers, encouraging them to dream boldly, think differently, and pursue excellence with passion. It is here that ideas will converge, collaborations will flourish, and the seeds of future discoveries will be sown. I am confident that this conference will leave an indelible mark on the global scientific community and strengthen our collective resolve to push the boundaries of knowledge.

I extend my heartfelt wishes for the resounding success of AFMD-2026 and look forward to the transformative impact it will inspire.

Vice Chancellor

Prof. C. MUTHAMIZHCHELVAN
Vice Chancellor
SRM Institute of Science and Technology
SRM Nagar, Kattankulathur - 603 203.
Chengalpattu Dist., Tamilnadu, India.

Dr. S. Ponnusamy, Ph.D.
Registrar

SRM
INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)



Greetings from SRM Institute of Science and Technology!!!

I am delighted that the **Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology**, is organizing the *2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026)*, scheduled from March 19-24, 2026. The enthusiastic participation of distinguished scientists, industry experts, and promising young researchers from across the globe reflects the growing importance of advanced functional materials in shaping next-generation technologies.

AFMD 2026 serves as a leading international platform for knowledge exchange, interdisciplinary collaboration, and innovation in the rapidly evolving domains of materials science and nanotechnology. As functional materials continue to drive transformative advancements in energy conversion and storage, catalysis, electronics, photonics, biomaterials, and sustainable technologies, this conference offers an invaluable opportunity for researchers to present pioneering work, engage in meaningful discussions, and build strategic partnerships.

The conference stands as a dynamic forum to foster research collaborations, inspire creativity, and promote academic excellence. The overwhelming response to this edition underscores the pivotal role of advanced materials research in accelerating technological progress and addressing global societal challenges. I am confident that the deliberations and interactions during AFMD 2026 will spark new ideas, strengthen international networks, and motivate participants to pursue impactful innovations that define the future of materials science and device engineering.

I extend my best wishes for the grand success of AFMD 2026.

Registrar
Registrar
SRM Institute of Science and Technology
SRM Nagar, Kattankulathur - 603 203
Chengalpattu Dist, Tamilnadu, India.

SRM
INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)

Dr. Leenus Jesu Martin M, Ph.D.

Dean, CET



Message

It is with great pride that I extend my heartfelt felicitations to the **Nanotechnology Research Centre at the SRM Institute of Science and Technology for organizing the 2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026), scheduled from March 19–24, 2026.**

Advanced functional materials and device engineering form the backbone of modern technological advancement. From renewable energy systems and intelligent electronics to high-performance structural components and smart sensing platforms, the role of materials innovation is transformative. AFMD 2026 provides an important academic forum for researchers, faculty members, industry professionals, and young scholars to deliberate on emerging trends and cutting-edge research.

The conference reflects SRMIST's commitment to nurturing a research-driven academic environment that promotes interdisciplinary collaboration and global engagement. The convergence of experts from diverse domains will undoubtedly enrich scientific dialogue and foster meaningful partnerships.

My sincere wishes for the grand success of AFMD 2026.

Warm regards,

Dean, CET

2/3/2026

Dean
College of Engineering and Technology
SRM Institute of Science and Technology
SRM Nagar, Kattankulathur - 603 203
Chengalpattu Dist. Tamilnadu, India.

डॉ. समिर वी. कामत
Dr. Samir V. Kamat

सत्यमेव जयते
भारत सरकार
Government of India

स्वच्छ भारत
एक कदम स्वच्छता की ओर

सचिव, रक्षा अनुसंधान तथा विकास विभाग
एवं
अध्यक्ष, डीआरडीओ
Secretary, Department of Defence R&D
&
Chairman, DRDO



MESSAGE

I would like to convey my greetings on the occasion of the 2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026), to be held from March 19–24, 2026, at the SRM Institute of Science and Technology, organised by the Nanotechnology Research Centre.

The theme of AFMD 2026 underscores the critical role of advanced functional materials and integrated device technologies in shaping future-ready systems. Innovations in nanostructured materials, high-performance ceramics, smart coatings, energy storage materials, quantum systems and advanced electronic architectures are central to strengthening strategic capabilities and ensuring technological self-reliance.

Modern defence and aerospace platforms increasingly depend on multifunctional materials with enhanced thermal stability, mechanical strength, electromagnetic performance, and environmental resilience. The integration of such materials into intelligent devices and adaptive systems represents a transformative direction in engineering and applied science.

By bringing together researchers, technologists and industry leaders, AFMD 2026 provides an important forum to accelerate interdisciplinary collaboration and translational research aligned with national priorities. The scientific deliberations at this conference are expected to inspire innovative solutions and foster partnerships that contribute to resilient and advanced technological ecosystems.

My best wishes for a grand success of AFMD 2026.

Kamat

(Dr. Samir V. Kamat)

Date : 03/03/26

Place : New Delhi

रक्षा मंत्रालय, रक्षा अनुसंधान तथा विकास विभाग, डीआरडीओ भवन, नई दिल्ली-110011
Ministry of Defence, Department of Defence R&D, DRDO Bhawan, Rajaji Marg, New Delhi-110011
दूरभाष/Phone : 011-23011519, 23014350 फैक्स/Fax : 011-23018216 ई-मेल/E-mail : secydrdo@gov.in

Shizuoka University

Message for the 2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026)

I am delighted to deliver a welcome speech for the 2nd International Conference on Advanced Functional Materials and Devices (AFMD 2026) which is organized at the SRM Institute of Science and Technology (SRMIST), India. It is an honor for Shizuoka University to join the hands with SRMIST in the academic and research activities.

Shizuoka University has currently seven Faculties such as Humanities and Social Science, Education, Informatics, Science, Engineering, Agriculture, Global Interdisciplinary Science and Innovation, and School of Regional Development. There are six Graduate Schools for master and doctoral course. In addition to that, we have Research Institute of Electronics and Research Institute of Green Science and Technology to promote the research activity. Shizuoka University's staff and students uphold the philosophy of "freedom and enlightenment" as a mainstay of education, research and collaboration with society, industry and overseas.

Collaboration between Shizuoka University and SRMIST started in 2009 before the Memorandum of Understanding was signed in 2014. Since then, the colleagues in both Universities have been fostering the relationship steadily, which have led to the promotion of Double Degree Program (DDP) in the doctoral course and exchange program of students. This collaboration is now one of the most active frameworks among the collaborations between the other foreign Universities and Shizuoka University. Moreover, we proposed India-Shizuoka Partnership for Innovation, Research, and Education (InSPIRE) Program which strengthens ties with partner universities in India, primarily SRMIST, and it begins in October, 2025.

Shizuoka University is grateful to SRMIST for their tremendous support as host of many joint conferences including AFMD and ICONN which is another conference hosted jointly by Shizuoka University and SRMIST. I hope that all the speakers and researchers will enjoy the scientific discussions and strengthen the collaboration.

Finally, I would like to express my sincere thanks to all members of conference committee, and participants.

Kazuyuki Hizume

Prof. Kazuyuki Hizume

President of Shizuoka University

March 4, 2026

Felicitation message from Daegu Gyeongbuk Institute of Science and Technology (DGIST), Republic of Korea!!

It is a great honour for the Daegu Gyeongbuk Institute of Science and Technology (DGIST), Republic of Korea, to extend our warmest congratulations to the Nanotechnology Research Centre, SRM Institute of Science and Technology, for organizing the 2nd International Conference on Advanced Functional Materials and Devices (AFMD-2026), to be held from March 19–24, 2026.

As science advances at an unprecedented pace, the future of technology increasingly depends on the intelligent design of advanced functional materials and innovative device architectures. From sustainable energy systems and quantum technologies to smart electronics and environmental solutions, the research themes at AFMD-2026 are central to shaping a resilient, technology-driven global society.

We believe that meaningful innovation emerges where disciplines intersect, and international collaborations thrive. AFMD-2026 provides an exceptional global platform for researchers, industry leaders, and young scientists to exchange transformative ideas, explore interdisciplinary approaches, and establish lasting research partnerships. Such forums are essential in translating fundamental discoveries into impactful technologies.

DGIST, as a leading research-oriented institution dedicated to convergence science and advanced technology development, strongly values international academic engagement. We are confident that AFMD-2026, taking place from March 19–24, 2026, will stimulate insightful discussions, inspire pioneering research directions, and strengthen scientific networks across continents.

We commend the organizing committee for its vision and dedication in bringing together a distinguished community of global experts. On behalf of DGIST, we wish AFMD-2026 every success and look forward to continued collaboration in advancing science and innovation for the benefit of society.

Dr. Sangaraju SHANMUGAM
Senior Professor,
Department of Energy Science and Engineering,
Daegu Gyeongbuk Institute of Science & Technology (DGIST),
Deagu-42988, Republic of Korea,
Tel: 82 53785 6413; Fax: 82 53 785 6409.
Email: sangaraju@dgist.ac.kr

1862
RIGA TECHNICAL UNIVERSITY
Riga Technical University, Reg. No. 90000068977, Kīpsalas street 6A, Riga, LV- 1048, Latvia
Phone: +371 67089999, fax: +371 67089710, e-mail: rtu@rtu.lv, www.rtu.lv

Rīgā

03.03.2026. No. 04000 2.2.1-e/8

International Conference on Advanced Functional Materials and Devices-2026 (AFMD-2026)

Address on the occasion of the opening of the conference "International Conference on Advanced Functional Materials and Devices-2026 (AFMD-2026)" in Nanotechnology Research Centre of SRM Institute of Science and Technology, Chennai, India

Dear colleagues and participants,

It is with great pleasure and excitement that I address you on behalf of Riga Technical University (RTU). AFMD-2026 stands as a testament to the power of international cooperation – fostering interdisciplinary research, encouraging visionary ideas, and building bridges across cultures and continents that together shape the future of science and engineering. Such collaborative platforms empower us not only to share breakthroughs and discoveries but also to inspire the next generation of researchers and innovators.

At Riga Technical University, we are committed to advancing research excellence and international partnerships that fuel transformative scientific progress. I am confident that this conference will be a fertile ground for thought leadership, meaningful dialogue, and synergistic collaborations that resonate far beyond this venue. As you engage in discussions, enjoy inspiring keynote lectures, and present your outstanding research contributions, may this gathering serve as a beacon of shared curiosity, creativity, and scientific achievement.

In closing, I wish all participants a highly productive and inspiring conference. May AFMD-2026 foster ideas and collaborations that advance our collective pursuit of knowledge and innovation.

Vice-Rector for Research

M. Indrikova

UNIVERSITAS INDONESIA
FACULTY OF ENGINEERING

Gedung Dekanat Fakultas Teknik
Kampus UI Depok 16424
P. 62.21.7863504, 7863505, 78888430
F. 62.21.7270050
E. humas@eng.ui.ac.id
www.eng.ui.ac.id

Greetings from Universitas Indonesia.

It is a privilege to extend my warm greetings to all distinguished guests, speakers, and participants of the International Conference on Advanced Functional Materials and Devices (AFMD-2026), organized by the Nanotechnology Research Centre, SRM Institute of Science and Technology.

This conference provides an excellent platform for researchers worldwide to exchange ideas and present advancements in advanced functional materials, nanotechnology, and emerging device applications. Such discussions are essential for driving innovation in sustainable and environmentally responsible technologies.

The Department of Electrical Engineering, Faculty of Engineering, Universitas Indonesia, remains committed to promoting sustainability through renewable energy initiatives, green campus programs, and responsible environmental practices.

I sincerely appreciate the organizers and contributors for making this event possible and wish all participants a productive and inspiring conference experience.

UNIVERSITAS INDONESIA
FAKULTAS TEKNIK

ditandatangani
secara elektronik
digitally signed

Dr. Muhammad Salman, S.T., M.IT.
Head of Electrical Engineering Department
Faculty of Engineering, Universitas Indonesia

Dokumen ini telah ditandatangani secara elektronik menggunakan sertifikat elektronik yang diterbitkan oleh Balai Besar Sertifikasi Elektronik (BSrE) Badan Siber dan Sandi Negara.

Greeting message from Faculty of Physics, Alexandru Ioan Cuza University of Iași, Romania

On behalf of the academic community at the Faculty of Physics, Alexandru Ioan Cuza University of Iași, Romania, it is our pleasure to extend warmest greetings and congratulations to the organizers of the 2nd International Conference on Advanced Functional Materials and Devices (AFMD-2026), scheduled for March 19–24, 2026.

The advancements since the inaugural edition underscore the leadership and the orientation towards international collaboration upheld by the Nanotechnology Research Centre at SRM Institute of Science and Technology. AFMD has emerged as a international forum, fostering interdisciplinary discourse and collaborative endeavours in advanced functional materials, nanotechnology, and cutting-edge device engineering.

We hold in high regard our enduring affiliation with AFMD and its partner institutions, which collectively elevate its international stature. Events such as AFMD-2026 are instrumental in fortifying academic partnerships, nurturing emerging scholars, and promoting scientific interchange across borders.

It is our aspiration that this second edition will further solidify research consortia, spark innovative collaborative ventures, and yield to new scientific networks. The Faculty of Physics, Alexandru Ioan Cuza University of Iași, reaffirms its commitment to international cooperation and the pursuit of excellence in materials science and related fields.

We extend our sincerest best wishes to the AFMD-2026 organizers and convey our gratitude to the organizing committee for their dedication and foresight in convening this scientific conference!

Dean,

Prof. dr. Ionut Topala

FACULTY OF PHYSICS
Iași, blvd. Carol I, no. 11, code 700506
Tel. +40232 20 10 50
e-mail: fizica@uaic.ro
https://www.phys.uaic.ro/

Patrons

Dr. T. R. Paarivendhar, Founder Chancellor, SRMIST, India

Dr. Ravi Pachamuthu, Pro-Chancellor (Administration), SRMIST, India

Dr. P. Sathyanarayanan, Pro-Chancellor (Academics), SRMIST, India

Dr. R. Shivakumar, Chairman, SRM Trichy & Ramapuram Campus, India

Advisory Committee

Prof. C. Muthamizhchelvan, Vice Chancellor, SRMIST, India

Prof. S. Ponnusamy, Registrar, SRMIST, India

Prof. Leenus Jesu Martin, Dean (CET), SRMIST, India

Prof. B. Neppolian, Dean (Research), SRMIST, India

Prof. M. Arthanareeswari, Chairperson (SOBS), SRMIST, India

Prof. D. K. Aswal, NDMA, Government of India, India

Prof. Arindam Ghosh, IISc Bangalore, India

Prof. S. Balakumar, University of Madras, India

Prof. Guillaume Maurin, University of Montpellier, France

Prof. Kaniska Biswas, JNCASR, Bangalore, India

Dr. D. Kanjilal, IUAC, New Delhi, India

Prof. Kazushi Ikeda, NAIST, Japan

Prof. Majdi Hochlaf, University of Gustave Eiffel, France

Prof. Mohd Khairul Ahmad, UTHM, Malaysia

Prof. Nafarizal Bin Nayan, UTHM, Malaysia

Dr. M. Saravanan, CSIR-NPL, New Delhi, India

Prof. Umesh Waghmare, JNCASR, India

Prof. Vivek Polshettiwar, TIFR, Mumbai

Prof. Yashuhiro Hayakawa, Shizuoka University, Japan

Prof. Kazuyuki Hizume, Shizuoka University, Japan

Prof. Kazuhide Kimbara, Shizuoka University, Japan

Prof. Koichiro Awai, Shizuoka University, Japan

Prof. Toru Aoki, Shizuoka University, Japan

Prof. Mitsuhiro Fukuta, Shizuoka University, Japan

Prof. Jun Kondoh, Shizuoka University, Japan

Prof. Kazuhiko Hara, Shizuoka University, Japan

Conference Chair

Prof. M. Navaneethan, SRMIST, India

Organizing Committee

Prof. E. Senthil Kumar, SRMIST, India

Prof. J. Archana, SRMIST, India

Prof. M. Krishnamohan, SRMIST, India

Dr. S. Harish, SRMIST, India

Prof. Daniel Moraru, Shizuoka University, Japan

Prof. Hiroya Ikeda, Shizuoka University, Japan

Prof. Mohamed Chehimi, University of Paris Cité, France

Prof. Mohamed Jouini, University of Paris Cité, France

Prof. Guillaume Maurin, University of Montpellier, France

Prof. M. Prakash, SRMIST, India

Prof. Majdi Hochlaf, University of Gustave Eiffel, France

Dr. Mohd Faiz Bin Mohd Salleh, Universiti Malaya, Malaysia

Prof. Naoki Wakiya, Shizuoka University, Japan

Dr. Arief Udhiarto, Universitas Indonesia, Indonesia

Dr. Pavels Onufrijevs, Riga Technical University, Latvia

Prof. Kazushi Ikeda, NAIST, Japan

Prof. Nafarizal Bin Nayan, UTHM, Malaysia

Prof. Chien-Hsiang Chang, National Cheng Kung University, Taiwan

Dr. S. Sakthinathan, National Taipei University of Technology, Taiwan

Prof. Rajesh Kumar, IIT Indore, India.

Prof. A. Karthigeyan, SRMIST, India

Local Organizing Committee

Dr. K. D. Nisha, SRMIST, India

Dr. P. Justin Jesuraj, SRMIST, India

Dr. E. Vinoth, SRMIST, India

Dr. P. Bharathi, SRMIST, India

Dr. V. Vijay, SRMIST, India

Dr. K. P. Mohamed Jibri, SRMIST, India

Dr. C. Kanagaraj, SRMIST, India

Dr. Govind Ambadas Vangari, SRMIST, India

Dr. T. Govindaraj, SRMIST, India

Dr. D. Simon Patrick, SRMIST, India

Dr. S. Kamalakannan, SRMIST, India

Dr. M. S. Nithyapriya, SRMIST, India

Dr. Parvathi Krishna, SRMIST, India

Dr. S. Priyadharshini, SRMIST, India

Dr. K. Arun, SRMIST, India

Dr. R. Aysha Parveen, SRMIST, India

Dr. K. Monikapani, SRMIST, India

Dr. V. Saranya, SRMIST, India

Dr. D. Elumalai, SRMIST, India

Dr. A. Gowdhaman, SRMIST, India

Dr. N. Charumathi, SRMIST, India

Dr. D. Kanchan Kumar, SRMIST, India

Dr. R. Amuthan, SRMIST, India

Dr. Abin Philip, SRMIST, India

Dr. S. Suganya, SRMIST, India

Dr. K. Lakshmanamoorthy, SRMIST, India

Dr. S. Chandramohan, SRMIST, India

Dr. Anuja Datta, SRMIST, India

Dr.Anand Mohan Shrivastav, SRMIST, India

Dr. Elangovan Elamurugu, SRMIST, India

Dr. G. Bharath, SRMIST, India

Dr. Mohit Saraf, SRMIST, India

Dr. Rajaboopathi Mani, SRMIST, India

Dr. Shailendra K Saxena, SRMIST, India

Dr. Sougata Mallick, SRMIST, India

Dr. A. Naga Rajesh, SRMIST, India



2nd International Conferene on
Advanced Functional Materials and Devices (AFMD - 2026)
March 19 - 24, 2026

Time (IST)	Program Schedule (Day 1) 19th March 2026 (Thursday)						
12.00 - 14.00	**Registration**						
14.00 - 14.40	Venue	Dr. T. P. Ganesan Auditorium (TPGA)					
	Distinguished Plenary Lecture	**Prof. Ganapathy Vaitheeswaran** *University of Hyderabad* *"Evidence for multifold phonon degeneracies in cubic Nb_3Bi"*					
14.40 - 15.00	***Coffee Break***						
Parallel Session - I							
15.00 - 15.35	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614
	Keynote Lecture	KN 01	KN 02	KN 03	KN 04	KN 05	KN 06
		Prof. A. M. Kannan *Arizona State University, USA* *"Vanadium redox flow battery for large scale Energy storage for load management"*	**Prof. Vijayamohanan Pillai** *Indian Institute of Science Education and Research, Tirupati* *"Van der Waals Gap Engineering of Two Dimensional (2D) Materials: Applications for Energy Storage"*	**Prof. Srinivasan Natarajan** *Indian Institute of Science, Bangalore* *"Minerals as Future Solid-State Materials"*	**Prof. Ivo B. Rietveld** *University of Rouen Normandy, France* *"Vibrational Circular Dichroism and Second Harmonic Generation: Tools for Detecting Chirality and Symmetry Breaking"*	**Prof. Birabar Ranjit Kumar Nanda** *Indian Institute of Technology Madras, Chennai* *"Generation of tunable Quantum Transport in SOC active 2D materials"*	**Prof.V. Kanchana** *Indian Institute of Technology, Hyderabad* *"Computational Pathways in Topological Quantum Materials and Their Device Applications: Insights from DFT"*
15.35 - 16.05	Invited Talk	IT 01	IT 02	IT 03	IT 04	IT 05	IT 06
		Dr. Aravind Kumar Chandiran *Indian Institute of Technology Madras, Chennai* *"Polarized halide perovskite materials for photoelectrochemical water splitting"*	**Prof. N. Kamaraju** *Indian Institute of Science Education and Research, Kolkata* *"Probing Magnetic Order and Spin–Charge–Lattice Coupling in van der Waals Magnets Using Femtosecond Time-Resolved Reflectivity"*	**Dr. Naonori Sakamoto** *Shizuoka University, Japan* *"Excess water vapor absorption and structure deformation of cage-structured crystal $12CaO{\cdot}7Al_2O_3$"*	**Dr. Mihai Irimia-Vladu** *Johannes Kepler University Linz, Austria* *"Stability of Hydrogen-bonded Semiconductors for Organic Electronic Devices"*	**Prof. Anil Kumar Singh** *National Institute of Technology Rourkela* *"Tuning Multiferroic Properties in Y-Type Hexaferrite through Doping"*	**Prof. Yu-Jane Sheng** *National Taiwan University, Taiwan.* *"High-strength Poly(vinyl alcohol) Physical Eutectogels: Effects of polymer molecular weight, DES composition, and heat treatment"*
16.05 - 16.35	Invited Talk	IT 07	IT 08	IT 09	IT 10	IT 11	IT 12
		Dr. Vikum Premalal *University of Sri Jayewardenepura, Sri Lanka* *"Facile Synthesis of High-Performance CuS-Coated CuI Cathode for Seawater-Activated Magnesium Batteries"*	**Dr. Pavels Onufrijevs** *Riga Technical University* *"Laser-Structured Stainless Steel for Low-Temperature Friction Reduction"*	**Prof. Shikha Varma** *Institute of Physics (IOP), Bhubaneswar* *"Bioconjugation on Nanopatterned Surfaces for Biosensing: Experimental Insights and First-Principles DFT"*	**Dr. Mangal Roy** *Indian Institute of Technology, Kharagpur* *"Degradation Customization of Degradable Metallic Biomaterials"*	**Prof. De-Hao Tsai** *National Tsing Hua University, Taiwan* *"Gas-phase Electrophoresis-based Characterization for Real-time Quantifying Synthesis of Advanced Nanomaterials"*	**Dr. Kei Shigematsu** *Institute of Science Tokyo, Japan* *"Domain Structure and Magnetic Reversal by Electric Field in Cobalt-substituted Bismuth Ferrite Thin Films and Nanodots"*
17.00 - 19.00	***Culturals***						
19.00 - 21.00	***Dinner***						

	AC - Advanced Characterizations	EH - Environmental & Health Monitoring	BM - Biomaterials & Soft Materials
	QD - Quantum Materials & Devices	EL - Electronics, Optics & Photonics	AF - Advanced Functional Materials
	EN - Energy and Sustainable Materials	CM - Computational Materials Science & Materials Informatics	TF - Thin Films & Surfaces
	TP - Tech Park II		IA - Industry–Academia Partnership

2nd International Conferene on
Advanced Functional Materials and Devices (AFMD - 2026)
March 19 - 24, 2026

Time (IST)		Program Schedule (Day 2) 20th March 2026 (Friday)							
09.00 - 09.40	Venue	Dr. T. P. Ganesan Auditorium (TPGA)							
	Plenary Lecture	**Prof. Satishchandra B Ogale** *Research Institute for Sustainable Energy, Kolkata* *"Materials and Processing Innovations for Performance Enhancements in Emergent Battery Systems"*							
Parallel Session - II									
09.55 - 10.30	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - CLS 19
	Keynote Lecture	KN 07 **Prof. Dominic Bresser** *Helmholtz Institute Ulm (HIU) & Karlsruhe Institute of Technology (KIT), Germany* *"Towards an Enhanced Understanding of the Reactivity and Morphological Evolution of Lithium-Metal Electrodes"*	KN 08 **Prof. Tanmoy Maiti** *Indian Institute of Technology, Kanpur* *"High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene "*	KN 09 **Dr. Mukesh Kumar Sinha** *ASL- DRDO* *"Innovative Functional Fibrous Materials for Technical Textiles"*	KN 10 **Prof. Pau-Loke Show** *UCSI University, Malaysia* *"Emerging Materials and Intelligent Processes in Microalgae Biorefinery Technology"*	KN 11 **Dr. Jayakumar Balakrishnan** *Indian Institute of Technology, Palakkad* *"Thermal transport in 2D materials"*	KN 12 **Prof. Amin Bahrami** *Leibniz Institut für Festkörper und Werkstoffforschung, Germany*	***Oral Presentation (OP 001 - OP 007)***	***Young Researcher's Talk***
10.30 - 11.05	Keynote Lecture	KN 13 **Prof. Aninda Jiban Bhattacharyya** *ICER and SSCU, Indian Institute of Science, Bengaluru* *"Aqueous Batteries: Prospects and Challenges"*	KN 14 **Prof. Senthil Murugan Ganapathy** *University of Southampton,United Kingdom* *"Integrated Photonic Devices and AI-Driven On-Chip Spectroscopy for Rapid Biomedical Diagnostics"*	KN 15 **Prof. Jun Kondoh** *Shizuoka University, Japan* *"Study of Wicking Materials for Surface Acoustic Wave Atomizer Toward Chemical Spraying Applications"*	KN 16 **Prof. Ying-Chih Liao** *National Taiwan University, Taiwan* *"Green Fabrication of Conductive Patterns on Eco-Friendly Substrates"*	KN 17 **Prof. Naratip Vittayakorn** *Advanced Materials Research Unit (AMR), KMITL, Thailand* *"Advanced Hybridized Nanogenerators for Multifunctional Self-Powered Systems: Synergistic Materials Design, Principles, and Sustainable Applications"*	KN 18 **Prof. Tomoya Ohno** *Kitami Institute of Technology, Japan* *"How to Improve the coating homogeneity on primary particles using chemical reaction and physical deposition"*		
11.05 - 11.20	***Coffee Break***								
Parallel Session - III									
11.20 - 11.50	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - CLS 19
	Invited Talk	IT 13 **Prof. Ho-Hsiu Chou** *National Tsing Hua University, Taiwan* *"Molecularly Engineered Semiconducting Polymers for Solar-Driven Hydrogen Evolution and Circular Waste Upcycling via Photoreforming"*	IT 14 **Dr. Vibha Saxena** *Bhabha Atomic Research Centre (BARC), Mumbai* *"Beyond the Monolayer: Translating Langmuir-Blodgett WO3 Assembly into Solar Cell Metrics"*	IT 15 **Prof. Slawomir Boncel** *Silesian University of Technology, Poland* *"From functionalization to functionality: physicochemical design principles of sp2-carbon nanoallotropes across dimensions"*	IT 16 **Prof. Mohamed Jouini** *Univerite Paris Cite, France* *"Electroactive and electrochromic smart organic coatings functionalized with polymer brushes"*	IT 17 **Prof. C. Venkateswaran** *University of Madras, Chennai* *"Magnetic Properties of $GdMnO_3$ Films on Epitaxial and Non-Epitaxial Substrates"*	IT 18 **Prof. Yuki Maruno** *Kansai University, Japan* *"Deep Learning–Based Screening for Sarcopenic Dysphagia to Support Clinical Decision Making"*	***Oral Presentation (OP 008 - OP 016)***	***Young Researcher's Talk***
11.50 - 12.20	Invited Talk	IT 19 **Dr. Partha Saha** *National Institute of Technology, Rourkela* *"Cobalt-Free, High-Energy Ni-Rich Cathodes Enabled by Structural and Interface Engineering"*	IT 20 **Prof. Hiroshi Masumoto** *Tohoku University, Japan* *"Magneto-Functional Effects in Magnetic Metal–Ceramic Nano-Granular Thin Films"*	IT 21 **Prof. Naoki Wakiya** *Shizuoka University, Japan* *"Phase separation and metal-insulator transition in TiO2-VO2 thin films using dynamic aurora PLD"*	IT 22 **Dr. Ekaterina Brodovskaya** *National Research Ogarev Mordovia State University, Russia* *"In vitro formation of 3D cell structures using magnetic nanomaterials"*	IT 23 **Dr. Rabindra Nath Mahato** *Jawaharlal Nehru University, New Delhi* *"X-ray Photoelectron Spectroscopy and Critical Exponent Study of Nanocrystalline Pr0.7-xYxBa0.3MnO3 (x = 0, 0.05 and 0.1)"*	IT 24 **Prof. Paul Joseph** *National Institute of Technology, Warangal* *"Thin Film Electrodes for Photo-degradation of pollutants and Power Generation in Microbial Fuel Cells – Doping and Coating Strategies"*		
12.20 - 12.50	Invited Talk	IT 25 **Dr. Shigeto Hirai** *Kitami Institute of Technology, Japan* *"Surface structure engineering of highly active and durable oxygen evolution catalysts"*	IT 26 **Dr. Koteswara Rao Peta** *University of Delhi, New Delhi* *"Metal Oxide Semiconductor Nanostructures for Energy Conversion and Energy storage Applications"*	IT 27 **Prof. Yuichi Sakumura** *Nara Institute of Science and Technology (NAIST), Japan* *"Toward Explainable Breath Analysis Using Semiconductor Sensor Arrays"*	IT 28 **Dr. Chia Wen Yi** *Nanyang Environment & Water Research Institute (NEWRI), NTU, Singapore* *"Resource Recovery from Seawater Reverse Osmosis (SWRO) Desalination Brine"*	IT 29 **Prof.M.M. Shaijumon** *Indian Institute of Science Education and Research, Trivandrum* *"Engineering Metal Anodes for High-rate Solid-state Batteries"*	IT 30 **Prof. Daniel Moraru** *Shizuoka University, Japan* *"Probing Dopant-Induced Quantum Structures by Tunneling Spectroscopy in Silicon Nanodevices"*		
12.50 - 14.00	***Lunch Break***								
Inauguration Ceremony (Venue: T P Ganesan Auditorium)									
14.00 - 14.45	***Inauguration and Award Ceremony***								
14.45 - 15.25	Venue	Dr. T. P. Ganesan Auditorium (TPGA)							
	Distinguished Plenary Lecture	**Prof. Kanishka Biswas** *Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru* *"Phonon-Glass Electron-Crystal like High Performance Thermoelectrics"*							
15.25 - 15.45	***Coffee Break***								
Parallel Session - IV									
15.45 - 16.20	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - CLS 19
	Keynote Lecture	KN 19 **Prof. Ravichandar Babarao** *RMIT, Australia* *"Accelerating Materials Discovery for Clean Energy and Environmental Application: Integrating Simulations and Experiments"*	KN 20 **Prof. Rougier Aline** *Institut de Chimie de la Matière Condensée de Bordeaux, France* *"Towards Thin Films Advanced Deposition for Improved Electrochromic Properties"*	KN 21 **Prof. Mei- Jywan Syu** *National Cheng Kung University, Taiwan* *"Proposing an Imprinted Poly (2-vinyl-4-nitroaniline) Modified Electrode for Differential Pulse Voltammetry Detection of Urinary Uric Acid"*	KN 22 **Prof. Awadhesh Mani** *Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam* *"Comparative studies on some novel quantum systems at extreme pressures and magnetic fields"*	KN 23 **Prof. S. Balakumar** *University of Madras, Chennai* *"A Dual Bioceramic Strategy for Integrated Bone and Wound Regeneration Using Hydroxyapatite and Bioactive Glass Systems"*	KN 24 **Prof. Kazushi Ikeda** *Nara Institute of Science and Technology (NAIST), Japan* *"Topological Data Analysis for Materials Informatics"*	***Oral Presentation (OP 017 - OP 022)***	***Young Researcher's Talk***
16.20 - 16.50	Invited Talk	IT 31 **Dr. M. Saravanan** *CSIR-National Physical Laboratory, New Delhi* *"Cost-effective reference materials development using spark plasma sintering for thermoelectric applications"*	IT 32 **Dr. S Ganesamoorthy** *Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam* *"Detector Grade CdZnTe Single Crystals for Room Temperature Gamma-ray Detector Applications"*	IT 33 **Prof. Masanori Koshimizu** *Shizuoka University, Japan* *"Development of Plastic Scintillators Having Fast Response Using Perovskite Quantum Dots"*	IT 34 **Dr. Jevgenijs Kaupužs** *Riga Technical University, Latvia* *"Finite-Difference Steepest Descent (FDSD) Method for Modeling Light Propagation in Structures with Metal Nanoparticles"*	IT 35 **Prof. Tetsu Yonezawa** *Hokkaido University, Japan* *"Low-Temperature Sintering Copper Particle Technology - Figure Joining and Conductive Materials for Semiconductor Industry"*	IT 36 **Dr. A. Mercy Latha** *CSIR-Central Electronics Engineering Research Institute, Chennai* *"Terahertz Spectroscopic and Imaging of Composite Materials"*		
17.00 - 19.00	***Culturals***								
19.00 - 21.00	***Dinner***								

2nd International Conferene on
Advanced Functional Materials and Devices (AFMD - 2026)
March 19 - 24, 2026

Program Schedule (Day 3)
21st March 2026 (Saturday)

Time (IST)										
09.00 - 09.40	Venue	TPGA Mini Hall 01				TPGA Mini Hall 02				
	Plenary Lecture	**Prof. R. Murugavel** *Indian Institute of Technology Bombay, Mumbai* *"Role of Metal Phosphates in Energy Transition"*				**Prof. Tapas Kumar Maji** *Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru* *"Developing Photocatalyst by Post-Synthetic Modification Metal-Organic Frameworks"*				
Parallel Session - V										
09.50 - 10.25	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - LH 606	TP - CLS 19
	Keynote Lecture	KN 25 **Dr. Sudakar Chandran** *Indian Institute of Technology Madras, Chennai* *"Engineering Halide Perovskites for Photonic and Optoelectronic Applications"*	KN 26 **Prof. Judy Wu** *University of Kansas, USA* *"Designing advanced quantum dots/graphene broadband photodetectors"*	KN 27 **Prof. Govind Gupta** *CSIR-National Physical Laboratory, New Delhi* *"Two-Dimensional Metal Chalcogenides: Exploring Exciting Opportunities for Neuromorphic Computing"*	KN 28 **Prof. Chien-Hsiang Chang** *National Cheng Kung University, Taiwan* *"Modulating Physical Properties and Enhancing stability of Catanionic Vesicles Using Fatty Acid Additives"*	KN 29 **Prof. Anjan Barman** *S. N. Bose National Centre for Basic Sciences, Kolkata* *"Hybrid interface for Magnonics: A quantum technology platform"*	KN 30 **Dr. Suresh Sundaram** *Georgia Tech, France* *"Layered boron nitride and its III-nitride heterostructures"*	KN 31 **Dr. Vanchiappan Aravindan** *Indian Institute of Science Education and Research, Tirupati* *"Na-ion Batteries via Solvent-co-Intercalation"*	***Oral Presentation (OP 023 - OP 028)***	***Oral Presentation (OP 029 - OP 034)***
10.25 - 10.55	Invited Talk	IT 37 **Prof. Maheswaran Shanmugam** *Indian Institute of Technology Bombay, Mumbai* *"Molecular based Magnetoelectric Materials for Sustainable Energy Harvesting"*	IT 38 **Prof. Vincent K.S. Hsiao** *National Chi Nan University, Taiwan* *"Fluorescence Anisotropy and Chiroptical Luminescence: From Anisotropic Photoluminescence Probing to Cholesteric Liquid Crystal Control"*	IT 39 **Dr. Srabanti Ghosh** *CSIR - Central Glass and Ceramic Research Institute, Kolkata* *"Structure–Function Modulation in Semiconductor Heterostructures for Efficient Solar Fuel Production"*	IT 40 **Prof. Ratno Nuryadi** *BRIN, Indonesia* *"MEMS Microcantilever Sensors Functionalized with ZnO Nanorods for High-Sensitivity Gas Detection"*	IT 41 **Dr. Binoy Krishna Hazra** *Indian Institute of Technology, Guwahati* *"Non-collinear antiferromagnets for spintronic applications"*	IT 42 **Prof. Keun Heo** *Jeonbuk National University, South Korea* *"Van der Waals and Ferroelectric polymer based Artificial Neural Devices for Neuromorphic Applications"*	IT 43 **Dr. Amarnath R Allu** *CSIR - Central Glass and Ceramic Research Institute, Kolkata* *"Reactive Glass–Metal Interaction under Ambient Conditions Enables Surface Modification of Gold Nano-islands"*		
10.55 - 11.15	***Coffee Break***									
Parallel Session - VI										
11.15 - 11.45	Invited Talk	IT 44 **Prof. Chandra S Sharma** *Indian Institute of Technology, Hyderabad* *"From Earth to Mars: Pioneering Metal-Carbon Dioxide (Metal-CO2) Battery Solutions for a Greener Tomorrow"*	IT 45 **Dr. Bruce (Jun-Yu) Ou** *University of Southampton, United Kingdom* *"Nanomechanical metamaterials and multifunctional metalenses"*	IT 46 **Dr. Shintaro Yasui** *Institute of Science Tokyo, Japan* *"Water-based Solid Battery using 3D-Slime Interface quasi-Solid Electrolyte (3D-SLISE)"*	IT 47 **Prof. Bing -Hung Chen** *National Cheng Kung University, Taiwan* *"Utilizing CO2 for Synthesis of Organic Carbonates via Direct Carbonylation of Glycerol"*	IT 48 **Dr. Swarup Deb** *Saha Institute of Nuclear Physics, Kolkata* *"Excitonic Signature of 2D Sliding/Interfacial/Moiré Ferroelectrics"*	IT 49 **Prof. Chi-Cheng Chiu** *National Cheng Kung University, Taiwan* *"Modulation of the Interfacial Lithium-Ion Transport within Lithium Ion Batteries:Insights from Multi-Scale Simulations"*	IT 50 **Prof. Heng-Kwong Tsao** *National Central University, Taiwan.* *"Microstructural dynamics of stretching nanofilm of hydrogels:effects of film thickness on mechanical properties"*	***Oral Presentation (OP 035 - OP 043)***	Special Talk **Prof. Mitsuhiro Fukuta** *Shizuoka University, Japan*
11.45 - 12.15	Invited Talk	IT 51 **Prof. Atsushi Nakamura** *Shizuoka University, Japan* *"Development of an electron beam–pumped, localized surface plasmon–enhanced nanoscale light source for electron-beam–assisted optical microscopy"*	IT 52 **Prof. Svitlana Bugaychuk** *University of Lille, France* *"Surface-induced photorefractive effect (SIPRE) in liquid crystal nanocomposites for applications in fast switchable devices"*	IT 53 **Prof. Tadachika Nakayama** *Nagaoka University of Technology, Japan* *"Application of Pulsed Electric Fields in Inorganic Materials Science"*	IT 54 **Dr. Jitendra Bahadur** *Bhabha Atomic Research Centre (BARC), Mumbai* *"Complex interactions driven assembly in the multi-component colloids: Insights from synchrotron SAXS"*	IT 55 **Prof. Pranaba Kishor Muduli** *Indian Institute of Technology, Delhi* *"Spintronics using 2D materials"*	IT 56 **Dr. Arnab Bose** *Indian Institute of Technology, Kanpur* *"Generation and detection of orbital currents"*	IT 57 **Prof. Chang Hee Hong** *Jeonbuk National University, South Korea* *"InGaN LED Technology Trends for Agriculture and Bio-industry Applications: From Spectral Engineering to Van der Waals Epitaxy"*		**Prof. Dmitrijs Stepanovs** *Riga Technical University, Latvia*
12.15 - 12.45	Invited Talk	IT 58 **Dr. Chinmoy Ranjan** *Indian Institute of Science, Bengaluru* *"Solid oxide electrolysis of CO2 : Power to X"*	IT 59 **Dr. Tomoki Maeda** *Ibaraki University, Japan* *"Quantum Beam Approaches to Advanced Functional Polymer Composites"*	IT 60 **Dr. Arup Dasgupta** *Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam* *"Application of Probe Aberration Corrected STEM techniques in understanding some fascinating features of melt-cast (Fe,Cr)₂B"*	IT 61 **Dr. Kazuo Shimizu** *Shizuoka University, Japan* *"From Reactive-Species Composition to Function: A Design Framework for Non-Ablative, Reversible Biointerface Modulation"*	IT 62 **Prof. Md. Ehesan Ali** *Institute of Nano Science and Technology, Mohali* *"Quantum spin sensors for open-shell molecules"*	IT 63 **Dr. Sakura Takeda** *Nara Institute of Science and Technology (NAIST), Japan* *"Deriving Interface Physics from Correlations Between Electrical Properties and XPS in PECVD-SiO₂/Si"*	IT 64 **Dr. Hiroki Kase** *Shizuoka University, Japan* *"Representation of 3D X-ray CT Using Mixed Reality with Force Feedback for Density Information"*		***Industrial Talk***
12.45 - 14.00	***Lunch Break***									
Parallel Session - VII										
14.00 - 14.35	Keynote Lecture	KN 32 **Prof. Tharamani C. Nagaiah** *Indian Institute Of Technology, Ropar* *"Designing greener energy conversion system for a sustainable future"*	KN 33 **Prof. Toru Aoki** *Shizuoka University, Japan* *"Impact of Carbon Doping and Device Structure on the X-ray Response of GaN Detectors"*	KN 34 **Prof. Harri Lipsanen** *Aalto University, Finland* *"Broadband miniaturized spectrometers with van der Waals junctions"*	KN 35 **Prof. Yoshimasa Kawata** *Shizuoka University, Japan* *"Live Cell Imaging and Cell Stimulations with Direct Electron-Beam Excitation Assisted Microscoopy"*	KN 36 **Prof. Yogendra Kumar Mishra** *Mads Clausen Institute, University of Southern Denmark, Denmark* *"Tetrapods based Advanced Materials for Advanced Technologies"*	KN 37 **Prof. Benoît Piro** *Université Paris Cité, France* *"An Innovative Printed Device for Sensing of Exhaled Gas"*	KN 38 **Dr. Tetsuo Kodera** *Tokyo Institute of Technology, Tokyo* *"Progress and prospects in research of semiconductor spin qubit devices toward quantum computers"*	***Oral Presentation (OP 044 - OP 049)***	***Oral Presentation (OP 050 - OP 055)***
14.35 - 15.05	Invited Talk	IT 65 **Prof. Tomoaki Yamada** *Nagoya University, Japan* *"Domain Engineering of Ferroelectric Nano-structures and Their piezoelectric properties"*	IT 66 **Prof. Hiromasa Shimizu** *Tokyo University of Agriculture & Technology, Japan* *"Sensing experiments based on collaborative research activities in Tokyo University of Agriculture and Technology"*	IT 67 **Dr. Madhurya Chandel** *Warsaw University of Technology, Poland* *"Exploring MBene: 2D Materials Pathways in Synthesis and Characterization for Optoelectronics devices"*	IT 68 **Prof. Ionut Topala** *Alexandru Ioan Cuza University Lasi, Romania* *"Measurement of hydrogen to carbon ratio in amorphous hydrogenated carbon products and the effect ion irradiation"*	IT 69 **Dr. Kaushalya Jhuria** *Indian Institute of Technology, Delhi* *"Telecom band silicon based optical defects for quantum technologies"*	IT 70 **Prof. K.G. Suresh** *Indian Institute of Technology, Bombay* *"Heusler alloys as spintronic and spin-caloritronic applications"*	IT 71 **Prof. Felicia Iacomi** *Alexandru Ioan Cuza University, Romania* *"Studies on the structure and functional properties of some nanocomposite layers based on graphene and graphene oxide"*		
Parallel Session - VIII										
15.05 - 16.15	***Oral Presentations***	***OP 056 - OP 062***	***OP 063 - OP 069***	***OP 070 - OP 076***	***OP 077 - OP 083***	***OP 084 - OP 090***	***OP 091 - OP 097***	***OP 098 - OP 104***	***OP 105 - OP 111***	***OP 112 - OP 118***
16.15 - 16.30	***Coffee Break***									
16.30 - 18.00	Venue	Dr. T. P. Ganesan Auditorium (TPGA)								
	Poster Presentation									
18.30 - 21.30	***Banquet Dinner***									

2nd International Conferene on
Advanced Functional Materials and Devices (AFMD - 2026)
March 19 - 24, 2026

Time (IST)	Program Schedule (Day 4) 23rd March 2026 (Monday)								
08.30- 10.00	Venue	Dr. T. P. Ganesan Auditorium (TPGA)							
	Poster Presentation								
Parallel Session - IX									
10.00 - 11.10	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - LH 606	TP - CLS 19
	Oral Presentations	*OP 119 - OP 125*	*OP 126 - OP 132*	*OP 133 - OP 139*	*OP 140 - OP 146*	*OP 147 - OP 153*	*OP 154 - OP 160*	*OP 161 - OP 167*	*OP 168 - OP 174*	*OP 175 - OP 181*
11.10 - 11.30	*Coffee Break*									
Parallel Session - X										
11.30 - 12.05	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - LH 606	TP - CLS 19
	Keynote Lecture	KN 39	KN 40	KN 41	KN 42	KN 43	KN 44	KN 45	*Oral Presentation* (OP 182 - OP 188)	*Young Reseacher's Talk*
		Prof. Ramesh Chandra Mallik *Indian Institute of Science, Bangalore* *"Improved Thermoelectric Figure of Merit in Cu2Se Material"*	**Prof. Somobrata Acharya** *Indian Association for the Cultivation of Science (IACS), Kolkata* *"Dimension Controlled Ferroelectricity and Bulk Photovoltaic Effect in CsPbBr 3 Perovskite Nanocrystals"*	**Dr. M. Sathish** *Central Electrochemical Research Institute, Karaikudi* *"Functionalized Carbon-based Materials for Rechargeable Zinc-Air Batteries"*	**Prof. Suhrit Ghosh** *Indian Association for the Cultivation of Science (IACS), Kolkata* *"Supramolecular Assembly of Donor-Acceptor (Macro) molecular Systems for Low-Power Energy Harvesting"*	**Prof. Shaikh M Mobin** *Indian Institute of Technology, Indore* *"Crystal Engineered MOFs and Interfacial Chemistry for Next Generation Ammonium Ion Sustainable Energy Storage Devices"*	**Prof. Rajesh Kumar** *Indian Institute of Technology, Indore* *"Electrochromic materials and device: smart windows for multifunctional applications"*	**Prof. Dipak Kumar Goswami** *Indian Institute of Technology, Kharagpur* *"Flexible OFET Platforms for Secure and Affordable Diagnostics: From Synaptic Phototransistors to Wearable Sensors"*		
12.05 - 12.35	Invited Talk	IT 72	IT 73	IT 74	IT 75	IT 76	IT 77	IT 78		Invited Talk
		Dr. Vivek Kumar *Indian Institute of Information Technology Design & Manufacturing, Kancheepuram* *"2D Materials for High performance Hybrid supercapacitors"*	**Dr. Arup Samanta** *Indian Institute of Technology, Roorkee* *"High Temperature Quantum Transport using deep dopant in Silicon"*	**Dr. Srinivasan Anandan** *International Advanced Research centre for Powder Metallurgy & New Materials (ARCI), Hyderabad* *"Development of Indigenous Electrode Materials for Li- and Na-Ion Batteries: From Lab-Scale Innovation to Technology Demonstration"*	**Dr. Goutam Ghosh** *Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru* *"Peptide-Based Nanomaterials for Organic Electronics: Tailoring Piezoelectric Properties through Nanostructural and Chiroptical Modulation"*	**Dr. Ashutosh Kumar Singh** *Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru* *"Efforts Toward Developing High-Performance Aqueous Rechargeable Zn-Ion Batteries"*	**Dr. Pritam Sadhukhan** *Indian Association for the Cultivation of Science (IACS), Kolkata* *"Stimuli-Responsive Molecular Systems for Nanoscale Energy Harvesting Prospects"*	**Dr. Rana Saha** *Indian Institute of Science Education and Research, Tirupati* *"Topological spin textures in van der Waals magnets"*		***Prof. Rajan Jha*** *Indian Institute of Technology, Bhuvaneshwar* *"Fiber Cavity: A Versatile System for Sensing and Quantum Technology"*
12.35 - 14.00	*Lunch Break*									
Parallel Session - XI										
14.00 - 14.35	Venue	TP - LH 711	TP - LH 604	TP - LH 605	TP - LH 613	TP - LH 712	TP - LH 614	TP - LH 615	TP - LH 606	TP - CLS 19
	Keynote Lecture	KN 46	KN 47	KN 48	KN 49	KN 50	KN 51	KN 52	KN 53	*Young Researcher's Talk*
		Prof. C Subramaniam *Indian Institute of Technology, Bombay* *"Nanostructured carbons for bottling and utilizing sunlight for sustainable energy and environmental applications"*	**Prof. Riabochkina Polina** *National Research Mordovia State University, Russia* *"Optical laser ceramics for solid-state lasers in the two-micron spectral range"*	**Dr. Takeshi Maeda** *Osaka Metropolitan University, Japan* *"Impact of Intermediate Diradical Character on Optical and Magnetic Properties in Croconaine Dyes"*	**Prof. Mathieu Etienne** *LCPME-CNRS-UNIVERSITE DE LORRAINE, France* *"Materials Development and Characterization for Redox Flow Technologies"*	**Prof. Abdelmajid Taki** *University of Lille, France* *"Characterization of complex dynamics in a chain of plasmonic nanoparticles"*	**Prof. Anatoly Lysyakov** *National Research Mordovia State University, Russia* *"Interaction between Universities and Industry: The Case of National Research Mordovia State University"*	**Prof. Indranil Sarkar** *Institute of Nano Science and Technology, Mohali* *"Unraveling interface physics of ferromagnet/nonmagnet heterostructures for development of efficient spin orbit torque applications"*	**Prof. Sebastian Lourdudoss** *KTH-Royal Institute of Technology, Sweden* *"Heteroepitaxial structures and high growth rate of semi-insulating InP for buried heterostructure quantum cascade lasers by hydride vapour phase epitaxy"*	
14.35 - 15.05	Invited Talk	IT 79	IT 80	IT 81	IT 82	IT 83	IT 84	IT 85	IT 86	
		Prof. Masato Nakaya *Nagoya University, Japan* *"Thermoelectric Properties of Nanocluster Composites consisting of Fullerene Molecules and Metal Oxide Nanoclusters"*	**Dr. Chao-Wei Huang** *National Cheng Kung University, Taiwan* *"MOFs-derived and Chitosan-based Photocatalysts for Scalable VOCs Degradation in Photocatalytic Fluidized Beds"*	**Prof. Makiko Kobayashi** *Kumamoto University, Japan* *"Design of Sol–Gel Composite Materials for High-Temperature Ultrasonic/Piezoelectric Devices"*	**Dr. Mani Ulaganathan** *Amrita Vishwa Vidyapeetam, Coimbatore* *"Redox Flow Batteries for Large Scale Energy Storage Application"*	**Prof. Hiroya Ikeda** *Shizuoka University, Japan* *"Seebeck-Coefficient Evaluation of Si Microribbon by Kelvin-Probe Force Microscopy"*	**Prof. Yueh-Heng Li** *National Cheng Kung University, Taiwan* *"A Traceable Digital Thread for UAV Propulsion: MBSE Architecture Linked with Performance Simulation"*	**Prof. Tamihiro Gotoh** *Gunma University, Japan* *"Bandgap widening of evaporated In-Se films by room temperature annealing"*	**Prof. Rodrigo Ferrao Paiva Martins** *NOVA University Lisbon and CEMOP/UNINOVA, Portugal* *"Transforming Electronics: The Future of Transparent and Paper Electronics"*	
15.05 - 15.35	Invited Talk	IT 87	IT 88	IT 89	IT 90	IT 91	IT 92	IT 93	IT 94	
		Dr. Manas K Panda *Jadavpur University, Kolkata* *"Stimuli-Responsive Soft Molecular Materials"*	**Prof. Sergei Gushchin** *National Research Mordovia State University, Russia* *"Upconversion luminescence of SrF2-ErF3 solid solutions"*	**Prof. Kitani Tomoya** *Shizuoka University, Japan* *"A Proposal for Infrastructure Management Using Motorcycle Dynamics Data and Rider Vital Signals"*	**Dr. Bharati Debnath** *Research Institute for Sustainable Energy (RISE), TCG CREST, Kolkata* *"Design of Electrodeposition-Driven Phosphide Catalysts for Green Hydrogen and Ammonia Synthesis"*	**Dr. Miki Mochizuki** *Shizuoka University, Japan* *"Toward a Resilient Society: Dialogue between Engineering and the Social Sciences in Disaster Contexts"*	**Dr. Yasuhide Mochizuki** *Institute of Science Tokyo, Japan* *"Theoretical Study of Phonon-Induced Negative Thermal Expansion Materials"*	**Dr. Tetsushi Ohki** *Shizuoka University, Japan* *"The Expanding Attack Surface of AI-Enabled Biometric Infrastructures"*	**Prof. A. M. Jastrzębska** *Warsaw University of Technology, Poland* *"Effect of tandem-type stabilization of two-dimensional (2D) Nb2CTx MXene on their colloidal and cytotoxic properties"*	
15.35 - 16.30	**Award Distribution & Valedictory Ceremony**									
16.30 - 16.45	*Coffee*									

2nd International Conferene on
Advanced Functional Materials and Devices (AFMD - 2026)
March 19 - 24, 2026

Time (IST)	Program Schedule (Day 5) 24th March 2026 (Tuesday)
09.00 - 17.00	**Collaborative Discussion Meeting and Research Facility Visit**

Abstract ID	Abstract Title	Page No
	Plenary Lecture	
PL-001	Evidence for Multifold Phonon Degeneracies in Cubic Nb_3Bi	1
PL-002	Materials and Processing Innovations for Performance Enhancements in Emergent Battery Systems	2
PL-003	Phonon-Glass Electron-Crystal like High Performance Thermoelectrics	3
PL-004	Role of Metal Phosphates in Energy Transition	4
PL-005	Developing Photocatalyst by Post-Synthetic Modification Metal-Organic Frameworks	5
PL-006	Engineering Photo-and Electrocatalytic Materials for Sustainable Environment	6
	Keynote Lecture	
KN-001	Vanadium Redox Flow Battery for Large Scale Energy Storage for Load Management	7
KN-002	Van der Waals Gap Engineering of Two Dimensional (2D) Materials: Applications for Energy Storage	8
KN-003	Minerals as Future Solid-State Materials	9
KN-004	Vibrational Circular Dichroism and Second Harmonic Generation: Tools for Detecting Chirality and Symmetry Breaking	10
KN-005	Generation of tunable Quantum Transport in SOC active 2D materials	11
KN-006	Computational Pathways in Topological Quantum Materials and Their Device Applications: Insights from DFT	12
KN-007	Towards an Enhanced Understanding of the Reactivity and Morphological Evolution of Lithium-Metal Electrodes	13

KN-008	High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene	14
KN-009	Innovative Functional Fibrous Materials for Technical Textiles	15
KN-010	Emerging Materials and Intelligent Processes in Microalgae Biorefinery Technology	16
KN-011	Thermal transport in 2D materials	17
KN-014	Electroactive and Electrochromic Smart Organic Coatings Functionalized with Polymer Brushes	18
KN-015	Study of Wicking Materials for Surface Acoustic Wave Atomizer Toward Chemical Spraying Applications	19
KN-016	Green Fabrication of Conductive Patterns on Eco-Friendly Substrates	20
KN-017	Advanced Hybridized Nanogenerators for Multifunctional Self-Powered Systems: Synergistic Materials Design, Principles, and Sustainable Applications	21
KN-018	How to Improve the Coating Homogeneity on Primary Particles using Chemical Reaction and Physical Deposition	22
KN-019	Accelerating Materials Discovery for Clean Energy and Environmental Application: Integrating Simulations and Experiments	23
KN-020	Towards Thin Films Advanced Deposition for Improved Electrochromic Properties	24
KN-021	Proposing an Imprinted Poly(2-vinyl-4-nitroaniline) Modified Electrode for Differential Pulse Voltammetry Detection of Urinary Uric Acid	25
KN-022	Comparative Studies on Some Novel Quantum Systems at Extreme Pressures and Magnetic Fields	26
KN-023	A Dual Bioceramic Strategy for Integrated Bone and Wound Regeneration Using Hydroxyapatite and Bioactive Glass Systems	27

KN-024	Topological Data Analysis for Materials Informatics	28
KN-025	Engineering Halide Perovskites for Photonic and Optoelectronic Applications	29
KN-026	Designing Advanced Quantum Dots/Graphene Broadband Photodetectors	30
KN-027	Two-Dimensional Metal Chalcogenides: Exploring Exciting Opportunities for Neuromorphic Computing	31
KN-028	Modulating Physical Properties and Enhancing stability of Catanionic Vesicles Using Fatty Acid Additives	32
KN-030	Layered Boron Nitride and its III-Nitride Heterostructures	33
KN-032	Designing Greener Energy Conversion System for A Sustainable Future	34
KN-033	Impact of Carbon Doping and Device Structure on the X-ray Response of GaN Detectors	35
KN-034	Broadband miniaturized spectrometers with van der Waals junctions	36
KN-035	Live Cell Imaging and Cell Stimulations with Direct Electron-Beam Excitation Assisted Microscoopy	37
KN-036	Tetrapods based Advanced Materials for Advanced Technologies	38
KN-037	An Innovative Printed Device for Sensing of Exhaled Gas	39
KN-039	Improved Thermoelectric Figure of Merit in Cu_2Se Material	40
KN-040	Dimension Controlled Ferroelectricity and Bulk Photovoltaic Effect in $CsPbBr_3$ Perovskite Nanocrystals	41
KN-041	Functionalized Carbon-based Materials for Rechargeable Zinc-Air Batteries	42

KN-042	Supramolecular Assembly of Donor-Acceptor (Macro)Molecular Systems for Low-Power Energy Harvesting	43
KN-043	Crystal-Engineered MOFs and Interfacial Chemistry for Next-Generation Ammonium-Ion Sustainable Energy Storage Devices	44
KN-046	Nanostructured Carbons for Bottling and Utilizing Sunlight for Sustainable Energy and Environemental Applications	45
KN-047	Optical Laser Ceramics Y_2O_3 Doped with Tm^{3+}, Ho^{3+} for Solid-State Lasers in the Two-Micron Spectral Range	46
KN-048	Impact of Intermediate Diradical Character on Optical and Magnetic Properties in Croconaine Dyes	47
KN-049	Materials Development and Characterization for Redox Flow Technologies	48
KN-050	Unraveling Interface Physics of Ferromagnet/Nonmagnet Heterostructures For Development of Efficient Spin Orbit Torque Applications	49
KN-051	Interaction between Universities and Industry: The Case of National Research Mordovia State University	50
KN-052	Characterization of Complex Dynamics in A Chain of Plasmonic Nanoparticles	51
KN-053	Heteroepitaxial Structures and High Growth Rate of Semi-Insulating InP for Buried Heterostructure Quantum Cascade Lasers by Hydride Vapour Phase Epitaxy	52

Invited Lecture

IT-001	Polarized Halide Perovskite Materials for Photoelectrochemical Water Splitting	53
IT-002	Probing Magnetic Order and Spin–Charge–Lattice Coupling in van der Waals Magnets Using Femtosecond Time-Resolved Reflectivity	54

IT-003	Excess Water Vapor Absorption and Structure Deformation of Cage-Structured Crystal $12CaO{\cdot}7Al_2O_3$	55
IT-004	Stability of Hydrogen-bonded Semiconductors for Organic Electronic Devices	56
IT-005	Tuning Multiferroic Properties in Y-Type Hexaferrite through Doping	57
IT-006	High-Strength Poly (Vinyl Alcohol) Physical Eutectogels: Effects of Polymer Molecular Weight, DES Composition, and Heat Treatment	58
IT-007	Facile Synthesis of High-Performance CuS-Coated CuI Cathode for Seawater-Activated Magnesium Batteries	59
IT-008	Laser-Structured Stainless Steel for Low-Temperature Friction Reduction	60
IT-009	Bioconjugation on Nanopatterned Surfaces for Biosensing: Experimental Insights and Firs tPrinciples DFT	61
IT-010	Degradation Customization of Degradable Metallic Biomaterials	62
IT-011	Gas-phase Electrophoresis-based Characterization for Real-time Quantifying Synthesis of Advanced Nanomaterials	63
IT-012	Domain Structure and Magnetic Reversal by Electric Field in Cobalt-substituted Bismuth Ferrite Thin Films and Nanodots	64
IT-013	Molecularly Engineered Semiconducting Polymers for Solar-Driven Hydrogen Evolution and Circular Waste Upcycling via Photoreforming	65
IT-014	Beyond the Monolayer: Translating Langmuir-Blodgett WO_3 Assembly into Solar Cell Metrics	66
IT-015	From Functionalization to Functionality: Physicochemical Design Principles of Sp^2-Carbon Nanoallotropes Across Dimensions	67

IT-016	Integrated Photonic Devices and AI-Driven On-Chip Spectroscopy for Rapid Biomedical Diagnostics	68
IT-017	Magnetic Properties of $GdMnO_3$ Films on Epitaxial and Non-Epitaxial Substrates	69
IT-018	Deep Learning–Based Screening for Sarcopenic Dysphagia to Support Clinical Decision-Making Cobalt-Free High-Energy	70
IT-019	Ni-Rich Cathodes Enabled by Structural and Interface Engineering	71
IT-020	Magneto-Functional Effects in Magnetic Metal–Ceramic Nano-Granular Thin Films	72
IT-021	Phase Separation and Metal-Insulator Transition in TiO_2-VO_2 Thin Films Using Dynamic Aurora PLD	73
IT-022	In vitro formation of 3D cell structures using magnetic nanomaterials	74
IT-023	X-ray Photoelectron Spectroscopy and Critical Exponent Study of Nanocrystalline $Pr_{0.7-x}Y_xBa_{0.3}MnO_3$(x = 0, 0.05 and 0.1)	75
IT-024	Thin Film Electrodes for Photo-degradation of pollutants and Power Generation in Microbial Fuel Cells – Doping and Coating Strategies	76
IT-025	Surface Structure Engineering of Highly Active and Durable Oxygen Evolution Catalysts	77
IT-026	Metal Oxide Semiconductor Nanostructures for Energy Conversion and Energy storage Applications	78
IT-027	Toward Explainable Breath Analysis Using Semiconductor Sensor Arrays	79
IT-028	Resource Recovery from Seawater Reverse Osmosis (SWRO) Desalination Brine	80
IT-029	Engineering Metal Anodes for High-rate Solid-state Batteries	81

IT-030	Probing Dopant-Induced Quantum Structures by Tunneling Spectroscopy in Silicon Nanodevices	82
IT-031	Cost-Effective Reference Materials Development using Spark Plasma Sintering for Thermoelectric Applications	83
IT-032	Detector Grade CdZnTe Single Crystals for Room Temperature Gamma-ray Detector Applications	84
IT-033	Development of Plastic Scintillators Having Fast Response Using Perovskite Quantum Dots	85
IT-034	Finite-Difference Steepest Descent (FDSD) Method for Modeling Light Propagation in Structures with Metal Nanoparticles	86
IT-035	Low-Temperature Sintering Copper Particle Technology - Figure Joining and Conductive Materials for Semiconductor Industry	87
IT-036	Terahertz Spectroscopic and Imaging of Composite Materials	88
IT-038	Fluorescence Anisotropy and Chiroptical Luminescence: From Anisotropic Photoluminescence Probing to Cholesteric Liquid Crystal Control	89
IT-039	Structure-Function Modulation in Semiconductor Heterostructures for Efficient Solar Fuel Production	90
IT-040	MEMS Microcantilever Sensors Functionalized with ZnO Nanorods for High-Sensitivity Gas Detection	91
IT-041	Non-collinear antiferromagnets for spintronic applications	92
IT-043	Reactive GlassMetal Interaction under Ambient Conditions Enables Surface Modification of Gold Nano-islands	93
IT-044	From Earth to Mars: Pioneering Metal-Carbon Dioxide (Metal-CO_2) Battery Solutions for a Greener Tomorrow	94
IT-045	Nanomechanical Metamaterials and Multifunctional Metalenses	95

IT-046	Water-based Solid Battery using 3D-Slime Interface quasi-Solid Electrolyte (3D-SLISE7	96
IT-047	Utilizing CO_2 for Synthesis of Organic Carbonates via Direct Carbonylation of Glycerol	97
IT-048	Microstructural dynamics of stretching nanofilm of hydrogels: effects of film thickness on mechanical properties	98
IT-049	Modulation of the Interfacial Lithium-Ion Transport within Lithium Ion Batteries: Insights from Multi-Scale Simulations	99
IT-050	Telecom Band Silicon Based Optical Defects for Quantum Technologies	100
IT-051	Development of an electron beam–pumped, localized surface plasmon–enhanced nanoscale light source for electron-beam–assisted optical microscopy	101
IT-052	Surface-Induced Photorefractive Effect (SIPRE) In Liquid Crystal Nanocomposites for Applications in Fast Switchable Devices	104
IT-053	Application of Pulsed Electric Fields in Inorganic Materials Science	103
IT-054	Complex Interactions Driven Assembly in the Multi-Component Colloids: Insights from Synchrotron SAXS	104
IT-055	Spintronics using 2D materials	105
IT-056	Excitonic Signature of 2D Sliding/Interfacial/Moiré Ferroelectrics	106
IT-057	InGaN LED Technology Trends for Agriculture and Bio-industry Applications: From Spectral Engineering to Van der Waals Epitaxy	107
IT-058	Solid Oxide Electrolysis of CO_2: Power to X	108
IT-059	Quantum Beam Approaches to Advanced Functional Polymer Composites	109

IT-060	Application of Probe Aberration Corrected STEM Techniques in Understanding Some Fascinating Features of Melt-Cast $(Fe,Cr)_2B$	110
IT-061	From Reactive-Species Composition to Function: A Design Framework for Non-Ablative, Reversible Biointerface Modulation	111
IT-062	Quantum Spin Sensors for Open-Shell Molecules	112
IT-063	Deriving Interface Physics from Correlations Between Electrical Properties and XPS in PECVD-SiO_2/Si	113
IT-064	Representation of 3D X-ray CT Using Mixed Reality with Force Feedback for Density Information	114
IT-065	Domain Engineering of Ferroelectric Nano-structures and Their piezoelectric properties	115
IT-066	Sensing Experiments Based on Collaborative Research Activities in Tokyo University of Agriculture and Technology	116
IT-067	Exploring MBene: 2D Materials Pathways in Synthesis and Characterization for Optoelectronics devices	117
IT-068	Measurement of Hydrogen to Carbon Ratio in Amorphous Hydrogenated Carbon Products and the Effect Ion Irradiation	118
IT-069	Studies on the Structure and Functional Properties of Some Nanocomposite Layers Based on Graphene and Graphene Oxide	119
IT-070	Heusler Alloys as Spintronic and Spin-Caloritronic Applications	120
IT-071	Generation and Detection of Orbital Currents	121
IT-073	High Temperature Quantum Transport using Deep Dopant in Silicon	122
IT-074	Topological Spin Textures in Van der Waals Magnets	123

IT-075	Peptide-Based Nanomaterials for Organic Electronics: Tailoring Piezoelectric Properties through Nanostructural and Chiroptical Modulation	124
IT-076	Efforts Toward Developing High-Performance Aqueous Rechargeable Zn-Ion Batteries	125
IT-077	Stimuli-Responsive Molecular Systems for Nanoscale Energy Harvesting Prospects	126
IT-078	Development of Indigenous Electrode Materials for Li- and Na-Ion Batteries: From Lab-Scale Innovation to Technology Demonstration	127
IT-079	Thermoelectric Properties of Nanocluster Composites consisting of Fullerene Molecules and Metal Oxide Nanoclusters	128
IT-080	MOFs-derived and Chitosan-based Photocatalysts for Scalable VOCs Degradation in Photocatalytic Fluidized Beds	129
IT-081	Design of Sol–Gel Composite Materials for High-Temperature Ultrasonic/Piezoelectric Devices	130
IT-083	Seebeck-Coefficient Evaluation of Si Microribbon by Kelvin-Probe Force Microscopy	131
IT-084	A Traceable Digital Thread for UAV Propulsion: MBSE Architecture Linked with Performance Simulation	132
IT-085	Bandgap Widening of Evaporated In-Se Films By Room Temperature Annealing	133
IT-086	Transforming Electronics: The Future of Transparent and Paper Electronics	134
IT-087	Stimuli-Responsive Soft Molecular Materials	135
IT-088	Upconversion Luminescence of SrF_2-ErF_3 Solid Solutions	136
IT-089	A Proposal for Infrastructure Management Using Motorcycle Dynamics Data and Rider Vital Signals	137

IT-090	Design of Electrodeposition-Driven Phosphide Catalysts for Green Hydrogen and Ammonia Synthesis	138
IT-091	Toward a Resilient Society: Dialogue between Engineering and the Social Sciences in Disaster Contexts	139
IT-092	Theoretical Study of Phonon-Induced Negative Thermal Expansion Materials	140
IT-093	The Expanding Attack Surface of AI-Enabled Biometric Infrastructures	141
IT-094	Effect of Tandem-Type Stabilization of Two-Dimensional (2D) Nb_2CTx Mxene on their Colloidal and Cytotoxic Properties	142
	Theme: Advanced Characterizations (AC)	
AC-001	Structural, Morphological, and Magnetic Properties of Eu – Doped Nanocrystalline $La_{0.9}Ba_{0.1}MnO_3$	143
AC-002	Designer Colour-Tunable NIR-Reflective Cool Pigments in the Ternary Vanadate Phenacite-Inverse Spinel Phase Regime	144
AC-003	Multifaceted Characterization of PVDF/$Bi_{12}GeO_{20}$ Nanocomposite Films: Insights into Structural, Optical, Thermal, Mechanical and Dielectric Properties	145
AC-004	Microstructural and Mechanical Performance of Laser Beam Welded Joint between Inconel 625 and SAE 304 Stainless Steel	146
AC-005	Tailoring Laser Fluence to Enhance Piezoresistive Sensitivity in Laser-Induced Graphene-Based Flexible Sensors	147
AC-006	Investigation on the Linear and Non-Linear Optical Properties of Indole-Ringed Amino Acid Infused Thiourea-Metal Complexes	148
AC-007	An Experimental Analysis of Zinc MMCs Reinforced with SiC and Graphite	149

AC-008	Advancements in Soft/Hard Ferrite Nanocomposites: Magnetic, Dielectric, and Optical Perspectives	150
AC-009	Fatigue Behaviour of FeMnSi Shape Memory Alloy	151
AC-010	Investigations on the Structural and Photoluminescence Properties of Alkali-Doped Cesium Copper Iodide Single Crystals	152
AC-011	Structural and Magnetic Properties of Tryphtophan-capped Iron Oxide Nanocomposites	153
AC-012	Disorder Induced Inter-band Dynamics of Spin–Orbit Coupled Tilted Nodal Line Semimetals	153
AC-013	Application of X-Ray Radiography for Detection and Repair of Bulges Observed in Composite Rocket Motor Casing	154
AC-014	Additive manufacturing of Anisotropic Honeycomb Lattice materials embedded with Shape Memory Alloys: Mechanical and microstructural characterization	155
AC-015	Phase Evolution and Dielectric Response of Lead-Free $BiTiO_3$, NBT, and KBT-Based Perovskites	155
AC-016	A comparative analysis of alternate refrigerant-lubricant pairs for enhanced and sustainable VCR system performance	156
AC-017	Disorder Induced Interband Dynamics of Spin–Orbit Coupled Tilted Nodal Line Semimetals	157
AC-018	Effect of Pre-Milling (Ni And Al) on the Oxidation Behaviour of Nialfecocr High Entropy Alloy	157
AC-019	Fe–Co–Gd Alloy Synthesized by Mechanical Alloying: Structural and Magnetic Properties	158
AC-020	Effect of Graphene Filler in ARB Fibers in Araldite LY 556 Epoxy Resin and Aradur HY 951 Hardener Polymer Composites: Experimental Study of Fractography and Moisture Absorption	159

AC-021	Lightweight and Absorption-Dominant PVA/PANI/$CeNiO_3$@GNP Polymer Nanocomposites for EMI Shielding	160
AC-022	Extraordinary Magnetoresistance and Temperature-Dependent Electronic Transport in WTe_2	161
AC-023	Microstructural Evolution and Mechanical Tailoring of Fe-Al-Ni Alloys via Controlled Annealing and Normalizing Heat Treatments	162
AC-024	Multi-Scale Microstructural and Indentation Evaluation of Glass Fibre Reinforced Expired ABS for Sustainable Additive Manufacturing	163
AC-025	Raman Spectroscopic Characterization of Fly Ash and Bottom Ash from a Coal Power Plant of Eastern India	164
AC-026	Synthesis of high purity Zeolite from Water Treatment Sludge for Fluoride Removal from Coal Mine Water	165
AC-027	Alginate – Silica Functionalized Magnetic Nanoparticle for Targeted Cancer Cell Isolation	166
AC-028	A Comprehensive Review on PVDF Nanocomposites Reinforced with Maleic Anhydride and Silane-Treated Short Carbon Fiber	167
AC-029	Titanium Dioxide Nanoparticles: An Eco-Friendly Material for Versatile Applications with Self-Cleaning Abilities	168
AC-030	High Hardness Lanthanum Borate Glasses Containing Eu^{3+}, Dy^{3+} and Er^{3+}	169
AC-031	Electrical and Electrochemical Properties of Barium Vanadate Glass Cathode	169
AC-032	Analysis of Steel Structure infilled with ACC Blocks Subjected to Seismic Loads	170
AC-033	A Review on Polyaniline Based Hybrid Nanocomposites: The Role of Maleic Anhydride Compatibilizer and Silane-Treated Short Carbon Fibers	171

Theme: Quantum Materials & Devices (QD)

QD-001	Strategies for Light Management in Thin and Flexible C-Si Solar Cells Utilizing Cadmium Selenide (CdSe) Nanoparticles	172
QD-002	Effect of B-Site Doping on the Structural, Morphological, AC Susceptibility, and Magnetic Properties of Nanocrystalline $Pr_{0.7}Ba_{0.3}Mn_{1-x}NixO_3$ (x=0.1,0.2)	173
QD-003	Disorder-Induced Orbital Hall Conductivity in Three-Dimensional Weyl Semimetals	173
QD-004	Quantum-Aided Deepfake Detection: A Critical Review of Classical Techniques, Existing Challenges, and the Emerging Role of Quantum Approaches	174
QD-005	Collective Enhancement and Suppression of Coupling Strength Due to Photon-Mediated Magnon-Magnon Interaction	175
QD-006	Planar Hybrid System for Photon-Magnon Coupling	176
QD-007	Structural, Morphological and Optical Properties of Surfactant-Mediated ZnS QDs	177
QD-008	A New Semiconductor Quantum Dot for Optoelectronic Applications	178
QD-009	Morphology-Driven Magnetization Reversal in Functional Ni Nanostar Chains	179
QD-010	Impact of Intermediate Diradical Character on Optical and Magnetic Properties in Croconaine Dyes	180
QD-011	pH-Tunable Dual-Target Fluorescent Sensor for Selective Detection of Tartrazine and Ascorbic Acid Using N/O-Doped Carbon Quantum Dots	181
QD-012	Tailoring Topological Deflection and Mobility of Skyrmions in Synthetic Ferrimagnets	182
QD-013	Exploring Static and Dynamic stability conditions of Skyrmions in Synthetic Ferrimagnets	183

Theme: Energy and sustainable Materials (EN)

EN-001	Thermoelectric and Phase Change Materials for Waste Heat Recovery	184
EN-002	Catalyst-Enhanced ChCl-Ethylene Glycol Deep Eutectic Electrolytes for High-Performance Zinc-Ion Batteries	185
EN-003	Development and Characterization of Sustainable Metal Matrix Composites Reinforced with Industrial Waste and Minor Graphite Additives	186
EN-004	Lewis Acid Site Engineering for Sustainable Ethanol-to-Ethylene Conversion	187
EN-005	Hydrothermal synthesis of $CuMn_2O_4$/rGO composite and investigation of electrochemical properties for high performance supercapacitor electrode materials	188
EN-006	Thermoelectric Properties of Γ-Phase In_2Se_3 Thin Films Prepared by RF Magnetron Sputtering	189
EN-007	Microwave-Synthesised Vanadium Oxide Incorporated $Mose_2$/Polypyrrole Nanocomposites for Improved Hydrogen Evolution Reaction	190
EN-008	Upcycled Paper Cup-Based Porous Activated Carbon for High-Performance Supercapacitors	191
EN-009	Structural and Electrochemical Study of Template-Free Self-Standing MOF Electrocatalyst for OER in Alkaline Medium	192
EN-010	CoS/Water Hyacinth-Based -Natural Metals and Activated Carbon Nanocomposite for Supercapacitor Application	193
EN-011	Recycling of Spent Battery Electrode Materials for Textile Wastewater Remediation	194
EN-012	Exploring the Potential of Ag/NiO Cathode for the Fabrication of a Screen-Printed Silver-Zinc Rechargeable Microbattery	195
EN-013	Carbon-Integrated Co_3O_4 Cathodes with Enhanced Electrochemical Kinetics for Aqueous Zinc-Ion Batteries	196

EN-014	Interfacial Engineering of Nickel Sulfide with Graphitic Carbon Nitride for Advanced Zinc-Ion Storage	197
EN-015	Ag doped Activated Carbon as a Potential Energy Storage Material of Supercapacitor and Experimental Investigations	198
EN-016	$InVO_4$/ RGO Nanocomposite for Hybrid Supercapacitor Application	199
EN-017	Synergistic Bi_2WO_6/PANI Nanocomposites: Toward Sustainable and Efficient Energy Storage	200
EN-018	Superhydrophilic-Underwater Superoleophobic Cluster-Like TiO_2 Coated Mesh, a Tool for Oily Wastewater Treatment	201
EN-019	One-Pot Carbonization of Zn-Based Deep Eutectic Solvent for High-Performance Carbon Anodes in Aqueous Zinc-Ion Batteries	202
EN-020	Synthesis and Characterisation of Bio Hosted PCM for Thermal Management Application	203
EN-021	A Novel $NiMn_2O_4$@TiO_2 Core shell structure as a high-performance electrode for supercapacitor material	204
EN-022	α-MnO_2@C nanospheres cathode with enhanced electrochemical characteristics for aqueous zinc-ion battery applications	205
EN-023	$NaFePO_4$ as a Cathode Material for Sodium-ion Batteries	206
EN-024	Design of Zn-MOF/Ni–Co Bimetallic Oxide Hybrid Electrodes for Enhanced Asymmetric Supercapacitor Performance	207
EN-025	Electrodeposited Binder-Free Bi-Metallic Oxide Nanostructures and Vertical Graphene Nanosheets Hybrid Electrodes for Supercapacitor Applications	208
EN-026	Biomass-Derived Activated Carbon of Citrus Limon Derived Activated Carbon for Ultracapacitors Performance	209

EN-027	Ternary Nanocomposite of Polypyrrole/Graphener Oxide - MoO_3 for High-Performance Supercapacitor Electrode	209
EN-028	Design of Succinonitrile (SCN)-Modified LATP–PVDF-HFP Nanofiber Hybrid Electrolytes for High-Performance Flexible All-Solid-State Batteries	210
EN-029	Hydrothermally Synthesized Li-KNN And PVDF Based Flexible Composites for Piezoelectric Energy Harvesting	211
EN-030	Development of PVDF-HFP/Guar Gum Based Composite Polymer Electrolyte for Proton Conducting Battery Applications	212
EN-031	Hydrothermal Synthesis and Energy Related Performance of Vanadium Doped BaO Containing Layered Double Hydroxide Nanomaterials	213
EN-032	Engineering $NiMn_2O_4/NiMoO_4$ Heterobimetallic Oxides as Efficient Electrode Materials for Asymmetric Supercapacitors	214
EN-033	An Alternative Aluminum-Copper Galvanic Cell Model for Aluminum Ion Battery Systems Using Fe_2O_3 Nanoparticles in Acidic Mixture Electrolyte	215
EN-034	Design of Zn–Sr–Ni Trimetallic Nanocomposites for Environmental Remediation and Energy Storage	216
EN-035	Synthesis of Carbon-Based Materials for Positive Electrode Fabrication in Energy Storage Devices	217
EN-036	Hybrid Bio-leaching and AI-Assisted Optimization for REE Recovery from PCB and NdFeB E-Waste	218
EN-037	Egg Shell Mediated Ni5P4/Polypyrrole Electrocatalyst for Sustainable Water Splitting	219
EN-038	Experimental and Computational Analysis of PCM Assisted Cooling for Solar Collectors	220
EN-039	Synthesis and Characterization of Transition Metal (M = Co, Cu, Ni, Zn) Doped $SrTiO_3$ for Enhanced Photocatalytic Hydrogen Evolution	221

EN-040	Deciphering the Contribution of Quantum and Faradaic Capacitance in Er_2O_3 Decorated MXene Hybrid Composites for Supercapacitor Electrodes	222
EN-041	Sustainable Marine Algae-Derived Carbon/MXene/$HoFeO_3$ Nanohybrid for Photocatalytic Degradation of Persistent Agrochemical Pollutants in Water	223
EN-042	Preparation and Characterisation of the Nano-Enhanced Phase Change Material for Battery Thermal Management Applications	224
EN-043	One-Step Synthesis of a Dual Metal Chalcogendies Heterojunction Encapsulated in Carbon Nanotubes for High-Performance Supercapacitors	225
EN-044	Synergistic Composite Engineering of 0D Halide Perovskite in Cuse Enables Ultra-Low Thermal Conductivity and High Thermoelectric Performance	226
EN-045	Design of a Carbon-Modified $ZnMn_2O_4$ Cathode for High-Performance Aqueous Zinc-ion Batteries	227
EN-046	Electrochemical Investigation of Hydrothermally Synthesized $MnMoO_4$-Co-MOF Composite for Supercapacitor Applications	228
EN-047	Compositing NiFe Layered Double Hydroxide (LDH)/MXene for electrocatalytic water splitting application	229
EN-048	SnO_2 Quantum Dots: A New Frontier in Ultrafast Photocatalysis	230
EN-049	Design and Synthesis of Phenothiazine based Materials for Dye-Sensitized Solar Cells	231
EN-050	Samarium-doped Ni-Co Ferrite based Systems for Improved Magnetic and Electrochemical Properties	232
EN-051	Ni-Doped TiO_2/rGO Nanocomposites as High-Performance Electrode Materials for Supercapacitor Applications	233

EN-052	Synthesis of Substituted Carbazole based Materials for Dye Sensitized Solar Cells	234
EN-053	Facile Hydrothermal Synthesis of Bi_2O_3/MoS_2 (1:1) Heterostructure Electrodes with High Capacitance and Long-Term Stability for Supercapacitors	235
EN-054	Cr-Doped $NiCo_2O_4$ Nanoparticles Synthesized by a Hydrothermal Route for High-Performance Supercapacitor Applications	236
EN-055	Thermal Reliability of Graphene-Based Nanofluid Heat Pipes for Next – Generation Electronic Cooling	237
EN-056	Room-Temperature Magnetic Response in Co-Doped $Na_{0.5}Bi_{0.5}TiO_3$: A Lead-Free Perovskite System	238
EN-057	Hydrothermal Engineering of Ni–Co Layered Double Hydroxides for High-Performance Supercapacitor Electrodes	239
EN-058	Synthesis of Flexible Carbon-Based Electrodes for Supercapacitors through the Resistive Heating Method	240
EN-059	Metal-Free g-C_3N_4/Nitrogen-Doped Carbon Dots Nanocomposite for Enhanced Photocatalytic Hydrogen Generation	241
EN-060	Bimetallic (NiFe) Metal-Organic Framework for High Electrochemical Performance for Supercapacitor Applications	242
EN-061	Electrochemical Nitrate Reduction to Ammonia by $NiFe_2O_4/Fe_2O_3$	242
EN-062	Hydrophobic Concrete Using Admixtures and Industrial By-Products	243
EN-063	High Performance Electrospun Niobium Nitride Carbon Nanofibre Electrodes for Enhanced Lithium-ion Battery Efficiency	244

EN-064	Boosting Energy Density in Hybrid Supercapacitors with Fe MOF@GO Decorated Ni Nanoparticle Electrodes: A Robust Anode Electrode Material	245
EN-065	Sustainable and Scalable Low-VOC Inorganic Aqueous Coatings for Passive Daytime Radiative Cooling	246
EN-066	Carrier Modulation and Glassy Thermal Transport in Cu, Sb Co-Doped Ag8SnSe6 PGEC system	247
EN-067	Visible-Light-Driven Green Hydrogen Production Using 2D–2D WO_3/G-C_3N_4 Heterostructured Photocatalysts	248
EN-068	Copper-based Oxy selenide: Pioneering Single-Material Solution for Integrated Green Hydrogen Production and Environmental Remediation	248
EN-069	Effect of Annealing Temperature on the Structure and Electrochemical Performance of Nickel Vanadate/Nitrogen-Doped Graphene Oxide (NiV_2O_6/N-GO) Nanocomposites	249
EN-070	Asymmetric $CuFe_2O_4$ and Holey Reduced Graphene Oxide Electrodes for High-Performance Capacitive Deionization of NaCl and Heavy Metals	250
EN-071	Binary-Ternary Complex Oxide Nanoflower: Pulse Reverse Electrodeposited Electrode for Designing Supercapacitor Prototype	251
EN-072	Bayesian Reliability Analysis of Mineral-Tallow Oil Blends for Sustainable Dielectric Cooling in Electrochemical Energy Systems	252
EN-073	High-Performing Nickel Sulfide Nanoparticles Decorated 2D Mxene Electrocatalysts for the Valorization of Furfural	253
EN-074	Synergistic Catalytic Effect of Pt-Ni_2P/rGO Composite for Efficient Ammonia Oxidation Toward Greener Hydrogen Production	254
EN-075	To Improve Strength and Durability of Concrete with Biopolymer Additives and Sisal Fiber Reinforcement Concrete	255

EN-076	Modulation of the Interfacial Lithium-Ion Transport within Lithium-Ion Batteries: Insights from Multi-Scale Simulations	256
EN-077	Experimental and Computational Analysis of PCM Assisted Cooling for Solar Collectors	257
EN-078	Visible-Induced Photocatalysis by Cr Doped Fe_2O_3 Nanoparticles on Methylene Blue	258
EN-079	Performance Evaluation of GGBS and Nano-Titanium Modified Concrete Beams Under Flexural Loading	259
EN-080	Waste-Derived Bacterial Cellulose Acetate Composite Membrane for high performance Microbial electrochemical Systems	260
EN-081	Structural and Catalytic Effect of Partial Substitution of Nickel by Niobium on the Hydrogen Storage Behaviour of Mechanically Alloyed Mg-Mg_2Ni Composites	261
EN-082	Tuning p-Type and n-Type Thermoelectric Transport in VFeSb Half-Heusler Alloys via Site-Specific Substitution	262
EN-083	Green Synthesis of CdS Nanostructures Using Plant Extracts and Their Morphological, Optical, and Photocatalytic Properties	263
EN-084	Polyaniline Coupled MoS2-MoO3 Heterostructures for High Performance Supercapacitors	264
EN-085	Hydrothermally Synthesized NiS Nanoparticles: Optical Properties and Electrocatalytic Performance for Hydrogen Evolution	265
EN-086	Sol–Gel Auto-Combustion Synthesis and Photocatalytic Activity of 5% Co-Doped Bismuth Ferrite ($BiFe_{0.95}Co_{0.05}O_3$)	266
EN-087	Selective CO_2 Reduction to Formate using Copper Phosphide Based Electrocatalyst	267
EN-088	Exploring the Thermoelectric Potential of $Bi_2Te_xSe_{3-x}$ Topological Insulators through Raman Thermometry and Theoretical Analysis	268

EN-089	Improved Thermoelectric Performance of $SrTiO_3$-Based Entropy-Stabilized Perovskite Oxide for High-Temperature Waste Heat Recovery	269
EN-090	Water-in-Glass Additives: Synergistic Enhancement of Alkaline Hydrogen Evolution Reaction via Electrolyte Engineering	270
EN-091	Lattice Thermal Conductivity of $SrSnO_3$: A Combined Experimental and Theoretical Study	271
EN-092	Ca and Fe doping effect on Structural, Spectral and Dielectric properties of $Sr_{1-x}Ca_xTi_{1-y}Fe_yO_3$	272
EN-093	Ideating at Interfaces: Enhancing the Performance and Longevity of Sustainable Energy Systems	273
EN-094	Structural and Magnetic Properties of Rare Earth-Doped $Co_{0.8}Zn_{0.2}$ Ferrites Synthesized via Solid-State Reaction	274
EN-095	Numerical Investigation of High-Efficiency Two-Terminal Rb_1MAFA/In_2S_3 Tandem Perovskite Solar Cells	275
EN-096	Molarity Driven Electrochemical Optimization of Zn-Co LDH@CS Supercapacitor	276
EN-097	Developing $Rh_{2-Y}cr_yo_3$ Cocatalysts to Outperform Platinum in Semiconductor-Based Photocatalytic H_2 Evolution	277
EN-098	Investigation of WO_3 Nano-Structured Materials for Hydrogen Evolution Reaction	278
EN-099	Enhanced Thermoelectric Performance in Mn-Doped $AgCrSe_2$: Synergistic Optimization of Carrier Concentration and Lattice Thermal Conductivity	279
EN-100	Interfacial Polysulfide-Rich Nickel Iron Vanadium-LDH/Cobalt Oxysulfide Heterostructures for Durable and Efficient Overall Water Electrolysis	280
EN-101	Synergistic Ni-MOF/MoS_2-based heterostructures for efficient bifunctional hydrogen electrocatalysis	281

EN-102	Hybrid Fe_3O_4/PANI Nanocomposites for Advanced Electrochemical Energy Storage	282
EN-103	Band Gap Engineered Cd-Pb Co-Doped SnS Nanoparticles via Microwave Solvothermal Route for DSSC Photoanodes	283
EN-104	Electronic Structure and Interface Modulation in Bi_2WO_6–Carbon Nitride Heterostructures Via Transition Metal Doping for Boosted Photocatalytic Nitrate-To-Ammonia Conversion	284
EN-105	Synergistic Effect of Ni Doped in Zno Enhancing Charge Separation for Efficient Eco-Friendly Sun Light Driven Photodegradation	285
EN-106	Mesoporous Silica Dispersed Polyethylene Glycol Nano-Phase Change Material Embedded Rooftop Tiles for Thermal Comfort and Energy Savings in Green Buildings	286
EN-107	Efficient and Stable Triple Cation Perovskite Precursor-Based Solar Cells Empowered by Interface with 2-2'-Dihydroxy-4-Methoxy Benzophenone Stabilizer	287
EN-108	3D flower cobalt oxide nanoarchitectures for supercapacitor applications	288
EN-109	Microwave-Assisted $Bi_{2-x}Sb_xS_3$ Alloy Nanoparticles for Enhanced Visible-Light Photocatalytic Dye Degradation	289
EN-110	Band Structure Modulation in Co-Doped SnO_2 Nanoparticles for High-Performance UV Photocatalytic Dye Degradation	290
EN-111	Comparative Study of Reflux and Autoclave-Assisted Transesterification of Jatropha Oil Using Cao-Doped Mesoporous SBA-15	291
EN-112	High-Performance Ru50/Pt50-MoS_2/rGO Bifunctional Electrocatalyst for Sustainable Overall Water Splitting and Seawater Electrolysis	292
EN-113	Synergistic High-Entropy Oxide/Graphene Hybrids: Advancing Energy and Environmental Remediation	293

EN-114	Exploring the Role of Interstitial Occupation of Cobalt on the Thermoelectric Properties of Co-Rich Te-Substituted Skutterudite.	294
EN-115	Tailoring the Electrochemical Performance of ZnO/NiS/MWCNT Ternary Composites for Supercapacitor Application	295
EN-116	Unlocking Synergy in MXene-Supported W-Cr-Ni_2P for Overall Water Splitting	296
EN-117	Electrodeposited Gadolinium-Doped Nickel Selenide: An Efficient Electrocatalyst for Hydrogen Evolution Reaction in Alkaline Media	297
EN-118	Structural, Optical, Magnetic, and Dielectric Properties of (1-x) NCFO + (x)BCZT Composites Synthesized via Solid-State Reaction	298
EN-119	Electrocatalytic Water Splitting Performance of $SrTiO_3$/rGO Composite for Hydrogen Evolution Reaction in Acidic Medium	299
EN-120	Structural and Magnetic Properties of Rare Earth-Doped $Ni_{0.8}Zn_{0.2}$ Ferrites Synthesized via Solid-State Reaction	300
EN-121	Strategic Integration of Sns on Boronized Ni-ZIF for High-Performance Electrocatalysis and Energy Storage	300
EN-122	Study on the Thermoelectric Properties of BiCuOS-CuS Composites	301
EN-123	Optimizing $ZnCl_2$ Activation Temperature for Biomass-Derived Porous Carbons with Superior Energy and Power Density in Supercapacitors	302
EN-124	Sustainable Green Synthesis of CuO–ZnO Nanocomposite Heterostructures Using M. spicata L. for Catalytic Reduction of Various Dyes and Photocatalytic Degradation of Tetracycline	303
EN-125	Structure–Function Modulation in Semiconductor Heterostructures for Efficient Solar Fuel Production	304

EN-126	Engineering Next-Generation Photoelectrochemical Flow Reactors for Integrated Bio-oil Valorisation and CO_2 Reduction	305
EN-127	The Impact of Catalyst Engineering, Solution Chemistry and Operational Conditions on the Photocatalytic Performance of SnS Thin Films	306
EN-128	Engineering Non-Centrosymmetric Bismuth-Based Photocatalyst and Investigation of Their Influence on Mixed Pollutant Degradation	307
EN-129	Flexible Silver Chalcogenide Architectures on Carbon Fabric for Wearable Thermoelectric Energy Harvesting	308
EN-130	Comparative Intercalation Behavior of Li, Na, and K Ions in Bilayer Graphene: An Experimental and DFT Study	309
EN-131	Microwave-Assisted Synthesis of Gold-Graphene Quantum Dots Composite for Sensitization of TiO_2 in Dye-Sensitized Solar Cells	310
EN-132	Upgrading Industrial Waste–Derived Carbon via Chemical Purification for Sustainable Environmental and Energy Applications	311
EN-133	Doping-Induced Carrier and Phonon Transport Modulation in $Bi_2Sn_2O_7$ Pyrochlore Oxide for Flexible Wearable Thermoelectric Energy Harvesting	312
EN-134	Phase-Engineered NiTi Shape Memory Alloy for Enhanced Alkaline Hydrogen Evolution	313
EN-135	Ni-rich with reduced Ni-content $LiNi_{0.7}Mn_{0.15}Co_{0.15}O_2$ cathode delivered enhanced rate and cycle life in Li-ion batteries	314
EN-136	Nanoclusters of Metal–Organic Frameworks on NiO Nanosheets for Water	315
EN-137	Synergistic Charge Separation in $ZnMn_2O_4/Cu_3P$ Composites for Photocatalytic Hydrogen Evolution	315

EN-138	UV Light Induced Structural Transformation Enhances Electrocatalytic and Photoelectrocatalytic Efficiencies of Novel Metal-Organic-Materials	316
EN-139	Fabrication of Zinc Oxide Nanocomposites with carbon paste as a modified Platinum Electrode for Electrocatalytic conversion of substituted alcohols	317
EN-140	Enhanced Rate Performance of $Na_xLi_{1/5}Ni_{1/5}Mn_{2/3}O_2$ Hybrid Supercapacitor in Monovalent and divalent Aqueous Electrolytes	318
EN-141	Synergistic Ni_3Se_2/CoFeLDH Heterostructure Electrocatalyst as an Efficient Bifunctional Electrocatalyst for Overall Water Splitting	319
EN-142	Tuning Oxygen Evolution via Dual-Mode Fe Incorporation in CaO and $KCaPO_4$ Catalysts	320
EN-143	Temperature-induced Antisite Defects in Dopamine-based Carbon-$LiFePO_4$ Cathodes for Lithium-ion Batteries	321
EN-144	A Cyber-Physical Automation Framework for Intelligent Energy Management and Safety in Hydrogen Fuel Cell Autonomous Vehicles	322
EN-145	Synthesis of Surface-Modified ZrO_2 via Non-Thermal Plasma for Enhanced Photocatalytic Degradation of Ciprofloxacin and Crystal Violet	323
EN-146	Synthesis of Activated Carbon from Biowaste Materials for Energy Storage Applications	324
EN-147	Vanadium Oxide–Sulfide Nanocomposites as Efficient Electrocatalysts for Overall Water Splitting in Alkaline Media	325
EN-148	Investigations of the Charge Storage Behaviour in the rGO-$CuWO_4$ Encapsulated PANI Nanocomposite based Symmetric Supercapattery Device	326
EN-149	Development of Biomass-derived Activated Carbon/Impregnated with NMC111 composites for Supercapacitor Applications	327

EN-150	Optimizing Thermoelectric Properties of Mixed Metal Oxide/Metal Molybdate Material by Doping	328
EN-151	Solar Hydrogen Production by $Cu_2ZnTi(S,Se)_4$, $Cu_2ZnTi(S,Se)_4$, and $Cu_2ZnTi(S,Se)_4$ Quaternary Chalcogenide Nanocrystals as Visible-Light Photocatalysts	329
EN-152	Green-Derived Ni–Co–Ti Ternary Oxide Nanocomposites: A Comparative Electrochemical Insights for High-Performance Supercapacitors	330
EN-153	In-situ Hydrothermally Prepared Honeycomb-Like Structured NiO Electrode for Acetaminophen Drug Detection and Supercapacitor Applications	331
EN-154	Bi-MOF@$NiCo_2O_4$ Composite Electrodes: A Synergistic Approach Toward Superior Electrochemical Performance	332
EN-155	Enhanced Electrochemical Performance of Nickel Phosphide/CeO_2 Nanocomposite for Supercapacitor Applications	333
EN-156	Synergistic Effect and Thermal Performance of Poly-Hydroxyethyl Methacrylate Encapsulated Graphene Quantum Dot-Paraffin Hybrid Nanofluid	334
EN-157	Time dependent synthesis of a Cu_9S_5/CuS@Ni Foam Heterostructure for Visible-Light-Driven Photocatalytic Degradation and Supercapacitor Applications	335
EN-158	Impact of Ag and Mn Co-Doping on Carrier Enhancement and Thermoelectric Performance of Cu_2SnSe_3 at Intermediate Temperatures	336
EN-159	Understanding the Green Hydrogen Production Capability in Copper (Cu) and Vanadium (V) based Materials	337
EN-160	Dual Z-Scheme $BiVO_4$/CuO/g-C_3N_4 Ternary Heterojunction for Enhanced Visible-Light-Driven Ciprofloxacin Degradation	338
EN-161	Development of Biomass-Derived Electrode Material for Supercapacitor Applications	339

EN-162	Real-Time Experimental Validation of Thermally Enhanced Nano Composite Phase Change Materials for Photovoltaic Module Cooling.	340
EN-163	In-Situ Synthesized Gel Polymer Electrolyte for Long-Life Sodium-Ion Batteries	341
EN-164	Carbon Nanotube-Integrated Co-phthalocyanine/NiFe-LDH Hybrid with Superior Bifunctional Activity for Water Splitting	342
EN-165	Electrochemical Fabrication of Self-Supported Pt-Nanoporous Gold for Efficient Hydrogen Evolution Reaction	343
EN-166	Environmentally benign synthesis of phase-pure Ni3V2O8 Nanoparticles with Enhanced Pseudocapacitance for Electrochemical Energy Storage Applications	344
EN-167	Synergistic CdTe@ Sulfur Doped g-C_3N_4 Nanocomposite as a High-Performance Electrode for Advanced supercapacitor Application	345
EN-168	CoAl-N Nanostructures Derived from Spent $LiCoO_2$ Cathodes for High-performance Bifunctional Oxygen Electrocatalysis	346
EN-169	Metal-Organic Framework–Based Architectures for High-Efficiency Supercapacitive Energy Storage	347
EN-170	Design and Fabrication of Flexible Solid-State Interdigitated Micro-Supercapacitors Using Activated Carbon Microfibers	347
EN-171	In-Situ Sulfidation-Derived Selenium-Doped β-Bi_2O_3/Bi_2S_3 Heterostructure as an Effective Electrode for Supercapacitor Applications	348
EN-172	Accelerated Discovery of Cu-Based Lead-Free Hybrid Halide Perovskitoids Using Machine Learning for Solar Water Splitting Application	349
EN-173	Electrospun ZnX_2O_4 (X=Co, Mn, Fe) Nanofibers as Efficient Electrocatalysts for Electrochemical Water Splitting	350

EN-174	Water Treatment and Microplastic Degradation by Carbon Nitride-Supported Single-Atom Catalyst	351
EN-175	Boron-Doped MOF-Derived NiO as an Enhanced Electrocatalyst for Alkaline Water Splitting: A Comparative Study with Pristine Ni-ZIF	352
EN-176	Integration of Metal Selenide with Rare Earth Element for Oxygen Evolution Reaction	353
EN-177	Investigation on Structural and Optical Properties of Quaternary Oxides for Energy Conversion and Storage Applications	354
EN-178	MnO_2 Cathodes for High Performance Aqueous Zinc-Ion Battery Applications	355
EN-179	Crystal Structure and Short-Range Order of Lithium Cobaltate by High Energy X-ray Diffraction and Neutron Diffraction Studies	356
EN-180	Valorization of pyrolysis-derived bio-oil into high-performance biodegradable polymers	356
EN-181	Metal Organic Framework Assisted Optical and Interfacial Engineering of TiO_2 Photoanodes For Efficient Quantum Dot Sensitized Solar Cells	357
EN-182	Synergistic Effects of $Ti_3C_2T_X$ MXene/Sm_2O_3 Electrode and PVA/H_2SO_4/KNN Gel Electrolyte for Flexible All-Solid-State Supercapacitor	358
EN-183	Solvent-Assisted Morphological Control and Structural Evolution of Nickel-Based Metal–Organic Frameworks (Ni-BTC)	359
EN-184	Titanium-induced Modulation of Phonon and Charge Transport Enables Enhanced Thermoelectric Performance in WS_2	360
EN-185	Bi_2O_3-Incorporated V_2O_5 Nanoparticles: Enhanced Structural, Optical, and Electrochemical Properties for Supercapacitor Applications	361

EN-186	PVA-Assisted Fabrication of $PrCoO_3$ Cubic Perovskites for Advanced Hybrid Energy Storage	362
EN-187	Numerical Investigation of High-Efficiency Two-Terminal Rb_1MAFA/In_2S_3 Tandem Perovskite Solar Cells	363
EN-188	Development of Chitosan based nanocomposites for enhanced adsorption of chromium from industrial waste water	364
EN-189	Surface Engineered Sulvanite Integrated with Layered Double Hydroxide for Asymmetric Hybrid Supercapacitor	365
EN-190	A phase-tuned layered 1T W-MoS_2/PEDOT:PSS hybrid: functional engineering towards self-binding supercapacitor cathodes	366
EN-191	Recycled Electroactive Materials from Batteries as Catalysts for Green Hydrogen Production	367
EN-192	Enhancing the Thermoelectric Power Factor via Carrier Energy Filtering in Ag-Decorated Bi_2Se_3 Nanostructures/Carbon Fabric for Wearable Thermoelectric Application	368
EN-193	Enhancing Thermoelectric Properties of Ag_2Se Nanoparticles on Carbon Fabric via ZnO Composite for Wearable Energy Harvesting	369
EN-194	Decoupling Thermal and Electrical Transport Through Halide-Chalcogenide Hybridization in Cu_2SnSe_4 Thermoelectrics	370
EN-195	Fabrication and Testing of High Performance Flexible Symmetric Supercapacitor Using Copper Cobaltite Spinel Nanostructures	371
EN-196	Experimental Investigation of a Passive Battery Thermal Management System Using OM42 Phase Change Material and Aluminum Enhancements	372
EN-197	Carbon Ion Implanted $Ti_3C_2T_x$ MXene as a Multifunctional Material for Hydrogen Evolution Reaction and Supercapacitor Devices	373

EN-198	Ternary MXene/CNT/WO_3 Hybrid Cathode for High Performing Rechargeable Zinc–Air Batteries	374
EN-199	Synergistic α-MnO_2/$Ni(OH)_2$ Heterostructure as a High-Performance Cathode for Aqueous Zinc-Ion Batteries: Separator-Dependent Electrochemical Evaluation	374
EN-200	Copper Metal Organic Framework Reinforced Sulfonated Polyether Sulfone Composite for Proton Exchange Membrane Fuel Cells	375
EN-201	Advancements in Activation Methods and Electrode Fabrication of Biomass-Derived Biochar for High-Efficiency Supercapacitors	376
EN-202	CNF-Reinforced Ag_2Se/PVDF Films with Enhanced Seebeck Coefficient and High Flexibility for Wearable Thermoelectrics	377
EN-203	High-Performance $Mg_2Si_{0.6}Sn_{0.4}$ Solid Solution through Decoupling of Carrier-Phonon Dynamics for Thermoelectric Application	378
EN-204	A Flexible Triboelectric Nanogenerator Based on Biodegradable MXene@Cellulose Acetate/Ag Nanofibers for Self-Powered Electronics	379
EN-205	Potassium Oxychloride Solid State Electrolytes for Energy Storage Applications	380
EN-206	Investigation of Ru-doped Higher Manganese Silicide for Thermoelectric Application	380
EN-207	Interface-Engineered $NiCo_2O_4$@rGO Nanostructures with Superior Redox Activity for Efficient Energy Storage Devices	381
EN-208	Solid-State Derived Crystalline Molybdenum Pyrophosphate for High-Energy and Stable Pseudocapacitive Supercapacitors	382
EN-209	Protonated g-C_3N_4 Coupled Ternary System with Dual S-Scheme Charge Transfer Dynamics for Adsorption studies	383

	and Visible Light Driven Photocatalytic degradation of Methylene Blue and Ciprofloxacin	
EN-210	Surfactant-Regulated Bismuth–Nickel Oxide Nanomaterials for Efficient Supercapacitors	384
EN-211	ZnO Anchored g-C_3N_4 Nanosheets as an Efficient Material for Environmental Remediation and Energy Storage Applications	385
EN-212	Electrochemical Performance of $ZnC0_2O_4$ Nanoparticle for Water Splitting Applications	386
EN-213	Enhanced Themoelectric Performance of Layered Chalcogenide Bi_2Se_3 Through Ag Nanoinclusion	387
EN-214	Enhanced Atomic Ordering Leads to Carrier Delocalization and High Thermoelectric Performance in Zn doped $AgSbSe_2$	388
EN-215	Tuning of Carrier Concentration and Secondary Phase Interfaces for Enhanced Thermoelectric Performance of $AgInSe_2$	389
EN-216	Investigation of Mg_3Sb_2 a Zintl Phase Material for Thermoelectric Applications	390
EN-217	Flexible Cu_2Se/PVDF Thermoelectric Film for Efficient Human On-Skin Energy Harvesting	391
EN-218	NiFeCo LDH/Transition Metal Sulfide Heterostructures as Bifunctional Electrocatalysts for Water Splitting	392
EN-219	Alloying-Driven Atomic Disorder Enables Phonon Suppression and Enhanced Thermoelectric Performance in BiSe	393
EN-220	Rare-Earth-Induced Spin-State Engineering of Co_3O_4 For Efficient Oxygen Evolution Reaction	394
EN-221	Application of Lead-Free $Cs_3Bi_2Br_9$ Halide Perovskite for Solar-Driven Photocatalytic and Photoelectrochemical Water Splitting	395
EN-222	Rare Earth Incorporated Bimetallic MOF for Efficient	396

	Electrocatalytic Watersplitting	
EN-223	Enhanced Electrocatalysis Performance of NiFe LDH through Doping with Rare Earth Element	397
EN-224	Flexible Ag_2Se Composite Films using Organic Insulating Polymers for Wearable Thermoelectric Applications	398
EN-225	Investigation of Rapid Thermal Explosion Synthesis of $CuFeS_2$ for Enhanced Thermoelectric Performance	399
EN-226	Cocatalyst-Free Solar Driven Photocatalytic Hydrogen Production Using a Bimetallic Copper–Iron BDC MOF	400
EN-227	Rational Design of Porous MOF-808 Based Material for Strong Physisorptive Hydrogen Storage	401
EN-228	Investigating the Effect of Co doping on the Thermoelectric Properties of Ti-Ni-Sn	402
	Theme: Environmental & Health Monitoring (EH)	
EH-001	Innovative Spectrophotometric Assay For 'Vitamin C' Quantification and Its Implementation in A Portable Smartphone-Based Analytical Platform	403
EH-002	Rapid Spectroscopic Detection of Methanol from Alcoholic Mixtures	404
EH-003	Cu doped β-Ga_2O_3 Nanostructures for Environmental Photocatalytic Remediation	405
EH-004	Band Gap Engineering In B-Ga_2O_3 by Hydrothermal Method for Gas Sensing Performance	406
EH-005	Reusable SnO_2/g-C_3N_4/Cellulose Acetate Films for Photocatalytic Treatment of Dye-Contaminated Wastewater	407
EH-006	Coordination-Induced Self-Assembly of Metallosalens Enables Sustainable Monitoring of Phytic Acid in Agricultural Foods	408

EH-007	Optimization of Hydrothermally Synthesized MoS_2 and MoS_2-GO Nanocomposite for Enhanced Uric Acid Detection	409
EH-008	Influence of Pyrolysis Temperature on the Characteristics of Borassus Flabellifer Fruit Husk-derived Biochar for Selective Cationic Dye Adsorption from Multi- Dye Mixtures	410
EH-009	High-Sensitivity Piezoelectric PVDF - Coal GO Composite for Wearable Arterial Pulse Monitoring application	411
EH-010	Synthesis and Characterization of Transition Metal Doped Gallium Nitride for Gas Sensing Application	412
EH-011	Machine Learning–Driven Assessment of Urbanisation and Land Surface Temperature Dynamics in Hyderabad (1994–2024) Using Multi-Temporal Landsat Data	413
EH-012	Synthesizing High-Performance Zr-MOFs via Mixed-Linker Strategy to Enhance Rhodamine B Removal	414
EH-013	Interfacial charge transport-Engineered ZnO–g-C_3N_4 Nanocomposites for Enhanced Ammonia Detection	414
EH-014	Synthesis and Characterization of Room Temperature, Surfactant-Free GO-Cuo Nanosheets for Photocatalytic Degradation and Antibacterial Efficacy	415
EH-015	Experimental Spatiotemporal Studies on Fire Spread Over Thin Solid Fuels: Observations and Mechanisms	416
EH-016	Novel Highly Porous Carbon Hygrogel for Selective Electrochemical Sensing Application	417
EH-017	Electrocoagulation for Sustainable Tannery Wastewater Treatment: Modeling, Optimization, and Reactive Species Analysis	418

EH-018	Enhanced Performance of Tungsten Oxide Gas Sensors through Bismuth Doping: A Pathway to Reduced Operating Temperature	419
EH-019	Enhanced Electrochemical Response of Sol-Gel TiO_2/rGO Electrodes for PFAS Sensing	420
EH-020	Low-Cost Spin-Coated ZnO–rGO Thin-Film Electrodes for Portable Electrochemical Detection of PFOA in aqueous Systems	421
EH-021	Evaluation of Raw and Boiled Eggshell Powders as Renewable Biosorbents for Efficient Uranium (VI) Removal	422
EH-022	Conducting Polymer-Based Flexible Electrodes for Non-Invasive Electrochemical Biomolecule Detection	423
EH-023	MXene-Modified Metal-Organic Frameworks for Non-Invasive Electrochemical Detection of Serotonin	424
EH-024	Electrochemical Monitoring of Nitrofurantoin as an Emerging Antibiotic Pollutant Using Transition Metal Chalcogenides	425
EH-025	Synthesizing High-Performance Zr-MOFs via Mixed-Linker Strategy to Enhance Rhodamine B Removal	426
EH-026	Bimetallic MOF Derived Metal Oxide Based Chemiresistive No_x Gas Sensor	426
EH-027	Comparative Screening of Metal Oxides for Nitrate Removal from Aqueous Solutions	427
EH-028	Plasma-Induced g-C_3N_4/BC-Derived LIG Electrodes for AChE-Assisted Pesticide Detection	428
EH-029	Removal of Reactive Dyes from Water by PANI–$CoCl_2$ Composite: Kinetic, Isotherm, and Thermodynamic Studies	429

EH-030	Tailoring the Physico-Chemical Characteristics of SnO_2-Based Binary & Ternary Oxide Nanocomposites for Selective Gas Sensing: A New Strategy by Light Activation	430
EH-031	Electrocatalytic Reduction of Carbon Dioxide Over Copper Delafossite Complex Electrode Surface	431
EH-032	SecureVision-Pro: A Real-Time AI Surveillance Suite for Violence, Hazard, and Safety Detection with Audio-Visual Intelligence	432
EH-033	Real-Time Cyberbullying Detection and Reporting System with Multimodal Analysis and Secure AI-Powered Interface	433
EH-034	Biogenic CdS Nanostructures Using Hibiscus Rosa-Sinensis, Azadirachta Indica, Aloe Barbadensis Miller, And Citrus Sinensis: Encapsulant-Driven Morphological, Optical, and Photocatalytic Properties	434
EH-035	Utilizing CO_2 for Synthesis of Organic Carbonates via Direct Carbonylation of Glycerol	435
EH-036	Photocatalytic Degradation of Norfloxacin Antibiotic under UV Light Using Brookite TiO_2/N-Doped Graphene Nanocomposites	436
EH-037	Synthesis and Morphological Investigation of Carbon Nanotube Reinforced Nd Doped Yttrium Oxide Nano Composite on The Effect of Calcination Temperature for Environmental Gas Monitoring	437
EH-038	Plasmon-Mediated Energy Distribution and SERS Activity of Copper-Coated Glass Substrates	438
EH-039	An Edge-Cloud Enabled Smart Agriculture Infrastructure Using ESP32 and AWS for Intelligent Irrigation	439
EH-040	A Machine Learning-Based Vocal Screening Method for Respiratory Conditions	440
EH-041	Multifunctional Ni–Zn Ferrite ($Ni_{0.5}Zn_{0.5}Fe_2O_4$) Nanoparticles for Efficient Photocatalytic Removal of Pharmaceutical and Agrochemical Pollutants from Wastewater	441

EH-042	Investigation on the Remediation of Malachite Green Dye from Aqueous Solutions Using Industrial Boiler Ash as Sustainable Adsorbent	442
EH-043	Layered Hierarchically Porous Carbon-Composite Polymer Foam Filtration Column for Oil-in-Water Demulsification	443
EH-044	Enhanced No_2 Gas Sensing Performance of MoO_3 Thin Film Deposited by Pulsed Laser Deposition (PLD)	444
EH-045	Recovery Of Valuable Metals from Effluent of Tannery Industry	445
EH-046	Enhanced CO_2 Methanation Over Ni-Doped $AlPO_4$ Catalysts in A Fixed-Bed Reactor	446
EH-047	Electrospun PZT-PVDF composite: A Pathway to Flexible Acoustic Sensors	447
EH-048	A Stable Piezoelectric Pressure-Sensing Device Based on Riboflavin-Poly(vinylidene fluoride) Composite Nanofibers for Potential Applications in Athlete Training	448
EH-049	Development of Synergistic rGO–ZnO Hybrid Nanocomposites for Flexible Wearable Ethanol Sensors	449
EH-050	Toxicological Evaluation of PET Micro-Nano Plastics	450
EH-051	Synthesis, Ageing, and Toxicity of Polypropylene Microplastic	451
EH-052	Tire Wear Particles: Controlled Generation and Characterization	452
EH-053	Unveiling LiF-Engineered MXene: A Novel $Ti_3C_2T_x$/ZnO Hybrid Composite for Highly Selective and Sensitive Chemiresistive NH_3 Detection via Schottky Barrier Modulation at Ambient Temperature	453
EH-054	Eco-Friendly Synthesis of Polyphenol Stabilized ZnO Nanoparticles from Pomegranate Peel Waste for Biomedical Energy Harvesting and Pre-Clinical Simulated Wound Monitoring Application	454

EH-055	Investigating the Effects of Microplastics Isolated from Personal Care and Cosmetic Products in Drosophila Melanogaster	455
EH-056	Sustainable Valorization of Onion Peel into Heteroatom-Doped Activated Carbon for Safranin-O Adsorption	456
EH-057	Fabrication and Performance Evaluation of WS_2/Ag NPs/ PVA Nanocomposite Dry Electrodes for Continuous ECG Monitoring	457
EH-058	Polymorphic and Co crystalline Architectures of Acetamiprid: Structural Elucidation, Enhanced Solubility, and Green Field Assay	458
EH-059	Microplastic Contamination in Aquatic Systems: Origins, Detection Techniques and Polymer Membrane-Based Removal Methods	459
EH-060	Carbamodithioate- Modified Nanoscale Zerovalent Iron: Redox-Active Hybrid for Cr (VI) and p-Nitrophenol Remediation	460
EH-061	Engineering Moisture-and Water-Resistant MOF-5 by Octa phenyl Polyhedral Oligomeric Silsesquioxane for Hydrophobic-Oleophilic Oil-Water Separation	461
EH-062	An Innovative Printed Device for Sensing of Exhaled Gas	462
EH-063	Atomic-Scale Engineering of Sr-doped Bi_2MoO_6 for Ultrasensitive and Stable NO_2 Detection: Synergistic Enhancement via Catalytic Activation and Cloaking Effects	463
EH-064	Binder-Free 3D CuO Nanowire Electrodes Decorated with Co and Ni Nanoparticles for Efficient Electrochemical Non-enzymatic Glucose Sensing	464
EH-065	A Comprehensive Characterization of Oxygen and Sulfur-Doped Graphitic Carbon Nitride for Enhanced Functional Performance	465
EH-066	Facile Green Synthesis of ZnO/g-C_3N_4/Chitosan Ternary Nanocomposites for Photocatalytic Ciprofloxacin Degradation and Wastewater Disinfection	466

EH-067	Engineering Redox-Active MOFs for Field-Deployable Detection of Organophosphate Pesticides and Antibiotic Residues	467
EH-068	Design and development of Ni MOF nanosheet-infused CA-modified PEI membrane for enhanced Congo red adsorption	468
EH-069	Synthesis of But-2-yne-1,4-Diol Stabilized Gold Nanoparticles: An Efficient Catalyst for Methylene Blue and Rhodamine B Dye Degradation	469
EH-070	A Redox-Active Electron Acceptor Enabling Catalytic Oxygenation and Microgram-Scale Charge-Transfer Cocrystal Formation.	470
EH-071	Development of $NaTaO_3/Co_3O_4$ Based Photocatalyst for Berberine Chloride Degradation	471
EH-072	Bimetallic Ce-Co-MOF with Enhanced Peroxidase-like Activity for the Highly Sensitive Colorimetric Detection of Amoxicillin	472
EH-073	Porous N-Doped Carbon from Musa Acuminata Stem for Adsorptive Removal of Toxic Dyes and Pharmaceutical Drugs from Wastewater	473
EH-074	Pyrene-Based Fluorescent Probes for Selective Detection of Ciprofloxacin in Food and Environmental Samples	474
EH-075	Biocatalytic Transformation of Benzil Using Endophytic Fungus Isolated from Tarlmounia Elliptica	475
EH-076	Heterostructured Co-MOF derived Co_3O_4/WS_2 Nanocomposites for Portable Electrochemical Detection of Allura Red	475
EH-077	Mechanistic Understanding of c-CNF/CA/KGM SAPs Through Swelling Kinetics, DFT Calculations, and Molecular Docking for Sustainable Personal Hygiene Application	476
EH-078	Interfacial Engineering of Bi_2S_3 Thin Films Using an rGO Seed Layer for Enhanced Room Temperature H_2S Sensor	477

EH-079	Room-Temperature Ammonia Detection Using 2H-Phase MoS_2 for Sustainable Environmental and Health Monitoring	478
EH-080	Sustainable Sequential Precipitation Strategy for Selective Recovery of Gold and Copper from E-Waste	479
EH-081	Mxene-Integrated $CuWO_4$ Nanocomposite by Hydrothermal Synthesis and its Characterization for Photocatalytic and Biological Application	480
EH-082	Bimetallic MOF for Wearable Electrochemical Glucose Sensor	481
EH-083	Real-Time Gastrointestinal Transit Tracking Using Intelligent Textile-Based Wearable Devices	482
EH-084	Enhanced Sensing properties of Y-doped Bi_2S_3 Nanostructures for NO_2 Detection	483
EH-085	Optimizing the Influence of Bimetallic Oxides $NiMoO_4$ for Ultra-Sensitive NO_2 Detection at Room Temperature	484
EH-086	Acoustic Feature Dynamics of Bowel Sounds Prior to Defecation	485
EH-087	Accelerating Carbon Capture Materials Discovery: A Machine Learning Framework for Predicting CO_2 Adsorption and Structure-Property Relationships in MOFs	486
EH-088	Portable LED-Photodiode Based Colorimetric Sensor for PFAS detection Integrated Pith Mobile App	487
EH-089	Defect-Induced Charge Separation in Ca-Doped $BiVO_4/AgFeO_2$ Heterostructures for Enhanced Photocatalysis of Ciprofloxacin	488
EH-090	Fabrication of Mothership Capsules using Polymers for Lipase Enzymes Delivery to Treat Pancreatic Insufficiency	489
EH-091	Catalytic Innovations and Transesterification Approaches for Sustainable Biodiesel Production from Diverse Lipid Feedstocks	490

EH-092	PVP-Capped Flower-like Bi_2WO_6 Nanostructures for Highly Selective H_2S Gas Sensing	491
EH-093	Low dimensional Bi_2S_3 nanorod network for highly sensitive and selective NO_2 sensor at room temperature	492
EH-094	Nano-Engineered **α**-MoO_3 for Environmentally Sustainable NO_2 Detection	493
EH-095	Fabrication and Application of a CuNi-MOF-Modified Electrochemical Sensor for Ultrasensitive Vitamin K Quantification.	494
EH-096	Charge Transport Dynamics in LiOH-Intercalated $Ti_3C_2T_x$ MXene: Highly Sensitive and Rapid NO_2 Sensor	495
EH-097	A Glutathione-Stabilized Copper Nanocluster-Molybdenum Disulfide Composite for Electrochemical Non-Enzymatic Detection of Dopamine and Uric acid	496
EH-098	Ultrasound-Enhanced Adsorption of Fluoride using Thermally Activated Al/Si-Rich Industrial Sludge: Performance, Mechanism and Safety Assessment	497
EH-099	Sunlight-Driven Photocatalytic Inactivation of E. coli and Staphylococcus aureus using Iron-doped ZnO Nanoparticles	498
EH-100	Toxicity of PET Microplastic and Nanoplastic in Human Lung Alveolar Epithelial Cells	499
EH-101	Hierarchical HOF-Templated Ru-Borophene Hybrid: Synergistic Interface Engineering Toward Efficient OER in Alkaline and Marine Media	500
EH-102	Enhanced Sunlight-Assisted Wastewater Treatment via SnO2-Coated Jute Fibers	501
	Theme: Electronics, Optics & Photonics (EL)	
EL-001	Revealing the Non-Linear Optical Properties in Lead-Free Potassium Sodium Niobate ($K_{0.5}Na_{0.5}NbO_3$) Thin Films Through Two-Wave Mixing Interactions	502

EL-002	Tuning the Photoconductivity of SnSe Thin Films Through Investigating the Impact of Deposition Pressure.	503
EL-003	Energy harvesting technologies: A robust technology for self-powered systems	504
EL-004	Real-Time Hazardous Gas Detection Using a Hybrid Nano-Material Assisted SPR Sensor	505
EL-005	Investigation of Structural, Intramolecular Charge Transfer, and Nonlinear Optical Characteristics of the Push-Pull Chromophore 1-[{2-Methyl-4-[(2-methylphenyl) diazenyl] phenyl} diazenyl] naphthalen-2-ol – Lipid Crimson: A Vibrational Analysis	506
EL-006	Nanohybrid Functionalized MEMS Cantilever: Chitosan/Graphene QDs for Mercury (II) Monitoring in Water	507
EL-007	Thickness Dependent Properties of ZnO Thin Films for Enhanced UV Photodetector Performance	508
EL-008	High Performance Multifunction Integrated Optical Chip with Emergent Materials for Fiber Optic Gyroscope Applications – An Analysis	509
EL-009	Performance Comparison of Five different Cs-Bi-I Perovskite Compositions for Solar Cells: A SCAPS-1D Study	510
EL-010	Growth, Structural, Linear and Non-Linear Optical Limiting Properties of a Novel Barium (II) Bis benzo (15-Crown-5 ether) Manganese (II) Thiocyanate (BBCMT) Single Crystal	511
EL-011	Unravelling Piezoelectricity in Surface Charge Tuned Two-Dimensional Poly (L-Lactide) for Self-Powered Sensors	512
EL-012	Pulsed Laser Ablation Derived Plasmonic Nanoparticles with Enhanced Antibacterial Efficacy and SERS Sensitivity	513
EL-013	Synergistic Exciton–Plasmon Coupling in Noble metal nanoparticle - Rhodamine system: A combined DFT and experimental Study	514

EL-014	Thermoelectric Properties of Chalcogenide Perovskite Exhibiting Ultra-Low Thermal Conductivity	515
EL-015	Lead-Free Halide Double Perovskite $Cs_2Ag_{0.4}Na_{0.6}In_{0.9}Bi_{0.1}Cl_6$ as a Cold White Emitter for Indoor Application	516
EL-016	Site-Occupation Engineering of Sm^{3+} in $NaLaInNbO_6$ Double Perovskite toward Enhanced Efficient Red-Emitting Phosphors for pc-WLEDs	517
EL-017	AWaV: Adaptive Wavelength-Multiplexed Optical Emulation Framework for Semantic Feature Extraction and Vision Classification in Photonic AI Systems	518
EL-018	pH-Controlled Synthesis and Optical Limiting Behavior of Phase Change Materials	519
EL-019	Fabrication and Characterization of PEDOT: PSS and Activated Charcoal Based Two Terminal Devices	520
EL-020	Theoretical investigation of Dark Current and Responsivity of AlGaN/GaN HEMT-based High-Performance UV-Detection Photodetector	521
EL-021	High-Sensitivity BK7–Ag–BN–BlueP/WSe_2–BP SPR Biosensor for Label-Free Detection of A549 Lung Cancer Cells	522
EL-022	Plant-Mediated Synthesis of Cu–ZnO Nanocomposites with Multifunctional Environmental Applications	523
EL-023	Formalin Detection Using a Multilayer Surface Plasmon Resonance Sensor Incorporating Blue Phosphorus/Tungsten Disulfide Heterostructure, Aluminum Oxide, and Barium Borate Functional Layers	524
EL-024	TPE-Based Donor-π-Acceptor AIE-Luminophores for Sensing and Solid-State Lighting Applications	525
EL-025	Oxygen Vacancy–Engineered Optical, Luminescent and Dielectric Response in $BaPO_4$& Re^{3+}Modified $BaPO_4$ Nanophosphors (Where Re = Dy^{3+}, Tb^{3+}, Eb^{3+})	526

EL-026	Color Modulation in Samarium-Doped Borotellurite Glass Embedded with Eu: Y_2O_3 Nanophosphor Composites	527
EL-027	Chiral Perovskite Device Stacks: Multifunctional Platforms for Energy, Sensing and Neuromorphic Computing	528
EL-028	Design and Investigation of Nanoscaled GaN-Based Truncated-Fin FET for High-Sensitivity Hydrogen Gas Sensing	529
EL-029	Interface Mode Excitation Optimization in Nanophotonic Structures using Machine Learning Approaches	530
EL-030	Growth, Structural, and Optical Characterization of Malachite Green (MG) Doped Triglycine Sulphate (TGS) Single Crystals	531
EL-031	Nonlinear Optical and Photoluminescence Studies of Malachite Green Doped Triglycine Sulphate Single Crystals	531
EL-032	Growth, Optical and Electrical Studies Of β-Alanine Crystals	532
EL-033	Functional Integration of Sensors, Arduino and Python Programming: Blueprint of a Low-Cost Early Warning for Underground Hard Rock Mines	533
EL-034	Solvent-Thermal Annealing-Induced Grain Growth in Triple-Cation Halide Perovskite Thin Films for Enhanced Solar Cell Performance	534
EL-035	Enhanced Second order Nonlinear Optical Properties of Hematene Nanosheets	535
EL-036	A Double Interlocking Strategy for Narrowband Ultra-Violet Emitters (CIEy ≈ 0.029) with Dual Functionality for Efficient OLEDs	536
EL-037	Stimuli-Responsive Molecular Systems for Nanoscale Energy Harvesting Prospects	537
EL-038	Phenothiazine-Linked Benzodithiophene Hole Transport and Interface Passivation Materials for Perovskite Solar Cells	538

EL-039	Enhance the Efficiency of n-ZnO /p-Si Thin Silicon Solar Cell Through Silver Caped Silica Nanoparticle Mirror	539
EL-040	Surfactant-Mediated Structural Evolution and Band Gap Engineering of Hierarchical BiOCl Nanostructures	540
EL-041	Achieving White Light Emission from A Hydrazone Through Three Different Channels: AIE,Solvatochromism and Excitation Wavelength	541
EL-042	Multi-colour and Red Emissions from a Small Donor-Acceptor Molecule by Breaching Kasha's Rule	542
EL-043	A Mechanistic Insight into the Emission Behavior of Boron Difluorohydrazones (BODIHYs): Suppression of Kasha's Rule	543
EL-044	Atomistic Tuning of Optoelectronic and Chiroptical Properties in π-Conjugated Systems	544
EL-045	Investigation of Energy gap, Optical Conductivity, real and imaginary dielectric values of Nano composite from UV-Visible Spectroscopy	545
EL-046	3D Plasmonic Ag Nanodendrites as Highly Efficient SERS Substrates for Ultra-Trace Detection of Ascorbic Acid	546
EL-047	Interface Engineering on Vertically Stacked MoS_2/In_2S_3 Photodiode for High Performance Photodetector	547
EL-048	Realization of Surface Plasmon Polariton Modes in Graphene coated Conducting Media	548
EL-049	Green Synthesis of Semiconductor-Embedded PCL Nanofibers Fabricated by Electrospinning for Optoelectronic Applications	549
EL-050	Low Dimensional Nanostructures Based Bi_2S_3/P-Si(100) Heterojunction Photodiodes For Photodetector Applications	550
EL-051	Chirality in New Hybrid Cu-Halides: Synthesis and Functional Properties	551

EL-052	Design and Simulation of Patch Antenna for 5G Millimetre Wave Applications	552
EL-053	A Hierarchical Self-Assembly-Induced Solid-State White-Light Emission from a Solution- Processed Single Polymer	553
EL-054	Corncruzer: An Autonomous Iot-Enabled Precision Seeding Rover for Corn Cultivation	554
	Theme: Computational Materials Science & Materials Informatics (CM)	
CM-001	Numerical Review on Dynamic Factor Evaluation of Pick and Carry Crane Cabin Structure	555
CM-002	Climate-Aware Materials Informatics for Designing Corrosion-Resistant Coatings under Future Environmental Scenarios	556
CM-003	DFA-based fault severity tracking in bearing with standard material grade used in Induction Motor	557
CM-004	Exploring Transport Properties and Rare-Earth-Substitution-Enhanced Magnetism in XFeSb (V, Nb, Ta) Intermetallics for Renewable Energy and Spintronics Applications	558
CM-005	Machine Learning-Driven Design and Applications of Carbon Quantum Dots in Environmental and Energy Nanotechnology	559
CM-006	Semiconductor to metallic transition with possible magnetism in coved armchair BP nanoribbons	560
CM-007	Hafnium based ferromagnetic half metals for spintronic and thermoelectric device applications	561
CM-008	Tantalum Based Ferrimagnetic Half Metals for Spintronic and Thermoelectric Device Applications	562
CM-009	Machine Learning-Assisted Image-Based Crack Detection and Self-Healing Evaluation in Functional Self-Healing Materials	562
CM-010	Quantum Kernel-Driven Learning of Nanoscale Transport Dynamics in Engineered Nanomaterials	563

CM-011	Atomistic Insights into the Role of Gd/W Co-doping on the ElectronicStructure and Phase Stability of $La_2Mo_2O_9$: A First-Principles Supercell Investigation	564
CM-012	Tuning the Transport Characteristics of Boron Phosphide Monolayers via Ad-Atom Functionalization and Substitutional Doping: A DFT - NEGF Study	565
CM-013	AI-Driven Design and Optimization of Advanced Functional Thin-Film Materials for Energy and Electronic Applications	566
CM-014	Copper and Zinc Doped Black Phosphorene Nanosheets as Promising Nanocarriers for Dacarbazine Delivery: A DFT Investigation	567
CM-015	First-Principles Exploration of Nb_2C MXene for Two-Dimensional Drug Delivery Nanocarriers	568
CM-016	Exploring Zr_2C MXene as a Two-Dimensional Nanocarrier for Drug Delivery: A First-Principles Study	569
CM-017	First-Principal Study of Toxic Gas Sensing on ZrS_2 Monolayer	570
CM-018	Enhanced H_2S Detection Using Selenium Vacancy-Induced $MoSe_2$ Monolayer: A Density Functional Theory Analysis	571
CM-019	First-Principles Investigation of Spinterface Magnetism and Spin Transport in 2D Molecular–Fe_3GeTe_2 Junctions	572
CM-020	Magnetism and Spin-Filtering in Benzene-Modified MTe_2 Monolayers	573
CM-021	Enhanced Waste Heat Recovery in Industrial Systems using Optimized Thermoelectric Generators	574
CM-022	Dynamic Conductance of Chiral Molecular Junctions: A First-Principles Study	575
CM-023	Transport characteristics of pure HfS2 monolayers influenced by cobalt doping: A DFT study	576
CM-024	Engineering Silicon-Doped Graphdiyne with Amino Acid Derivatives: A DFT Study Toward Targeted Drug Delivery	577

CM-025	Aluminum-Doped Penta-Graphene as a Promising Two-Dimensional Material for Hydrogen Storage	578
CM-026	Halogen Doped Boron Nitride Nanosheets as Metal-Free Electrocatalysts for Hydrogen Evolution Reaction	579
CM-027	Intrinsic Polarization Effects in Janus 2D Aluminum Nitride for Energy Applications	580
CM-028	Halogen-Substituted-Driven Band Engineering in Mixed-Metal Chalcohalides $CuBiSeI_2$	581
CM-029	Density Functional Theory Investigation of WS_2 for Drug Delivery Applications	582
CM-030	First-Principles Study of Structural, Electronic, and Magnetic Properties of Tetragonal Ce-Based Pnictides	583
CM-031	Halogen-Driven Modulation of Electronic and Thermoelectric Properties in $TiOX_2$ Monolayers: A DFT Study	584
CM-032	Study of 2D Janus Cdxi (X=Cl, Br) Monolayers for Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance	585
CM-033	Oxide TE-Predictor: An Interpretable Machine Learning Framework to Accelerate the Design of Oxide-Perovskite Thermoelectric Materials	586
CM-034	Zr-Induced Enhancement of Thermoelectric Performance in Li-Based Quaternary Heusler Alloys	587
CM-035	Cellular Automata Modelling of Layered Ternary Carbides and Nitrides	588
CM-036	A Traceable Digital Thread for UAV Propulsion: MBSE Architecture Linked with Performance Simulation	589
CM-037	Graph-Splicing as a Digital Twin for Nanoscale Fabrication	590
CM-038	Rh-Doped $TiCo_{1-x}Ir_xSb$ (x = 0,0.25,0.75,1) Half-Heusler Alloys: High-Efficiency Thermoelectric Materials for Sustainable Energy Applications	591

CM-039	Mechanistic Insights into Gas Selectivity of Noble Metal Functionalized WO_3 from First-Principles Calculations	592
CM-040	Material-Aware Computational Modeling of VAT-Based Detumbling Control for a 3U CubeSat	593
CM-041	Unlocking High Thermoelectric Performance in 2D GaN/WSeTe van der Waals Heterostructures: DFT + NEGF study	594
CM-042	Machine Learning-Assisted Optimization of CdS/Zn(O,S) Window Layers for CdTe Solar Cells using SCAPS-1D.	595
CM-043	Computational Screening of $Ti_3C_2T_x$ and $Ti_3C_2T_x$–Ag MXenes for Heavy-Metal Adsorption: Langmuir-Freundlich Isotherm Analysis in Python	596
CM-044	Machine Learning Integrated MoS_2-Functionalized AlGaN/GaN HEMT for Ultra-Sensitive Mercury Ion Detection under UV illumination	597
CM-045	Analysing the State of Lead Halide Perovskites through 38,000 Photovoltaic Device Records	598
CM-046	Design Analysis of a 4H-SiC Trench U-MOSFET with Breakdown Point Transfer Technology	599
CM-047	Machine Learning Assisted MoS_2-Functionalized HEMT for UV-Enhanced Ultra-Sensitive Hg^{2+} Detection	600
CM-048	CM Finite-Difference Steepest Descent (FDSD) Method for Modeling Light Propagation in Structures with Metal Nanoparticles	601
CM-049	White Light Emission Generation by Engineering Dopant Stoichiometry in Metal-Organic Frameworks using FRET-Mapped Optimization and Shanno Radii Method	602
CM-050	Mechanical and Optical Properties of SnO_2 Ceramic (Sintered At 200°C, 800°C,1000°C) Calculated by Using VASP	603
CM-051	Multipole Plasmonic Peaks in Metal-dielectric Nanospheres-Modelling, Tuning and Analysis	604

CM-052	Electronic Structure–Driven Design of Dual-Atom Active Sites on Iridagraphene for Efficient Electrochemical CO_2 Reduction: A First-Principles Study	605
CM-053	First-principles study on structural, electronic and optical properties of mixed halide perovskites $CsPbBr_{3-y}X_y$ (X = I, Cl, F; y = 0,1,2,3) using GGA, mBJ and HSE functionals	606
CM-054	Effect of Metal Based Anion in Ionic Liquid@Uio-66 MOF for Selective CO_2 Capture and Separation: A Computational Study	607
CM-055	Tuning CO_2 Activation via Choline–Amino Acid Ionic Liquids on Au (111): A First-Principles Study	608
CM-056	PEG-Functionalized Janus TiSSe Nanosheets as an Enhanced Nanoplatform for Targeted Drug Delivery	609
CM-057	First-Principle Investigation of NbS_2 TMDs for Two-Dimensional Drug Delivery Nanocarriers	610
CM-058	Electro-Thermal and Process-Induced Analysis of Nanosheet FET-based Hydrogen Gas Sensors	611
CM-059	DFT Investigation on Highly Efficient Nanostructures for Bio Sensing Application	612
CM-060	Ag-Doped Germanene as a High-Performance Platform for Breath-Based Detection of Lung Cancer Biomarkers: A DFT and Device-Level Investigation	613
CM-061	Thickness Driven Modulation of Structural, Electronic, Mechanical, Thermodynamic, and Thermoelectric Properties of 2D-Zrnisn Nanosheets	614
CM-062	Negative Capacitance Gate-Overlap Tunnel FET With Source Pocket Using KNN-Based Ferroelectric Parameter Extraction for Low-Power RF Applications	615
CM-063	Design and Analysis of Dielectric Modulated Hetero-Dielectric Tunnel FET-Based Label-Free Biosensor with Enhanced Sensitivity	616

CM-064	Size-Dependent Π-Metal Interactions on Gold Nanoclusters: A DFT Study of Aromatic Adsorption from Benzene to Graphene	617
CM-065	Selective Detection of Ovarian Cancer Biomarkers Using Atomically Engineered Black Phosphorene Nanosheets	618
CM-066	Decoupling Thermal and Electronic Transport in a Monolayer Mg-Based Ternary chalcogenides for Enhanced Thermoelectric Performance	619
CM-067	Solvation-Driven Tuning of Electronic Structure and Photovoltaic Performance in Purpurin Isolated from *Rubia cordifolia* for Dye-Sensitized Solar Cells: An Integrated Experimental and DFT/TD-DFT Study	620
CM-068	Transforming Waste into Infrastructure: Evaluation of High Temperature Strength and Structural Stability of Fully Waste Pavement Blocks	621
CM-069	Optimizing FFD 3D Printer Parameters for Printing of Bio-inspired Xylotus Lattice Structure using Taguchi Approach	622
CM-070	Electron Spin Resonance-shift of Gadolinium ion in p-type $Sn_{1-x}Gd_xTe$ ($0.0005 \leq x \leq 0.01$) Diluted Magnetic Semiconductor	623
CM-071	Magnetization Reversal in the Presence of Spin Textures in a Synthetic Antiferromagnet	624
CM-072	DFT study on the Structural and Electronic Properties of $Mg_xCa_{1-x}FeSiO_4$ as a Cathode for Magnesium–Ion Battery	625
CM-073	Molecular Dynamics Insights into Microstructure and Mechanical Behavior of PBSA/PHBH Biopolymer Blends for Sustainable Packaging	626
CM-074	Effect of Clay Nanomaterials on the Nanoscale Morphology of poly (benzimidazobenzophenanthroline)	627
CM-075	Functional $CuMoO_4$/f-CNF Nanocomposites for Machine Learning–Assisted Electrochemical Pesticide Monitoring	628

Theme: Biomaterials & Soft Materials (BM)

BM-001	Mechanical properties of polymer/natural infill composite fabrication by FDM process	629
BM-002	Enabling Visible Light Driven Chemo-Photodynamic Therapy and Imaging of Cancer Cells by pH-sensitive CD-Metal Organic Gel	630
BM-003	A Review on Antibacterial Growth Control in Additive Manufacturing Using Chromium–Cobalt Materials	631
BM-004	Modeling and Analysis of Dielectric Elastomer Actuator for Underwater Propulsion	632
BM-005	Optimizing Chitosan Extraction from *Squid Gladius* for Advanced Biomaterials in Cartilage Regeneration	633
BM-006	The effect of abrasives in Dynamic Chemical polishing of Additive Manufactured Features	634
BM-007	Effect of Hygrothermal Aging in Oil, Distilled Water, Saline Water and HCL Acid on the Mechanical Behaviour of Kenaf, Banana and Sisal Woven Fiber Composites	635
BM-008	Comparative Biomechanical Study of Natural and Synthetic Materials in Femoral Analysis Using FEA	636
BM-009	Fabrication of Diglycolic Anhydride - Functionalized G-C_3N_4/PVA Hydrogel Incorporated with Selected Plant Extract and Silver Nanoparticles for Enhanced Antibacterial and Wound Healing Application	637
BM-010	Drug-Loaded 3D-Printed Cellulose–Alginate Scaffolds Fabricated from Waste Cotton for Soft Tissue Engineering Applications	638
BM-011	Synthesis and characterization of Chitosan/ strontium Titanate/PVA based Triboelectric Nanogenerator for Energy Harvesting Applications	639
BM-012	Biological Assessment of Carboxymethyl Chitosan-based Scaffold for Pulp-Dentin Engineering Applications	640

BM-013	Biocompatible Magnesium Ferrite Nanoparticles for Magnetic Fluid Hyperthermia Therapy	641
BM-014	Artificial Synaptic Functions and Resistive Switching in Al-Doped ZnO/Polymer Nanocomposite Based Transparent and Flexible Memristors	642
BM-015	Biocompatible ZnO–Biopolymer Nanofilms and Electrospun Nanofibers for Moisture-Responsive Wearable Biosensors	643
BM-016	Sustainable CS-MWCNT doped Eutectogels synthesis via Rapid Frontal Polymerisation: High-Strength Conductive Composites	644
BM-017	$ZnFe_2O_4$-gC_3N_4 /PVDF Composite Film-Based Self-Poled Piezoelectric Nanogenerator for Efficient Energy Harvesting Applications.	645
BM-018	Charcoal (Carbon)- Cotton Networks for wearable and Sustainable Electronics	646
BM-019	Scalable Bio-Circular Radiative Cooling Coating: Simultaneous Extraction of Cellulose and Silica from Rice Husk	647
BM-020	Electroencephalogram (EEG) Signals in the Diagnosis of Various Mental Disorders	648
BM-021	Competing Capillary and Magnetic Forces in Self-Assembled Magnetic Monolayers	649
BM-022	Contribution Sustainable Manufacturing of a Component under Minimum Quantity Lubrication (MQL) Condition: A Comprehensive Review	650
BM-023	Surfactant-Mediated Control of Pattern Formation in Magnetic Swimmers	651
BM-024	Effect of Co-Precipitation Assisted Hydrothermal Synthesis Time on Thermal and Magnetic Properties of $CoFe_2O_4$ for Magnetic Hyperthermia Applications	652

BM-025	Heat Energy as Medicine Enabled by Fe_3O_4 Magnetic Nanoparticles for Cancer Treatment	653
BM-026	Magnetic and Dielectric Behaviour of Alkaline Doped $BiFeO_3$	654
BM-027	Microstructural Dynamics of Stretching Nanofilm of Hydrogels: Effects of Film Thickness on Mechanical Properties	655
BM-028	Synergistic Tamra-Yasad Bhasma and Cinnamaldehyde Nano-shield Hydrogels for Diabetic Wound Repair	656
BM-029	Trace Elemental Analysis of Benincasa hispida, an Anti-Jaundice Medicinal Plant from Telangana, India, Using ED-XRF Spectroscopy	657
BM-030	Advanced Bone Repair Solutions: A Mechanical-Assisted Post Bio-Printing Approach	658
BM-031	Trace Element Profiling of Anti-Asthmatic Medicinal Plant Tephrosia purpurea Using EDXRF Technique	659
BM-032	Activatable Sulphur Dioxide (SO_2)-Releasing Probe Triggers Ferroptosis via Redox Imbalance in Cancer Cells	660
BM-033	Physiologically Based Pharmacokinetic Modelling of Liposomal Drug Delivery Regulated by Oleic Acid from Enteromorpha Intestinalis	661
BM-034	Design of Electrospun Multi-Layered Nanofiber Platform for Improved Wound Healing in Diabetic Condition	662
BM-035	Biofunctional Polydopamine/Gelatin Layer-by-Layer Self-Assembled Polycaprolactone Nanofibers for Wound Healing	663
BM-036	Engineered Nano biofertilizers Integrating Metal Oxides for Improved Growth Performance and Biochemical Response in Amaranthus Viridis	664
BM-037	Curcumin-Loaded PCL/Chitosan Nanofibers: Comparative Evaluation of Antimicrobial Activity and Wound Healing Potential	665

BM-038	Green synthesis of seaweed derived carbon dots via microwave assisted method for biomedical and environmental applications	666
BM-039	Phytofabrication of Zeolitic Imidazolate Frameworks as Potential Wound Healing Agents	667
BM-040	Tailoring the Gelation Kinetics and Visco-Elastic Properties of Pluronic Hybrid Hydrogels: Insights from Rheological Analysis	668
BM-041	Design and Development of Novel ZnZr Alloy Phases for Advanced Biomedical Applications	669
BM-042	Multifunctional ZnO/Y_2O_3–Nd_2O_3 Nanocomposite: A Novel Ternary Material for Enhanced Photocatalytic and Anticancer Behaviour	670
BM-043	Design and Evaluation of a Bioactive Nanocomposite-Coated 3D-Printed PLA Cranial Implant for Enhanced Osseointegration and Antibacterial Performance	671
BM-044	Biomechanical Analysis of Biodegradable PLA-PCL Screws in Hammer Toe Surgery Using 3D Finite Element Modelling	672
BM-045	Tunable Magnetic Hyperthermia Performance of Superparamagnetic Iron Oxide Nanoparticles Through Zinc Doping: A Structural, Magnetic and Relaxation Mechanisms Analysis.	673
BM-046	Development of Manganese-Impregnated Nanohydroxyapatite Functionalised with Alendronate as a Synergistic Metalloimmunotherapeutic Adjuvant.	674
BM-047	Design and Development of Biomimetic Ti_6Al_4V Scaffolds Via Metal Additive Manufacturing: Bio-Functionalization, *In-Vitro* and *In-Vivo* Studies	675
BM-048	Sustainable Co-Doping Strategy in TiO_2 Nanoparticles Using Kalanchoe pinnata: A Green Route to Enhanced Functional Nanomaterials	676
BM-049	Evaluating the Influence of Material Composition on Dental Restoration Systems Using Finite Element Analysis	677

BM-050	Bioactive Thiolated Mesoporous Silica @ L-Arginine modified Sodium Alginate/ Guar Gum Thin films for Blood compatible Wound Healing	678
BM-051	Nanostructured Hydroxyapatite Derived from Cowrie Shells Incorporated into PCL for Enhanced Osteogenic Differentiation	679
BM-052	Liposomes Containing Zinc-Based Chemotherapuetic Drug Block Proliferation and Trigger Apoptosis in Breast Cancer Cells	680
BM-053	*Boerhavia Diffusa-Assisted Green Synthesis of Gold Nanoparticles with Enhanced Heavy Metal Sensing, Catalytic, and Antimicrobial Properties*	681
BM-054	Investigating the Antibacterial Activity of Homoleptic Bipyridine-Based Polypyridyl Iron (II) Complexes: Probing the Role of Ligand Design in Antibacterial Function	682
BM-055	A Strategy to Inhibit Protein Corona Formation and Bacterial Infection Using Fluorinated Silver Nanoparticles for Infection-Resistant Wound Dressings	683
BM-056	Structural and Functional Evaluation of a Protein-Derived Nanofibrillar Hydrogel for Skeletal Muscle Engineering	683
BM-057	Bagasse-Derived Graphene Quantum Dots Eco - Friendly Synthesis, Characterization and its Anti-oxidant Activity	684
BM-058	Hybridizing Coumarins with IMiDs: A Platform for Structure-Guided Design of Bioactive Small Molecules	685
BM-059	Rational Design of Enzyme-Responsive Fluorescent Organoruthenium Prodrug for Real-Time Tracking of Cargo Release and Cytotoxicity	686
BM-060	Mechanical Flexibility, Photosalience, and Acidochromism of Benzylidene Indanone-Based Molecular Crystals	687
BM-061	IoT-Enabled Paper-Based Colorimetric Sensor Using Nanomaterials for Detection of Urinary Biomarkers	688

BM-062	Mechanically Flexible Pentadienenitrile Derivative Based Molecular Crystals Exhibiting Distinct Photoresponsive Behavior	689
BM-063	Tuning Mechanical Flexibility and Photomechanical Bending in Cyanostilbene Cocrystals	690
BM-064	Design of Flexible Chiral Organic Molecular Crystals using Crystal Engineering Approach for Optical Waveguiding and Self-Powered Piezoelectric–Triboelectric Devices.	691
BM-065	Audible Sound Controlled Spatiotemporal Patterning of Supramolecular Aggregates	692
BM-066	Bioinspired Hierarchical Hydroxyapatite Nanorod-Reinforced Composite Coatings for Durable and Corrosion-Resistant Implant Surfaces	693
BM-067	Electrospun PVA/Kapok Gum (Ceiba pentandra) Nanofibrous Mats for Bioactive Wound Healing Applications	694
BM-068	Biogenic Mg-HAp from Salmacis Virgulata for Advanced Bone Tissue Engineering and Osteogenic Enhancement	695
BM-069	Preclinical Evaluation of Vitamin-C Boosted Nano-Liposome Curcumin for Targeted Breast Cancer Therapy	696
BM-070	Electrophoretic Deposition of Hybrid Nanostructured β-TCP/HAp/MWCNT Coatings for Enhanced Corrosion Resistance and Mechanical Stability of 316L Stainless Steel	697
BM-071	Characterization and Mechanical Evaluation of Biodentine with Nano Zirconia, Nano Graphene and Calcium Phosphate	698
BM-072	Multiscale Structural and Functional Analysis of Radular Teeth from Patella vulgata: Evaluating Natural Biomineral Architecture for Biomaterial Design	699
BM-073	Development of Magnesium sample using wire arc additive manufacturing for automobile and biomedical applications	700
BM-074	Eu^{3+}-Doped Fe_3O_4 Mesocrystals for Magneto–Optic Synergistic Cancer Therapy and Bioimaging	701

BM-075	Fabrication of Mothership Capsules using Polymers for Lipase Enzymes Delivery to Treat Pancreatic Insufficiency	702
BM-076	Investigation of Implant Corrosion-Induced Toxicity in Zebrafish (Danio rerio): A Systemic Evaluation of Cellular and Metabolic Stability	703
BM-077	Dissolution of Calcium Oxalate Kidney Stones Using Nutraceutical Phosphates	704
BM-078	3D Printing of Biocompatible Cobalt–Chromium Metals with Functional Hydroxyapatite Surface Layers	705
	Theme: Advanced Functional Materials (AFM)	
AFM-001	Material Innovation in FinFETs: Reviewing the role of Gate Metal, Gate Oxide, Channel Engineering	706
AFM-002	A Review on Self-healing Characteristics of Laminated Polymer Composites	707
AFM-003	Evaluation of Self-healing Characteristics of FRP Composite Honeycomb	708
AFM-004	Development and Testing of 3d Printable Natural Fiber Reinforced PLA Material	709
AFM-005	Performance Evaluation of Cutting Tools with Multi-Layered Nano Coating of Al_2O_3, Tin and Ti	710
AFM-006	Effect of tandem-type stabilization of two-dimensional (2D) Nb_2CT_x MXene on their colloidal and cytotoxic properties	710
AFM-007	A Comprehensive Review on Mechanical Properties of Metal Hybrid Nanoparticle–Modified Glass Fiber Polymer Composites	711
AFM-008	Dual-Ceramic Reinforcement-Enabled Functional Tribological Behavior in Zinc Metal Matrix Composites	712
AFM-009	Influence of Laser Remelting Parameters on Surface Integrity and Near-Surface Hardness of SS316 Deposits Fabricated by Directed Energy Deposition	713

AFM-010	Hierarchical Nanostructure and Optical Response of Ag-Modified reduced Graphene Oxide/La_2O_3 Electrospun Fibers	714
AFM-011	Designing Functional Graded Ceramics with High dc-Tunability Using Core-Shell Approach	715
AFM-012	High Durability Poly(styrene-b-isoprene-b-styrene) Nanocomposites for Corrosion-Resistant and Antifouling Coatings	716
AFM-013	Lanthanide Fluoroborates: Synthesis, Structure–Property Correlations and Eu^{3+} Photoluminescence for Efficient Red Emission	717
AFM-014	Exploration of structure-property evolution in non-equimolar high entropy rare-earth doped $(Na_{0.5}Bi_{0.5})TiO_3$ ferroelectric ceramics	717
AFM-015	Process–Geometry Relationships and Dimensional Fidelity in SS316 Deposits Fabricated by Directed Energy Deposition	718
AFM-016	Microstructural and Mechanical Characterization of Si-Modified Cu-Ni-Al Shape Memory Alloys Processed via Powdered Metallurgy	719
AFM-017	Effective Photocatalytic behavior of Gallium oxide-based nanocomposites for degradation of methylene blue and ciprofloxacin	720
AFM-018	Exploring MBene: 2D Materials Pathways in Synthesis and Characterization for Optoelectronics devices	721
AFM-019	Microstructural and Mechanical Analysis of Additive Manufactured Smart Materials with Metamaterials Design(Anisotropic Honeycomb Lattice)	722
AFM-020	Synthesis and Multifunctional Properties of UiO-66 MOF for Palladium (II) Adsorption from Aqueous Solutions	723
AFM-021	Design of Porous Superhydrophobic Metakaolin-based Geopolymer for Microplastic Remediation in Water	724

AFM-022	Hydrogen-Bonded Organic Framework Synthesized via Diffusion Method as Promising Candidate for Water Splitting	725
AFM-023	Study on the Synergistic Effect of Iron-Rich Copper Slag as a Binder and Aggregate in Alkali Activated Geopolymer for Thermal Resistance Application	726
AFM-024	Effect on Structural and Electrical Properties of Gd and Zr Co-Doped $La_2Ce_2O_7$ for LT-SOFC	727
AFM-025	Al-Powered Medical Chatbot for Early Detection and Explanation of Infectious Diseases Using Generative AI and Streamlit	728
AFM-026	Anion-Driven Tuning of Ferroelectric and Optoelectronic Properties in Chalcogenide–Oxide Perovskites	729
AFM-027	Investigation of Mechanical Performance of 3D Printed Lattice Structures for Next-Gen Mechatronic Devices	730
AFM-028	Kilogram-Scale Flash Synthesis of Waste-Derived Graphene for High-Performance Concrete Applications	731
AFM-029	Magnetic and Magnetocaloric Property Study of Nanocrystalline Gadolinium Hydride	732
AFM-030	Magnetism in multicomponent rare-earth intermetallic compound RAl ($R = Gd_{0.2}Tb_{0.2}Dy_{0.2}Ho_{0.2}Er_{0.2}Al$)	733
AFM-031	Studies of Microstructure and Electromagnetic Properties of $Li_{0.5}Zn_{0.1}Ti_{0.1}Fe_{2.3}O_4$ Spinel Ferrites with Ytterbium (Yb^{3+}) Substitution	734
AFM-032	Flexural Performance of Metakaolin – Enhanced Concrete Beams Reinforced with Basalt Fiber Reinforced Polymer Bars	735
AFM-033	Investigation of Flexural and Crack Behaviour of Hybrid Fibre-Reinforced Concrete Beams Using Banana and Polyester Fibre	736
AFM-034	DFT study on enhancing conductivity in alkali metal adsorbed AGNR	737

AFM-035	Tribological Characterization of LPBF Processed SS316L Pins Fabricated on a Self-Developed Indigenous Metal 3D Printer	738
AFM-036	MOFs-derived and Chitosan-based Photocatalysts for Scalable VOCs Degradation in Photocatalytic Fluidized Beds	739
AFM-037	Structural, Morphological and Dielectric Properties of Cerium (IV) Oxide Nanoparticles Prepared Via Co-Precipitation Method	740
AFM-038	A Table-Like Structured Magnetocaloric Effect in (1-x)PBMO-xPSMO	741
AFM-039	Experimental and Phy-X Based Assessment of Radiation Shielding (γ-ray & X-ray) and Optical Properties of Pb-Doped Rare-Earth Orthoferrite Ceramics ($Pb_xRe_{1-x}FeO_3$ where Re = Gd^{3+} & Pr^{3+})	741
AFM-040	Hybrid Organic-Inorganic Flame Retardant - Non-isocyanate polyurethane	742
AFM-041	Temperature-Engineered Hierarchical Porous Biochars derived from Invasive Biomass for Energy Storage Applications	743
AFM-042	Broadband spectral responsive $PtSe_2$/n-type GaN heterojunction photodetector ranging ultraviolet-visible-near-infrared wavelengths	744
AFM-043	In Situ Engineering of MOF on Zeolite Hybrid Architectures for Precision Acid Base Tuning and Enhanced Ethanol to Butadiene Selectivity	745
AFM-044	BCZT Nanocomposites as a High-Performance Lead-Free Piezoelectric Energy Generator	746
AFM-045	Defect-Engineered Trap Dynamics in $SrAl_2O_4$: Eu^{2+}, Dy^{3+} Functional Oxides via Glass Network Modification	747
AFM-046	Investigating the Potential of Zn Incorporated $CoFe_2O_4$/ α - Fe_2O_3 Nano-Composite Hetero-Structure for RRAM Application	748

AFM-047	Sustainably Produced, Low-Cost Graphene for High-Performance Concrete at Ultra-Low Loading	749
AFM-048	Tuning Resistive Switching Performance of Nickel Ferrite RRAM Through Annealing Temperature	750
AFM-049	A Novel Electrospun Taurine-Doped Polyaniline (TPANI)/ Hydroxypropyl methylcellulose (HPMC)–Curcumin Nanofibrous Composite with Enhanced Functional Properties	751
AFM-050	NiO Nanoparticles from a mer-Ni (II) Pyrazole-Carboxylate Complex	752
AFM-051	Waste Thermocol–Derived Polymer Nanofibrous Membranes via Electrospinning for Sustainable Water Filtration	753
AFM-052	Microstructural Evolution and Graphitization Trajectory of Carbon Derived from Diverse Biomass Materials	754
AFM-053	Controlled Defect Dynamics in MoS_2 Using a Splicing-Inspired Computational Framework	755
AFM-054	Report on Extended Infrared Absorption Spectrum in Cobalt Activated Erbium Aluminium Garnet Nanocrystals for Opto-thermal and Infrared Sensing Applications	756
AFM-055	Modulating Energy Harvesting Performance of PVDF Piezo-Polymer based Flexible Triboelectric Nanogenerator by Incorporation of Ferroelectric Ceramic Filler	757
AFM-056	High-Strength Poly (Vinyl Alcohol) Physical Eutectogels: Effects of Polymer Molecular Weight, DES Composition, and Heat Treatment	758
AFM-057	Electrostatic Self-Assembly of Carbon Nanotubes for Next-Generation Functional Materials – A Review	759
AFM-058	Effective Anti-Cancer Therapeutics Using Piezoelectric BCZT Nanostructures	760
AFM-059	Engineering a Core–Shell Ta-Doped $SrTiO_3$@PTC Structure for High Frequency Capacitor Applications	761

AFM-060	Fabrication of Copper-Reinforced Aluminum Alloy Processed by Friction Stir Processing with Statistical Data Analytics	762
AFM-061	Structural and Optical Properties of Gd^{3+}-Doped $Sm_2Ti_2O_7$ Pyrochlore Nanomaterials for Solid-State Lighting	763
AFM-062	Self – Sterilizing Nanofiber Air Filter for PM2.5 Filtration	764
AFM-063	Influence of Operating Parameters on the Surface Properties of SiOx-Coated PET Films via Ar/O_2 Glow Discharge Plasma for Improving Cytocompatibility	765
AFM-064	Rational Design of Coordination-Modulated NiCo MOFs as High-Efficiency Electrodes for Next-Generation Supercapacitors	766
AFM-065	Investigation of Room-Temperature Poling in $LiNbO_3$-Based Sol–Gel Composite Films	767
AFM-066	Cage Charge Modulation in C12A7 Through Alkali Metal Substitution for Enhanced Ionic Transport	768
AFM-067	Nanoclay Composites in Human Immunodeficiency Virus Pharmaceuticals Sensors	769
AFM-068	Free-Standing GaP/MWCNT Composite Film as an Efficient Cathode Material for Li–O_2 Batteries	770
AFM-069	Theoretically and Experimentally Assessment of Foldable Lightweight Sheet of Ceramic-PU-PMMA IPN for γ ray Shielding and Light Emitting	771
AFM-070	Thermal Shielding Performance of Geopolymer Composite Syntactic Foams	772
AFM-071	Effect of g-C_3N_4 Nanoparticles on the Mechanical, Thermal, and Fracture Behavior of Jute Fiber Reinforced Polymer Composites	773
AFM-072	Development of Al–Cr_2AlC MAX Phase Coating on AA2024 Alloy via HVOF Method	774

AFM-073	Disorder Driven Triphenylamine based Monolithic Covalent Organic Framework for the Efficient Removal of Toxic Oxo-anions from Water	775
AFM-074	Defect-Stabilized, Urbach-Energy–Controlled UV-to-Visible down Conversion in Bi^{3+} Doped $Y_2Zr_2O_7$ Disordered Pyrochlore-like Phosphors	776
AFM-075	Influence of Ca Substitution on the Structural and Dielectric Properties of $Ba_{1-x}Ca_xTiO_3$ Ceramics	777
AFM-076	Robust Superhydrophobic $V_2O_5/CoFe_2O_4@SiO_2$/PDMS Composite Membranes for Membrane Distillation	778
AFM-077	Superhydrophobic Carbamodithioate Functionalized Fluorinated Graphene Nanosheet Composite Membrane for Sea Water Desalination	779
AFM-078	Flexible PVA-Based KTNT/MXene Nanocomposite Films with Improved Dielectric and Electrical Performance	780
AFM-079	Mechanochemical Solid Solution Formation in Zeolitic Imidazole–Tetrazole Frameworks for Enhanced Oxygen Evolution Reaction	781
AFM-080	Independent Evaluation of Pyroelectric and Triboelectric Properties in PVDF/PZT Composite Films	782
AFM-081	pH-Responsive mPEG-b-PCL-b-PEC Triblock Micelles for Stabilization and Tumor-Selective Delivery of Camptothecin	783
AFM-082	Heterointerface-Driven Electronic Modulation in Bimetallic Sulfide Nanostructures for Accelerated Oxygen Evolution	784
AFM-083	Formulation and Characterization of Xanthan Gum-Shea Butter Bigels & Influence of Emulsifiers (SDS, CTAB, SL) on Structure and Properties	785
AFM-084	Development and Characterization of Novel Biopolymer-Based Bigels Formulated using Xanthan Gum, K-carrageenan and Agar for the Delivery of Linezolid	786
AFM-085	Stabilization of Hybrid Halide Perovskite by Schiff Base – A Colloidal Synthetic Approach	787

AFM-086	Fullerene (C60) Endowing Antistatic Properties to the Industrially Viable Biodegradable Polyurethane Nano-Composites	788
AFM-087	Quest for Designing PLA-based Engineered Toughened Nanocomposites for Packaging Applications	789
AFM-088	Metal-organic Framework Composite Incorporated PVDF UF Membranes for Efficient Wastewater Treatment	790
AFM-089	Advancing Hydrogen Storage with Functionalized Carbon Nanoribbons	791
AFM-090	Fe-Doped CoS_2 Nano-octahedra as Electrocatalysts for Hydrogen Evolution Reaction in Acidic Medium	791
AFM-091	Interface-Engineered Bimetallic LDH/Singlet-MOF Heterostructures for High-Performance Electrocatalytic Water Splitting	792
AFM-092	Light-Responsive Functionalized Dendritic Fibrous Nano-Silica for Crop Protection and Management	793
AFM-093	A Conductive Bimetallic MOF/CNT Hybrid as a Bifunctional Electrocatalyst for Water Splitting Applications	794
AFM-094	Lead-Free Ceramic-Polymer Nanocomposites for Sustainable Energy Harvesting	795
AFM-095	Percolative $MoSe_2$/rGO Conductive Networks in PVA Enabling Scalable Gel-Free Wearable Biosensing	796
AFM-096	Synergistic Dual-Anion Vacancy Engineering and Interfacial Charge Modulation in O–MoS_2/NiFe-LDH/MWCNT for Efficient Bifunctional Water Splitting	797
AFM-097	Defect Engineering of MIL-Derived VO_x/$NiFe_2O_4$/MWCNTs towards Efficient Oxygen Evolution Reaction	798
AFM-098	Nitrogen-Doped Borophene: A Metal-free Electrocatalyst for Oxygen Evolution Reaction	799

AFM-099	Sustainable Copper Recovery from Waste Printed Circuit Boards Using Cross-Linked β-Cyclodextrin Polymer for Energy Applications	800
AFM-100	Agro-Waste Derived Advanced Biochar for Sustainable Copper Recovery From e-Waste and Subsequent Cu_2o Formation Toward Electrochemical Application	801
AFM-101	MXene Nanocomposite for Ultrasensitive Two-terminal Artificial Synaptic Devices	802
AFM-102	Defect-Engineered Metal–Organic Framework/Layered Double Hydroxide Photoelectrodes for Enhanced Photoelectrochemical watersplitting.	803
AFM-103	Cu Metal Organic Framework for Adsorption based Reversible Hydrogen Storage	804
AFM-104	Dielectric–Magnetic PVDF Composites for Electromagnetic Interference Shielding (EMI) Applications	805
AFM-105	Sustainable Energy Harvesting by Molecular Ferroelectrics Based on Cu(II) Complexes	806
	Theme: Thin Films & Surfaces (TF)	
TF-001	Experimental and Simulation Study on Magnetic Abrasive Finishing Process of Inconel 625 and Inconel 718	807
TF-002	Impact of Growth and Thermal Annealing in Oxygen and Nitrogen Atmospheres on the Properties of Terbium Oxide Thin Films for Advanced Semiconductor Applications	808
TF-003	RF- Magnetron Sputtered, Electrochromic NiO-based Ion Storage Electrodes for Flexible Smart Window Applications	809
TF-004	Effect of Cu, Sn, and Ti Doping on the Structural, Morphological, Surface, Electrical and Optical Properties of ZnO Nanorods grown on FTO Substrates	810
TF-005	Structural, Optical, and Photoluminescence Studies of $BiFeO_3$ Thin Films Prepared by Sol–Gel Dip Coating	811

TF-006	Microstructure-Driven Oxidation of Sputtered Tungsten Films	812
TF-007	Impact of Deposition Parameters on Resistive Switching Behaviour of HZO ($Hf_{0.5}Zr_{0.5}O_2$) Thin Films.	813
TF-008	Activation Energy Calculation for Li Doped SnO_2 Thin Films via the Arrhenius Method	814
TF-009	Exploring the Dual Functionality of a Vacancy-Ordered Layered Double Perovskite ($Cs_4MnBi_2Cl_{12}$) as an Efficient Red Phosphor and UV Photodetector	815
TF-010	Ultrafast Chemical Bath Deposited FeOOH Nanostructures on Nickel Foam for Efficient Alkaline Water Splitting	816
TF-011	Microstructural Heterogeneity and Mechanical Behaviour of Inconel 690: A Nickel-Based Superalloy	817
TF-012	Bio-Chelating Assisted Spray Pyrolysis of Fe-Doped CeO_2 Thin Films: Structural, Optical, Magnetic, and Photocatalytic Studies	818
TF-013	Dual-Functional MnO_2-V_2O_5 based Heterostructure Film Prepared by Pulsed Laser Deposition for Enhanced Electrochromic Supercapacitor Display	819
TF-014	The Optoelectronic Performance of a Cu_2SnS_3 Photodetector at Key Wavelengths for Medical Diagnostics and Fiber Optic Communication Applications	820
TF-015	Ultrathin Hexagonal Boron Carbon Nitride Films as Universal SERS Substrate	821
TF-016	Effect of Post-Deposition Annealing on the Structural, Morphological, Optical, and Electrical Properties of $Cd_{1-x}Mn_xS$ Thin Films	822
TF-017	Tunable Photoresponse of Solution-Processed Cd-doped CuI/Si Self-Powered Photodetectors	823
TF-018	A Review of Ice-Resistant Coatings Enabled by Carbon Nanotube Composites	824

TF-019	Performance Study of Two Terminal Solution Processed Al Doped ZnO Thin Films for UV Sensing	825
TF-020	Opto-Electrical Optimization of Semi-Transparent Perovskite Tandems Using Advanced Interconnecting Layers via SETFOS	826
TF-021	Enhanced Magnetic Anisotropy and Dual Magnetoresistance in LSMO Thin Films Induced by Interface Effects on (001) Si Substrates	827
TF-022	White-Light Emission and Improved Electrical Performance in Graphene Oxide Modified Al-ZnO Thin Films	828
TF-023	AI-Driven Structural Analysis of Native Defects in Atomically-Thin $Mo_{1-x}W_xS_2$	829
TF-024	Tailored MoO_3-V_2O_5 Composite Thin Films for Functional Devices	830
TF-025	Ion Beam Induced Modulation of $ZnTiO_3$ Thin Films for Next Generation Optoelectronics	831
TF-026	Silk Fibroin–PVA Bio-Composite Films as a Platform for Algal Immobilization in Wastewater Treatment and Biosensing Application	832
TF-027	Development of an Electron Beam–Pumped, Localized Surface Plasmon–Enhanced Nanoscale Light Source for Electron-Beam–Assisted Optical Microscopy	833
TF-028	Hybridizing SnS and G-C_3N_4 for Self-Powering Ultrafast UV-NIR Photodetectors for Environmental Monitoring	834
TF-029	TF Investigations on Structural and Magnetic Properties of Fe-Ga Thin Films Grown in Presence of External Magnetic Field	835
TF-030	Preparation of garnet-type sacrificial layer for free-standing single-crystalline thin film of solid electrolyte LLZTO	836
TF-031	Influence of Lattice Volume on the Electrical Conductivity of Spinel-Type Transparent Oxide Thin Films Fabricated via Pulsed Laser Deposition	837

TF-032	Matrix-Composition-Dependent Tunnel Magnetoresistance in Co–(Ta_2O_5–Al_2O_3) Nanogranular Thin Films by Sputtering with Pressed Powder Target	838
TF-033	Curcumin-Loaded Ag-MOF@Carbon Dot Blended Agarose/PVA Nano thin film as a Synergistic Anticancer Drug Delivery Platform	839
TF-034	Impact of Interfacial Dielectric Engineering on the Performance and Reliability of HfO_2-Based NC-GAA Nanosheet FETs at the 10-nm Node for Low-Power and High-Speed Logic Applications	840
TF-035	A Review of Solution-Processing Strategies for Chalcogenide Ink Formation	841
TF-036	Sulfonated Cr-MIL-101 Anchored SPSEBS/PEG Polymer Blend as High-Performance Proton Exchange Membranes for Fuel Cells	842
TF-037	Tin Selenide Thin Films Grown on Surface-Textured Glass Substrates with Periodic Microstructures for Improved Optical Absorption	843
TF-038	Optimization of growth conditions of Thermally Evaporated SnSe Thin Films	844
TF-039	Optical and Vibrational Properties of MOCVD grown monolayer $Mo_{1-x}Nb_xS_2$ ternary alloys	845
TF-040	Elastic Moduli as Determinants of Lattice Thermal Conductivity in Layered MoS_2	846
TF-041	Synthesis and Development of MXene Composites for Wearable Thermoelectric Applications	847
	Theme: Industry-Academia Partnership (IA)	
IA-001	Hydrogen Reduction of Iron Scale for Sustainable Steelmaking	848
IA-002	Effect of Heat treatment on Corrosion Behaviour of F55 Duplex Stainless Steel	849

IA-003	CloudCover AI: ML-powered real-time data masking in cloud storage for GDPR/DPDP compliance	850
IA-004	Carbon Nanotube Morphology–Tribology Relationships	851
IA-005	Design and Standardization of Near Infra-Red (NIR) Spectral Sensor for Rapid Detection of Microplastics in Wastewater	852
IA-006	Development of 316L Stainless Steel Robot Assisted Additive Manufactured Sample for Energy and Space Applications	853
IA-007	Government-Supervised Community Delivery Model for Strengthening the Public Distribution System (PDS)	854
	Our Sponsors	855

PL-001

Evidence for Multifold Phonon Degeneracies in Cubic Nb_3Bi

G Vaitheeswaran

School of Physics, University of Hyderabad, Gachibowi, Hyderabad 500046, Telangana, India

***Corresponding author email:** vaithee@uohyd.ac.in

ABSTRACT

Topological materials are of considerable interest due to their unique properties and promising applications. Topological states with multifold band degeneracies extend beyond electronic systems to include phononic systems as well. In this study, we explore the higher-order symmetry-enforced topological characteristics of Nb_3Bi, an intermetallic compound with an A15 crystal structure. Using first-principles calculations and symmetry analysis, we characterize the topological phonon modes protected by nonsymmorphic symmetries. Our findings reveal significant degeneracies in the phonon dispersion relations of Nb_3Bi, most notably a sixfold degenerate point located at the R point of the Brillouin zone. Additionally, we identify cubic Dirac contact points and quadratic triple points at the R and Γ points, respectively. Phonon surface state calculations on two different terminations, (001) and (110), exhibit distinct twofold rotational symmetry patterns. These results provide valuable insights into the unique phononic features and surface states of Nb_3Bi, underscoring its potential significance in the study of topological phonons.

PL-002

Materials and Processing Innovations for Performance Enhancements in Emergent Battery Systems

Satishchandra Ogale

Research Institute for Sustainable Energy (TCG-CREST), Kolkata, India

Centre for Energy Science, Indian Institute of Science Education and Research, Pune, India

ABSTRACT

High performance, affordable, and safe batteries represent the central device technology theme that defines the scope, scale, and future of the implementation of clean and renewable energy. While batteries for the transportation sector are at the focus of the current scientific research and technological developments, batteries are also required in plenty in multiple sectors including the strategic sectors such as defence, space, agriculture, robotics, wearables etc. Hence this field is flooded with multiple materials and processing innovations around the globe, aimed at enhancing the battery performance keeping a particular application goal in mind. In this talk, I will outline this scenario by discussing some of our recent research results on composite polymer electrolyte (CPE) based flexible lightweight batteries, and anode-free Li/Na batteries, highlighting some materials and processing innovations incorporated in both the cases.

PL-003

Phonon-Glass Electron-Crystal like High Performance Thermoelectrics

Kanishka Biswas

New Chemistry Unit & International Centre for Materials Science,

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR),

Jakkur P.O., Bangalore 560064 (India)

***Corresponding author e-mail**: kanishka@jncasr.ac.in

ABSTRACT

With about 2/3 of all utilized energy is being lost as heat. Thermoelectric materials can convert waste heat to electrical energy, and it will have significant role in future energy management. Achieving glass-like ultra-low thermal conductivity in crystalline solids with high electrical conductivity, a crucial requirement for high-performance thermoelectrics, continues to be a grand fundamental challenge. Despite this inherent trade-off, the experimental realization of an ideal thermoelectric material with a phonon-glass electron-crystal (PGEC) nature has rarely been achieved. We demonstrated high thermoelectric performance with a near room-temperature figure of merit, zT ~1.5 and a maximum zT ~2.6 at 573 K by optimizing atomic disorder in Cd doped $AgSbTe_2$.[1-3] Cd doping in $AgSbTe_2$ enhances cationic ordering, which simultaneously improves electronic properties by tuning disorder-induced localization of electronic states and reduces lattice thermal conductivity via spontaneous formation of nanoscale (~2-4 nm) superstructures. Further, we showed that isovalent Yb-doping induced enhanced atomic ordering decreases the overlap between the hole and phonon mean free paths and consequently leads to a PGEC-like transport in $AgSbTe_2$. A twofold increase in electrical mobility is observed while keeping the position of the Fermi level nearly unchanged, which leads to zT ~2.4 at 573 K.[4] Recently, we discovered PGEC-like thermoelectric transport in entropy stabilized new telluride single crystal, $AgGeSnSbTe_4$. Local distortion caused by the off-centering of Ge atoms, driven by a stereochemically active $4s^2$ lone pair in a globally symmetric rock-salt structure, plays a key role in suppressing thermal conductivity to its glass limit while maintaining good electrical transport.[5]

References:

1. S. Roychowdhury, T. Ghosh, R. Arora, M. Samanta, L. Xie, N. K. Singh, A. Soni, J. He, U. V. Waghmare and K. Biswas, Science, 2021, 371, 722.
2. T. Ghosh, S. Roychowdhury, M. Dutta and K. Biswas, ACS Energy Lett., 2021, 6, 2825.
3. A. Bhui, S. Das, R. Aurora, U. Bhat, P. Dutta, T. Ghosh, R. Pathak, R. Datta, U. V. Waghmare and K. Biswas, J. Am. Chem. Soc. 2023, 145, 25392.
4. V. Taneja, S. Das, K. Dolui, T. Ghosh, A. Bhui, U. Bhat, D. K. Kedia, K. Pal, R. Datta and K. Biswas, Adv. Mater. 2024, 36, 2307058.

PL-004

Role of Metal Phosphates in Energy Transition

Ramaswamy Murugavel*

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076

***Corresponding author e-mail:** rmv@chem.iitb.ac.in

ABSTRACT

Reaction of phosphoric acid mono- and diesters with a divalent transition metal ion can produce molecular clusters, 1-D polymers, 2-D grids, or 3-D frameworks. Particularly interesting among this series of structural types are the 1-D polymers that are built from thermally labile di-tert-butyl phosphate. These polymers with an inorganic backbone and organic sidechains readily and cleanly decompose at temperatures close to 200 oC. The nanomaterials produced from such precursors have been studied extensively as both electro- and photocatalysts in OER, HER, and overall water splitting reactions.

The monoaryl phosphate, on the other hand, combines with M2+ cations in a donor solvent (L) and yields tetranuclear metal phosphates [(R)PO3M(L)]4 (R = alkyl/aryl or alkoxy/aryloxy), whose inorganic core resembles the zeolitic D4R secondary building units (SBUs). In recent times, we have unravelled that it is possible to isolate even larger SBUs through small variations in the reaction conditions. Rationalization of building principles along with the use of this class of compounds for energy applications will be highlighted in this lecture.

For further representative publications, see: Murugavel & co-workers, ACS Catalysis 2023, 13, 8535; Inorg. Chem. 2022, 61, 6807 & 2020, 59, 13233; J. Am. Chem. Soc. 2017, 139, 39; Chem. Commun. 2019, 55, 7994; Angew Chem., Int. Ed. 2019, 16844; Small, 2020, 1903334; Chem. Mater. 2024, 36, 6475; ACS Mater. Lett. 2024, 6, 2126; Chem. Asian. J. 2025, e202401177; Dalton Trans. 2026, 55, 1306; J. Mater. Chem. A. 2026, 14, 1136; Carbon, 2026, 249, 121260.

PL-005

Developing Photocatalyst by Post-Synthetic Modification Metal-Organic Frameworks

Tapas Kumar Maji[1]*

[1] *Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Molecular Materials Laboratory, Chemistry and Physics of Materials Unit, School of Advanced Materials (SAMat), Jakkur Post, Bangalore- 560064, India*

***Corresponding author e-mail:** tmaji@jncasr.ac.in

ABSTRACT

The much-needed renewable alternatives to fossil fuels can be achieved efficiently and sustainably by converting solar or mechanical energy to fuels via hydrogen generation from water or CO_2 reduction. Sunlight-driven H_2 production and CO_2 reduction are promising routes for the production of chemical feedstocks as fuel precursors to mitigate the CO_2 concentration in the atmosphere and also to alleviate the global energy crisis.[1-4] Nature's design of carrying out the photosynthetic redox cycle involving CO_2 and water inspired us to develop highly efficient integrated catalytic systems for artificial photosynthesis. The versatile and highly amenable structural tunability of metal-organic frameworks (MOFs) by post-synthetic modification (PSM) allows for tailoring inherent semiconducting and optoelectronic properties, compared to traditional inorganic semiconductors. Besides, PSM is an excellent choice for introducing a functional photosensitizer into the MOF matrices to galvanize the electronic, optical and piezoelectric properties towards H_2O and CO_2 reduction.[1-2] Our presented results demonstrated an excellent approach to green H_2 production and carbon neutralization for tackling the energy crisis.[1-6] The groundbreaking contributions to the design and development of metal–organic frameworks (MOFs) were globally acknowledged when the 2025 Nobel Prize in Chemistry was awarded, marking a milestone recognition of MOFs as one of the most important families of functional materials in modern chemistry and materials science.

My talk will focus on their broad significance as functional materials and on advancing integrated photocatalytic systems through post-synthetic modification of MOFs for H_2O and CO_2 reduction.

Keywords: Metal Organic Framework (MOF); Photocatalysis; *In-situ* DRIFTS; DFT Calculation.

References:

1. Karmakar, S.; Barman, S.; Rahimi, F. A.; Maji, T. K. *Energy Environ. Sci.,* 2021, *14*, 2429.
2. Karmakar, S.; Barman, S.; Rahimi, F. A.; Biswas, S.; Nath, S.; Maji, T. K. *Energy Environ. Sci.,* 2023, 16, 2187.
3. Verma, P.; Singh, A.; Rahimi, F. A.; Sarkar, P.; Nath, S.; Pati, S. K.; Maji, T. K. *Nat. Commun.,* 2021, 12, 7313.
4. Verma, P.; Rahimi, F. A.; Samanta, D; Kundu, A.; Dasgupta, J.; Maji, T. K.; *Angew. Chem. Int. Ed.,* 2022, 61, e202116094.
5. Ghosh, A.; Karmakar, S; Rahimi, F. A.; Roy, R.; Nath, S.; Gautam, U.; Maji, T. K. *ACS Appl. Mater. Interfaces*, 2022, 14, 25220.
6. Ghosh, A.; Surendran, D.; Barman, S;, Jena, R.; Bhakar, M,; Nath, S.; Sheet, G.; Zareba, J. K.; Maji, T. K., *Adv. Mater*., 2025, e11679

PL-006

Engineering Photo- and Electrocatalytic Materials for Sustainable Environment

Wonyong Choi*

Korea Institute of Energy Technology (KENTECH), Naju 58330, Korea

***Corresponding author e-mail:** wchoi@kentech.ac.kr

ABSTRACT

The global environment is challenged by excessive consumption of fossil fuels and resources, which perturbs the nature's sustainable cycles of various chemical elements such as C, N, O, and H. As solar energy is the major driving force of the global cycles of these key elements, photo(electro)catalysis is an ideal engineering method to mimic and restore the nature's element cycles. The photochemical conversion of H_2O, CO_2, N_2, and O_2 has been intensively investigated employing various methods among which photo(electro)catalysis using semiconductor materials has been established as the most popular method. This talk will introduce several examples of photocatalytic, photoelectrochemical (PEC), and electrocatalytic conversions of C, N, and O compounds and discuss their environmental implications. The photocatalytic and photoelectrocatalytic processes have been applied to denitrification, de-NOx, and nitrogen fixation reactions but the successful performance is limited. The direct conversion of nitrogenous pollutants to dinitrogen and dinitrogen to ammonia without using chemical reductants is an ideal solution but difficult to be realized. Here we introduce various engineered photo(electro)catalytic systems that selectively interconvert among NO_3^-, NO_2^-, NO, NH_4^+, and N_2. As for O conversion, some examples of photocatalytic and photoelectrochemical systems for sustainable production of H_2O_2 through O_2 reduction will be introduced. A PEC system enabled continuous H_2O_2 production over 100 h even under a bias-free condition.

References:

1. S. Lee, H.-S. Bae, W. Choi, Acc. Chem. Res. 2023, 56, 867-877
2. S. Zhao, W. Choi, Nature Commun. 2025, 16:11024
3. D. Pan, M. Austeria P, S. Lee, H.-S. Bae, F. He, G. H. Gu, W. Choi, Nature Commun. 2024, 15:7243
4. S. Lee, S. Kim, C. Park, W. Kim, S. Ryu, W. Choi, Energy Environ. Sci. 2021, 14, 4437-4450

KN-001

Vanadium Redox Flow Battery for Large Scale Energy Storage for Load Management

Prof. A.M. Kannan

Graduate Program Chair - Clean Energy Systems

Arizona State University, Mesa, 85212 USA

ABSTRACT

Vanadium redox flow battery (VRFBs) is one of the preferred systems for grid level energy storage due to longer service life (>20000 cycles), and higher efficiency (>85%) along with deep discharge capability (>95% DoD). This presentation evaluates various bipolar plate flow channel design and geometries, which influence flow characteristics of electrolyte, system performance and cost. In particular, the channel dimensions (width: 0.66 to 1.5 mm, depth: 1 to 1.5 mm and land width: 0.5 to 1.5 mm) lead to lower pressure drop (<10 kPa) and enhance energy efficiencies (~10%). Higher power density (>500 $mW.cm^{-2}$) and minimum auxiliary power consumption of the balance of plant help lowering the system cost (<$350 per kWh), approaching DOE targets of <$150 per kWh, with about 10 h operation. The presentation also highlights recent developments in bipolar plate manufacturability, and shunt current reduction strategies, for achieving highly efficient, durable and economically viable VRFB system.

KN-002

Van der Waals Gap Engineering of Two Dimensional (2D) Materials: Applications for Energy Storage

Vijayamohanan K Pillai

IISER - Tirupati

ABSTRACT

Most of the Two-Dimensional materials have a finite van der Waals gap (v-gap) in between the layers which provides a clear separation between the in-plane and through plane electronic interactions. Although the carrier transport and associated unique features are studied in accurately prepared and precisely characterized monolayers, many technological applications such as nanoelectronics, electrocatalysis, biosensing, solar energy conversion, and energy storage use multilayers which are conveniently prepared using inexpensive and scalable chemical methods. My group was workingon diverse type of materials including zero dimensional (quantum dots), one dimensional (Carbon nanotubes), and two dimensional (phosphorine) systems and their composites tailored for energy storage applications emphasising on their size/shape dependent properties. For example, among various two-dimensional (2D) materials, graphene possesses similar interlayer spacing of multiwalled carbon nanotubes (0.32−0.35 nm) which could be modulated by several strategies such as the intercalation of cations and anions, the nature of the solvent, and surface functionalization. The resultant graphene nanoribbons (~40 nm diameter) formed by the ionic liquid-assisted transformation of multiwalled carbon nanotubes of an average diameter (~21 nm) along with graphene quantum dots having an emission wavelength of 445 nm are more useful for some of the specific applications. This electrochemical approach not only reveals the introduction of multiple heteroatoms at room temperature but also modulates the van der Waals gap between the layers of multiwalled carbon nanotubes, which could have significant implications for the mechanical and electrical properties. The tunability of this spacing depends on the nature of the ionic liquid, the size of the incoming ions, the applied potential, and the time. In this lecture several examples of v-gap engineering will be demonstrated for specific application like Na/Li ion batteries and multifunctional electrocatalysts.

References:

1. Domain Size Modulation of Clay−Nanocellulose Composites for Enhanced Na-Ion Transport, Sneha Mandal et al., ACS Appl. Energy Mater., 8/9 (2025) 6071–6086
2. Electrochemical transformation of 2D materials to their quantum dots, BR Isaac, Vijayamohanan K Pillai, Chemical Physics Reviews 5 (2024) 15389

KN-003

Minerals as Future Solid-State Materials

Srinivasan Natarajan

Division of Chemical Sciences, Indian Institute of Science, Bangalore 560012

National Institute of Mizoram, Mizoram

***Corresponding author e-mail**: snatarajan@nitm.ac.in; rajan1960@gmail.com, snatarajan@iisc.ac.in;

ABSTRACT

Crystalline inorganic oxides displaying bright colours attracted much attention from early days for application as gemstones and pigments.[1] A scientific inquiry into the origin of colours of inorganic solids is essential for a rational design and synthesis of coloured materials. While there are several causes for the colour of solids, the main factor that causes colour in an inorganic oxide containing transition metal ion is the electronic transitions within the partially filled d-states arising from the ligand field effects around the transition metal ion. Transition metal ions in less symmetric geometries such as distorted octahedral and five-fold coordinated (square pyramidal and trigonal bipyramidal) geometries produce colours different from those in regular octahedral and tetrahedral geometries in materials. Many known crystal structures have been explored over the years in the development of important colored compounds. The largest family of structures that are known, those of minerals, have not been given much attention towards developing new inorganic pigments. Over the years, we have explored many mineral structures as possible host (chromophore) towards developing new and interesting-colored compounds. In addition, we have explored the mineral structures for developing white-light emission using minimal use of rare-earth ions. The present talk would address some of these issues and our efforts towards identifying new chromophores employing transition metal chemistry in mineral structures.[2]

References

1. P. Ball, Bright Earth: Art and the Invention of Color, 2001, The University of Chicago Press, Chicago.
2. S. Natarajan et al, Chemistry – An Asian J, 2017, 12, 2734; European. J. Inorg. Chem., 2018, 2277; Inorg. Chem., 2019, 58, 8560; Dalton Trans., 2020, 49, 17649; Chem. Asian J., 2020,15, 3104; Chemistry A European J. 2021, 27, 1995; Eur. J. Inorg. Chem., 2023, 26, e2023004; Eur. J. Inorg. Chem., 2023, 26, e202300305; Chemistry An Asian J 2024, 20, e202401230; Chem. Mater., 2024, 36, 5356 – 5369; Dalton Trans. 2025, 54, 2753–2764; Chem. An Asian J., 2025, 20, e202400868; Chem. An Asian J, 2025, 20, e202401230; Chem. Eur. J 2025, 31, e202404016; Chem. Eur. J., 2025, 31, e202501300; Dalton Trans., 2025, 54, 17784 - 17797.

KN-004

Vibrational Circular Dichroism and Second Harmonic Generation: Tools for Detecting Chirality and Symmetry Breaking

Ivo Rietveld

SMS Laboratory, University of Rouen Normandy, Mont Saint Aignan, Rouen

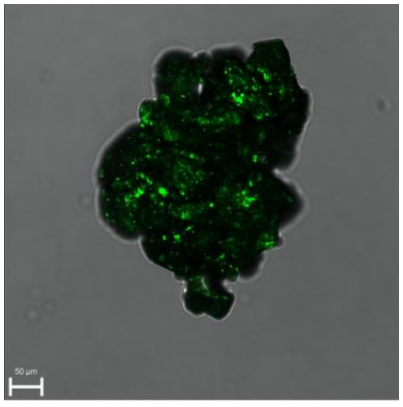
***Corresponding author e-mail:** ivo.rietveld@univ-rouen.fr

ABSTRACT

Vibrational circular dichroism (VCD) and second-harmonic generation (SHG) are two optical techniques that provide information about chirality and symmetry breaking in crystals. VCD measures the difference in infrared absorption of left- and right-circularly polarized light, delivering a direct, quantitative read-out of molecular handedness in crystals or of molecules in solution. SHG does not occur in centrosymmetric crystals, so any second-harmonic signal instantly flags non-centrosymmetric domains at the supramolecular level.

An interesting application of VCD in the solid state is the study of chiral crystals made up of achiral molecules, exhibiting chirality only in the solid state. This is demonstrated in the work involving achiral 1-(benzylsulfonyl)-4-methylbenzene crystals, which though molecularly achiral, crystallise in a chiral Sohncke space group. The handedness of the crystals can be confirmed either by single-crystal diffraction or by VCD. By selecting crystals of a chosen handedness with VCD, they can be used to seed the crystallisation of a racemic mixture, enabling preferential growth of the selected enantiomer. The VCD signal, normalised to the IR intensity, scales linearly with the enantiomorphic excess of the crystals. This linearity allows calculation of the enantiomeric excesses in the crystalline samples and demonstrates that VCD can reliably quantify chirality transferred from an achiral seed.

SHG enables detection of crystal handedness, whether pure or racemic, as long as the individual crystals are non-centrosymmetric. In a different example, racemic DL-histidine crystals belong to the centrosymmetric space group $P2_1/c$, yet SHG microscopy reveals micron-scale domains that emit second-harmonic light (see photo). These domains survive despite the overall centrosymmetric diffraction pattern and may correlate with the significantly slower nucleation rates of the racemic form compared with enantiopure L-histidine. SHG therefore exposes hidden, locally non-centrosymmetric regions that conventional X-ray analysis misses, suggesting that enantiopure crystallites grow concomitantly with racemic crystals.



Together, VCD provides precise enantiomeric-excess values for crystals that are exclusively chiral in the solid state, while SHG maps the spatial distribution of chiral domains that can reveal hidden enantiopure crystallites or indicate the onset of symmetry breaking. Using both methods delivers a multiscale toolbox for studying homochirality, improving chiral-resolution processes, and designing chiral materials.

KN-005

Generation of tunable Quantum Transport in SOC active 2D materials

B. R. K. Nanda

Center for Atomistic Modelling and Materials Design, IIT Madras

Department of Physics, IIT Madras

ABSTRACT

Spin–orbitronics has gained tremendous attention in recent years, offering a promising route for efficient information transfer and storage beyond traditional electronics. Two of the important phenomena in this context are the orbital/spin Hall effect (OHE/SHE), and the Rashba–Edelstein effect. Both correspond to a response to the applied electric field. While the former accounts for a transverse orbital/spin current, the latter leads to a non-zero accumulation of the magnetic moments and thus magnetizes the material. Thanks to strong spin-orbit coupling, topological features, and easy manipulation of symmetry, the SOC active 2D van der Waals materials have emerged as promising candidates for spin-orbitronics. In this talk, we will explore various mechanisms, such as heterostructure engineering, magnetic proximity effects, and time reversal symmetry breaking, etc. to tune the spin and orbital Hall conductivities in this class of materials. The emphasis of the talk will be on demonstrating Giant Damping-like Spin-Torque Conductivity in a GeTe/Py and $PtSe_2$/Py van der Waals Heterostructures, and Orbital and Spin Rashba Edelstein effect in Janus transition metal dichalcogenides. Finally, we will demonstrate possible ways of finding the best performing SHE materials out of a general class using AI&ML.

References

1. Giant Damping-like Spin-Torque Conductivity in a GeTe/Py van der Waals Heterostructure, H. Bangar, P. Sahu, A. Kumar, P. Gupta, A. Saxena, S. Dewan, S. Das, J. Åkerman, B. R. K. Nanda, and P. K. Muduli, arXiv:2601.12581
2. Active Learning Guided Computational Discovery of 2D Materials with Large Spin Hall Conductivity. A. J. Kale, S. Navaratna, P. Sahu, H. Chan, B. R. K. Nanda, and R. Batra, arXiv:2512.21077
3. Chiral orbital/spin textures and Edelstein effects in monolayer Janus TMDs, P. Sahu, S. Satpathy, and B. R. K. Nanda, arXiv:2511.09974 (2025).
4. Symmetry Enhanced Unconventional Spin Current Anisotropy in a Collinear Antiferromagnet, P. Gupta, K. Imtiyaz Ali Khan, A. Kumar, P. Sahu, R. Agarwal, A. Litvinenko, N. Kandwal, R. Singh Yadav, B. R. K. Nanda, J. Åkerman, Pranaba Kishor Muduli, Adv. Funct. Maters, 36, e06816 (2025).

KN-006

Computational Pathways in Topological Quantum Materials and Their Device Applications: Insights from DFT

V. Kanchana

Department of Physics, Indian Institute of Technology Hyderabad, Kandi, 502285, Sangareddy, Telangana, India

ABSTRACT

The advancement of next-generation quantum technologies relies critically on topological quantum materials, which enable energy-efficient operation, high-speed processing, and robust quantum information storage. These functionalities emerge from the interplay of magnetism, topology, electronic correlations, and superconductivity, particularly in systems with nontrivial electronic and phononic spectra. BeAu exemplifies this class by hosting exotic quasiparticles such as Weyl, Rarita–Schwinger–Weyl, and fourfold fermions, along with degenerate electronic nodal surfaces and multidimensional phononic degeneracies. Its strong spin Hall conductivity and large transverse magnetoresistance make it a promising platform for spintronics, quantum computing, and sensing applications [1]. GdCuSn, a C-type antiferromagnet with a Néel temperature of 27 K, exhibits symmetry-protected nodal surfaces and Dirac points near the Fermi level, consistent with observed positive magnetoresistance, while its sizable spin Hall effect enhances spin transport [2]. MnRuAs, based on a distorted kagome lattice, shows complex magnetic and electronic behavior, where DFT+U stabilizes a ferromagnetic ground state and reveals a quasi-one-dimensional Fermi surface and a nodal sphere [3]. MnPdGe further enriches this landscape by hosting nodal lines, Weyl nodal rings, and triple-point fermions; spin–orbit coupling generates strong Berry curvature, leading to large anomalous Hall, Nernst, and Kerr effects and significant spin Hall conductivity [4]. Beyond bulk materials, device-oriented studies demonstrate that MnGaGe operates as a two-terminal quantum transport device [5], while the MnAlGe/TiO_2 (001) heterostructure exhibits proximity-induced metallization and Ohmic contact formation, achieving a spin injection efficiency of 43% under a 0.2 V bias [6]. Additionally, 2D CrSBr/$ZrTe_5$ van der Waals spin-valves show strong proximity-induced magnetism, high magnetoresistance (~496%), and spin injection efficiencies exceeding 90%, enabling robust and thickness-independent spin filtering [7]. Collectively, these results highlight the strong potential of topological materials for quantum computing, energy-efficient electronics, and next-generation spintronic technologies.

References

1. A. Bhowmick, J. Singh, and V. Kanchana, *Spin Hall conductivity, magnetoresistance, and nontrivial topology in BeAu*, **Phys. Rev. B 111**, 115122 (2025).
2. S. S. Pradhan and V. Kanchana, *Exploring spin Hall conductivity and magnetotransport in the rare-earth topological antiferromagnetic Dirac semimetal GdCuSn*, Communicated.
3. C. V. Anusree *et al.*, *Correlation-stabilized ferromagnetism in MnRuAs with a distorted kagome lattice*, **Phys. Rev. B 111**, 035125 (2025).
4. S. S. Pradhan and V. Kanchana, *MnPdGe: A quasi-1D kagome Weyl nodal-ring semimetal for next-generation spin–orbit torque and magneto-optical applications*, (Communicated).

Towards an Enhanced Understanding of the Reactivity and Morphological Evolution of Lithium-Metal Electrodes

Ziyuan Lyu[1,2], Katrin Geng[1,2], Dominik Steinle[1,2], Dominic Bresser [1,2,3]

[1]*Helmholtz-Institute Ulm (HIU), Helmholtzstrasse 11, 89081 Ulm, Germany*

[2] *Karlsruhe Institute of Technology (KIT), P.O. Box 3640, 76021 Karlsruhe, Germany*

[3] *Ulm University, 89069 Ulm, Germany*

[*]**Corresponding author email:** dominic.bresser@kit.edu

ABSTRACT

Li-metal electrodes are considered the next great leap forward towards achieving higher energy density batteries. However, their high reactivity with essentially all liquid and solid electrolytes remains a formidable challenge – concerning both the cycle life of the cell and its safety owing to the commonly inhomogeneous,potentially dendritic lithium deposition upon continuous stripping and plating.Herein, we will report on our most recent efforts to deepen our understanding of the reactions and processes occurring at the lithium electrolyte interface. These efforts include the determination of the exchange current density as a measure for the reactivity and Coulombic efficiency, the use of X-ray tomography to study the impact of the electrolyte composition on the morphology of the plated lithium, and the development of an unsupervised data-clustering approach to identify characteristic cycle life stages of lithium-metal electrodes.The newly gained insights are anticipated to help guiding the development of further advanced electrolyte systems to eventually enable the widespread use of lithium-metal electrodes in next-generationbatteries.

KN-008

High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene

Tanmoy Maiti

Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Uttar Pradesh, India 208016.

***Corresponding author e-mail:** tmaiti@iitk.ac.in

ABSTRACT

Thermoelectric generators (TEGs) have emerged as promising technology for clean energy generation by directly converting waste heat into electrical power. However, it is challenging to design TEG with high energy conversion efficiency dictated by thermoelectric (TE) figure-of-merit, $ZT=S^2\sigma T/\kappa$ as it requires decoupling of electron and heat transport in solid bulk materials. One of the drawbacks of attaining better electron transport in polycrystalline bulk solids is the presence of 2-dimensional defects such as grain boundaries. Recently, we have shown that *ZT* values of thermoelectrics can be significantly enhanced by employing the strategy of making TE composites with highly conductive 2D materials such as graphene or MXene. We have used the matrix of various thermoelectric materials such as oxides, sulphides, skutterudites to make these composites. Challenges in oxide thermoelectrics are manifold as *ZT* values of oxides suffer from lower electrical conductivity as well as relatively higher thermal conductivity compared to intermetallics and chalcogenides. Electrons in oxide perovskites suffer from Anderson's localization due to the presence of multi-valent transition metals and point defects giving rise to variation in local electric field and strain. We have used the strategy of boosting the electron transport by manipulating semiconductor to metal transition temperature in donor doped $SrTiO_3$ by synthesizing nanocomposites with graphene, graphite and MXene. Presence of these inclusions in perovskite matrix provide high momentum electrons and impart enough strain to facilitate these localized electrons to attain the itinerant state. As a result, we could achieve single-crystal like electron mobility in ceramic nanocomposites. Furthermore, we could restrain the increase in thermal conductivity by attaining enhanced Umklapp scattering along with phonon-glass-like temperature-independent phonon mean-free-path above Debye temperature. We have fabricated 4-legged n-type thermoelectric power generator demonstrating milliwatt-level power output, hitherto remained unattainable for oxide thermoelectrics. Further we have synthesized composites of Bi_2S_3 and $CoSb_3$ Skutterudite with MXene and graphite to enhance their ZT values. The common observation from our study on incorporating highly conductive 2D materials in thermoelectric materials is the enhancement of electron transport by increasing carrier concentration and mobility. Most importantly the presence of these secondary phases in the composites induces enhanced phonon scattering, especially at high temperatures allowing us to achieve enhanced *ZT* values. Our proposed way of designing bulk composites with 2D materials can potentially open up the possibility of fabricating novel thermoelectric generators.

KN-009

Innovative Functional Fibrous Materials for Technical Textiles

Dr. Mukesh Kumar Sinha
Advanced Composite Centre (ACC), Advanced Systems Laboratory (ASL), DRDO
Hyderabad

ABSTRACT

This talk deals with special and advanced technology related to technical textiles and overall scenario of Indian textile industry. Indian textile industries were engaged for several decades in traditional products, due to high demands of such materials from the domestic and export markets. The developed products are of very cost competitive, because of availability of cheaper labours. At present, there is an increasing demand for innovative and smart apparels, home and functional technical textile products to be manufactured by using the new innovative technology of fibres and in that case, focused R &D efforts cannot be denied. At the same time, our capabilities in high performance and technical products are rather deprived.

An identified area, which is vital for Indian technical textile industry to fulfil technological gaps are; development of high performance (HP)/functional fibres (FF) and specialized coating & lamination process (SCL). Both of these areas are currently technological gaps and need to be addressed in a systematic long-term way for the technical textile industry to prosper in the country. Commercially available high performance and functional fibres like; Silicon Carbide (Nicalon), Carbon (Toray Industries Japan), p-aramid (Kevlar), PolyP-Phenylenebenzobisoxazole (PBO/Zylon), Ultra high molecular weight polyethylene-UHMWPE (Spectra & Dyneema) are finding increased importance in defence and technical textile applications. These high performance fibres are driven by special technical functions with specific physical properties. These properties are: higher tensile strength, chemical and thermal resistance as compared to the normal grade of polymeric fibres. Polymeric high performance fibres have a tenacity range of 15-50 g/d and tensile modulus of 150-400 g/d. Multinational companies like DuPont, Honeywell, DSM, and Niclon are having global trade monopolies for manufacturing such high performance fibres. Since defence sector is a primary consumer of these fibres for making NBC clothing, aerostat, inflatable tents & shelters for cold regions and ballistic textiles and its fibre mostly dependant on import.

Using high performance fibres and inherent functional fibres for a specific application will lead to product development, such as moisture management, conductive, hydrophilic, anti-bacterial, flame retardant, antistatic, smart & intelligent fibres & fabrics by exploiting their properties. Advantages of using such functional fibres could be tailored into various protective product applications e.g. sensors, EMI shielding clothing, fire retardant clothing, light weight cold weather protective clothing with high degree of comfort. Under the segment of medical textile products, which include like wound dressing & healing, face mask, tissue scaffolds, surgical gowns, artificial heart valves etc., where functional fibres like antimicrobial/fungal and hydrophilic and high strength modules fibres can play a vital role to develop such high valued product. Apart from Protech and Meditech, other end user applications, where such R & D efforts will be useful such as: Indutech, sporttech and mobiltech segments of technical textiles

Technical Textiles are one of the most important segement, which comprises of 12 core high tech. textiles & fabrics. Out of which, DPTs is subset of Protech (protective textiles). The old concept of DPTs was emphasised on functional properties of fabrics rather than aesthetics. Such concept has been changed and now, DPTs should be contained with both functional as well as aesthetics (surface properties), so that soldiers should look smart and intelligent with enormous fighting capability. Equally, at same note a military functional Defence protective textiles (DPTs) uniform are foremost vital, relevant and plays an important role for deciding the fate of war and causalities by protecting themselves and civilians and therefore, the importance of DPTs cannot be ignored. Now in this modern age, DPTs should fulfill the stringent army requirements during combat operations, emergency operations and critical survival situations to protect themselves and minimize casualties during war scenario. Therefore, the range of textile materials used in defence has highly diversified spectrum in the army: protective clothing for extreme temperature (heat and cold); chemical, biological, nuclear and radiological (CBRN) protective clothing (specific performance for neutralizing deadly warfare agents); bulletproof composite panels; camouflage fabrics; and inflatable boats & protective covers, aerostat, parachute fabrics inflatable tents & shelters. In order to design protective technical textiles, a continual long-term technological research could play a major role to compete with the international market.

KN-010

Emerging Materials and Intelligent Processes in Microalgae Biorefinery Technology

Pau-Loke Show

Director, Center of Excellence for Research, Value Innovation and Entrepreneurship (CERVIE), UCSI University, Malaysia

***Corresponding author e-mail:** ShowPL@ucsiuniversity.edu.my

ABSTRACT

Microalgae represent an emerging class of functional biological materials with broad applications in sustainable technologies, environmental remediation, and bio-derived product development. Recent advances in downstream processing have positioned Liquid Biphasic Systems (LBSs) as an effective and scalable platform for the separation and purification of microalgae-derived biomolecules and bioproducts, contributing to circular bioeconomy pathways. LBSs offer high selectivity, operational simplicity, and strong potential for industrial scale-up, making them attractive alternatives to conventional purification techniques in biorefinery workflows. Integration of Internet of Things (IoT) and artificial intelligence (AI) with LBS-based processing is enhancing real-time monitoring, control and optimization, enabling intelligent materials and process systems that respond dynamically to changes in biomass composition and operational conditions. This keynote reviews recent research progress on novel LBS configurations, their roles in clarifying, partitioning and partially purifying microalgae-derived materials, and how intelligent technologies are being deployed to achieve higher efficiency and sustainability. In addition, the talk will outline challenges and ethical considerations in adopting AI-enabled systems in bio-processing and highlight future opportunities for microalgae-derived functional materials in environmental and materials science applications. By framing microalgae technology within the context of advanced materials development and sustainable processing, this work aims to stimulate interdisciplinary research collaborations between materials scientists, bioprocess engineers, and industry innovators.

Thermal transport in 2D materials

Jayakumar Balakrishnan

Department of Physics, IIT Palakkad

***Corresponding author email address**: jayakumar@iitpkd.ac.in

ABSTRACT

Interfaces play an important role in modulating thermal conductivity in 2D materials, especially 2D-TMDs. In this talk, I will discuss a Micro-Raman based approach that enables the simultaneous determination of thermal conductivity and interface thermal conductance of supported 2D MoS_2 on crystalline and amorphous substrates [1]. We demonstrate a four fold increase in thermal conductivity in MoS_2 on crystalline substrate in comparison to MoS2 on amorphous substrate. Our studies emphasizes the importance of substrate vibrational properties and interfacial interactions in determining the thermal properties of supported 2D materials. In the final part of the talk I will briefly show our recent demonstration of a fast direct write laser lithography technique for large area 2D devices with out the need for sophisticated masks or techniques like e-beam [2].

Keywords: Raman spectroscopy, TMDs, Graphene, laser lithography

References:

1. A. Sampanraj et al., Phys. Rev. B, 2025, **111**, 075423.
2. N. J. Joy and J. Balakrishnan, J. Micromech. Microeng., 2026, **36**, 015003.

KN-014

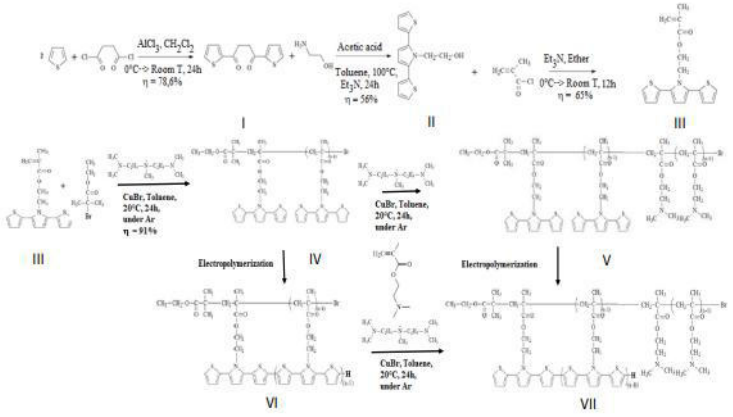
Electroactive and Electrochromic Smart Organic Coatings Functionalized with Polymer Brushes

Amani Chams*, Christian Perruchot, Mohamed M. Chehimi and Mohamed Jouini.

Université Paris Cité. CNRS, ITODYS, F-75013 Paris, France

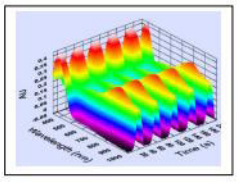
ABSTRACT

We report a strategy for preparing smart coating based on the synthesis, electrodeposition, and patterning of ultrathin films on electrode surfaces using the "precursor polymer" approach [1,2]. A passive polymer backbone (a polymethacrylate: PMM) is used as support functionalized with electroactive monomer group: 2-(2,5-di (thiophen-2-yl)-1H-pyrrol-1-yl)ethyl, a thiophene-pyrrole-thiophene noted SNS-ethyl. This coumpound is covalently linked to the PMM in the precursor polymer (PPHMA2). The electropolymerization on ITO substrates (scheme 1) resulted in a crosslinked conjugated copolymer material network through inter- and intra-chain coupling and leads to smooth, high optical quality films, which should be important for electro-optical coatings applications.



Scheme of the synthesis of the smart polymers material network using the "precursor polymer approach"

II:2-(2-5-di(thiophen-2-yl)-1H-pyrrol-1-yl)ethanol monomer number
III:2-(2-5-di(thiophen-2-yl)-1H-pyrrol-1-yl)ethyl 2-bromo methacryl y (SNS-MA)
IV: PolyMA-SNS
V: PolyMA-SNS-PolyMMA
VI: PolyMA-PolySNS
VII: PolyMA-PolySNS-PolyMMA



In-situ 3D spectroelectrochemical curves of Poly(MA)-Poly(SNS) film on ITO, CA square wave: E_{appl} = 0,00/30 sec to 1,05/30 sec V/SCE.

References:

1. D. Stanke, M. L. Hallensleben, L. Toppare, Synth. Met. 72 (1995) 95-98.
2. Rigoberto C. Advincula et al., Chem. Mater. 2002, 14, 10, 4073–4080

Study of Wicking Materials for Surface Acoustic Wave Atomizer Toward Chemical Spraying Applications

Jun Kondoh, Sohei Uno[1], Hiroki Ichihara[1]*

[1]Shizuoka University, Hamamatsu, Shizuoka, 432-8561 Japan

***Corresponding author e-mail**: kondoh.jun@shizuoka.ac.jp

ABSTRACT

Surface acoustic wave (SAW) devices play an important role in mobile communication systems such as smartphones, and they are also widely used as sensors and actuators[1],[2]. In this presentation, a SAW-based atomizer for chemical spraying applications is investigated. When a liquid droplet is placed on the SAW propagation surface, longitudinal waves are radiated into the liquid. As the applied electrical power to the SAW device increases, droplet vibration, droplet transport, and fine droplet ejection are observed. These phenomena originate from acoustic streaming and are therefore categorized as nonlinear acoustic phenomena. SAW-induced atomization[3] is generally regarded as a nonlinear acoustic phenomenon. However, atomization can occur even at relatively low applied electrical power when a thin liquid layer is formed on the SAW device. This suggests a different atomization mechanism. We have considered that capillary waves are generated on the thin liquid layer and that mist droplets are emitted from the wave fronts. To maintain a stable thin liquid layer on the SAW device, filter paper has been used as a liquid supply medium, where liquid is continuously delivered by capillary action. However, the influence of liquid supply materials on atomization performance has not been systematically investigated. In this study, various wicking materials are compared in terms of their liquid supply characteristics and atomization behavior. Furthermore, an experimental system simulating pulmonary drug delivery by chemical spraying was constructed. Using a pump that mimics inhalation during breathing, it was demonstrated that the generated mist can be dispersed over a distance of at least 20 cm.

Keywords: SAW device, atomization, chemical spray

References:

1. K. Hashimoto, Applied Physics Express, **18** (2025) 090103.
2. J. Kondoh, Japanese Journal of Applied Physics, **57** (2018) 07LA01.
3. M. Kurosawa et al., Sensors and Actuators A, **50** (1995) 69.

KN-016

Green Fabrication of Conductive Patterns on Eco-Friendly Substrates

Ying-Chih Liao[1]*

[1]*Department of Chemical Engineering, National Taiwan University, Taiwan*

***Corresponding author e-mail:** liaoy@ntu.edu.tw

ABSTRACT

The growing demand for sustainable, low-cost materials in biosensing has accelerated the development of green fabrication strategies for real-time and portable health monitoring devices. Conventional electrode fabrication typically involves multi-step processing and non-renewable materials, raising environmental concerns and limiting large-scale deployment. In this work, we report a sustainable and scalable approach for biosensor fabrication by directly converting biodegradable bacterial cellulose (BC) into conductive carbon thin films via CO_2 laser-induced carbonization under ambient conditions. BC, a biopolymer produced by microorganisms, possesses a highly porous nanoscale fibrous network, excellent mechanical robustness, and inherent biocompatibility, making it an attractive substrate for biomedical applications. The localized laser-induced heating enables in situ decomposition of organic components and reorganization of carbon atoms into conductive graphitic domains, forming a functional electrochemical electrode in a single step without chemical additives or post-treatment. The resulting laser-carbonized BC electrodes exhibit enhanced conductivity and electrochemical activity, enabling sensitive and simultaneous detection of glucose and lactate in phosphate buffer solution. Differential pulse voltammetry confirms good selectivity, reproducibility, and operational stability. Furthermore, the electrodes demonstrate reliable performance in real sweat samples, highlighting their applicability for non-invasive biomarker monitoring. This work establishes laser-induced carbonization of bacterial cellulose as a green, efficient, and versatile platform for developing sustainable, high-performance biosensors for portable and on-site health monitoring applications.

KN-017

Advanced Hybridized Nanogenerators for Multifunctional Self-Powered Systems: Synergistic Materials Design, Principles, and Sustainable Applications

Naratip Vittayakorn

Advanced Materials Research Unit, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang (KMITL), Bangkok, Thailand

***Corresponding author e-mail:** naratip.vi@kmitl.ac.th

ABSTRACT

The rapid proliferation of the Internet of Things (IoT) and wearable electronics has triggered an urgent demand for sustainable, flexible, and efficient autonomous power sources. This keynote addresses the frontier of mechanical energy harvesting through the development of hybridized Triboelectric (TENG) and Piezoelectric (PENG) nanogenerators, with a specific focus on materials engineering strategies to overcome the limitations of conventional energy harvesters. Our research at KMITL highlights the "synergistic integration" of functional fillers within diverse polymer matrices to create high-performance composite films. We elucidate the design principles of incorporating novel lead-free piezoelectric ceramics (e.g., $BaTiO_3$ nanorods, KNNS-based, BNT-based, and BF-BT-NZN systems) and 2D nanosheets (e.g., dielectric $Ti_{0.8}O_2$, MgAl-LDH, Ti_2NbO_7) into flexible matrices like PDMS or cellulose paper. These engineered interfaces significantly enhance the dielectric constant, surface charge density, and electromechanical coupling, resulting in giant output performance capable of powering portable electronics. Furthermore, we explore the paradigm shift towards sustainable and biocompatible electronics by utilizing nature-derived biopolymers specifically Bacterial Cellulose (BC) and Chitosan. We demonstrate how reinforcing these matrices with organic piezoelectric crystals (e.g., Triglycine Sulfate) or functional protein fillers (e.g., Silk fiber, albumin, egg-shell membrane) can manipulate molecular structures to boost triboelectricity. Beyond materials, we showcase device-level innovations, such as a 3D multi-layer Origami structure combined with a self-charge pumping module (SCPM), a strategy that dramatically amplifies energy conversion efficiency. Finally, the multifunctionality of these hybrid devices is highlighted through applications in thermal energy harvesting (textiles), photocatalytic environmental remediation (CCTO), and self-powered health monitoring. By bridging the gap between fundamental material synthesis—ranging from nanoparticles to nanosheets and practical device fabrication, this talk aims to provide a comprehensive roadmap for the next generation of eco-friendly, self-powered smart systems.

Keywords: Hybrid Nanogenerators; Self-Powered Sensors; Lead-free Piezoelectrics; Biopolymer Composites; Multifunctional Devices

References:

1. U. K. Khanapuram, G. M. Rani, S. Panda, T. Charoonsuk, ..., N. Vittayakorn, et al., "Harvesting Energy from Friction: The Revolutionary Decade of Triboelectric Nanogenerators," Adv. Powder Mater., Art. no. 100373, Nov. 2025.
2. S. Hajra, A. Ali, ..., N. Vittayakorn, ..., and T. H. Oh, "Synergistic integration of nanogenerators and solar cells: advanced hybrid structures and applications," Adv. Energy Mater., vol. 14, no. 21, p. 2400025, Jun. 2024.

KN-018

How to Improve the Coating Homogeneity on Primary Particles using Chemical Reaction and Physical Deposition

Tomoya Ohno[1]*, Jeevan Kumar Padarti[1], Shigeto Hirai[1]

[1]*Kitami Institute of Technology, Koen-cho 165, Kitami, Hokkaido, Japan, 090-8507*

***Corresponding author e-mail:** ohno@mail.kitami-it.ac.jp

ABSTRACT

Nano-coating of primary particles is widely recognized as an effective approach for material compositing in optical materials and electrochemical catalysts. However, systematic evaluation of the relationship between coating layer structure and material properties remains challenging, primarily due to the lack of appropriate structural indicators and the strong dependence of coating morphology on the specific coating process employed. Our research group has previously developed a nano-coating process that combines chemical reaction-driven film formation with physical deposition phenomena, applying it to introduce protective layers onto cathode materials for lithium-ion secondary batteries. In addition, we proposed a method for structural evaluation of coating layers based on complementary spectroscopic analyses using X-ray fluorescence (XRF) and X-ray photoelectron spectroscopy (XPS).

In this study, we investigate how pressure control during the coating process affects the coating layer homogeneity. Reduced pressure conditions are expected to increase the polymerization degree of the coating precursor molecules, thereby influencing the chemical reaction-driven coating formation and ultimately improving the uniformity of the coating layer. The homogeneity of the protective layer was quantitatively evaluated using the ratio of surface/bulk elemental concentrations obtained by XPS to those obtained by XRF. Furthermore, the impact of improved coating homogeneity on electrochemical performance of lithium-ion batteries was examined.

The results demonstrate that pressure control during the coating process enhances the uniformity of the protective layer on the cathode material surface. This improved homogeneity correlates with enhanced battery performance, highlighting the importance of precise control of coating layer structure. These findings provide a useful framework for quantitatively evaluating nano-coating structures and for designing advanced surface-modified electrode materials.

Keywords: particle, nano-coating, lithium-ion secondary batteries, cathode

References:

1. T. Ohno, J. K. Padarti, S. Hirai, T. Matsuda and H. Suzuki, *Adv. Powder Technol.*, 34 (2023) 104247
2. T. Ohno, J. K. Padarti, S. Hirai and T. Matsuda, *Adv. Powder Technol.*, 35 (2024) 104608

Accelerating Materials Discovery for Clean Energy and Environmental Application: Integrating Simulations and Experiments

Ravichandar Babarao

Centre for Advanced Materials and Industrial Chemistry (CAMIC), School of Science, RMIT University, Australia

Visiting Scientist, CSIRO Manufacturing Flagship, Clayton, Victoria, Australia

***Corresponding author e-mail**: ravichandar.babarao@student.rmit.edu.au

ABSTRACT

Porous materials especially, coordination polymers (CP) or metal-organic frameworks (MOFs) have emerged as a special class of hybrid nanoporous materials. The variation of metal oxides and the vast choice of controllable organic linkers allow the pore size, volume, and functionality of MOFs to be tailored in a rational manner for designable architectures. MOFs thus provide a wealth of opportunities for engineering new functional materials and are considered as versatile candidates for storage, separation, sensing, catalysis, drug delivery and other important applications. With ever-growing computational resources and advance in mathematical techniques, molecular simulations have become an indispensable tool for materials characterization, screening and design. At a molecular level, simulations can provide microscopic insights from the bottom-up and establish structure-function relationships. This presentation will highlight how molecular modelling, combined with experiments, can be a powerful tool in complementing experimental work, thereby aiding in the design of new smart porous materials for storage, sensing, catalysis, and separation applications.

References:

1. X. Shao, A. Maibam, F. Cao, H. Jin, M. Liang, M.G. Kim, K. M. Tran, H. S. Jung, R. Babarao and H Lee, Angew., Chem. Int. Ed., 2024, 63 (44), e202406273.
2. A. Maibam, I. B. Orhan, S. Krishnamurty, S. P. Russo, and R.Babarao, ACS Applied Materials and Interfaces, 2024, 16 (7), 8707 – 8716.
3. B. L. Mathews, N. C. Harvey-Reid, E. Jangodaz, V.J. Scot, M.J. J. Polson, A. Maibam, R. Babarao. S.G. Telfer and P.E. Kruger, J. Mater. Chem. A, 2024, 12, 15106 - 15114.
4. I. B. Orhan, Tu C. Le, R. Babarao and A. W. Thornton, Communications Chemistry, 6(1), 214.

KN-020

Towards Thin Films Advanced Deposition for Improved Electrochromic Properties

Aline Rougier

Université de Bordeaux CNRS Bordeaux INP, ICMCB, UMR5026, 87 av. Du Dr Schweitzer, F-33600 Cedex Pessac France

***Corresponding author e-mail**: aline.rougier@icmcb.cnrs.fr

ABSTRACT

Chromogenic materials and devices are known for the modulation of their optical properties under external stimuli. The later of various origins include light for photochromism or temperature for thermochromism. In this presentation, taking the example of Electrochromism (EC), corresponding to an optical modulation under an applied voltage, we will highlight how a fine tuning of the deposition conditions including the power source, the configuration (conventional or co-sputtering), single deposition or combinatorial, can enhance the EC properties of sputtered oxide films. In particular, we will demonstrate how a careful control of the deposition conditions of sputtered $W0_3$ films[1], known as the state of the art EC oxide switching from a colorless to blue under reduction, leads to save energy in buildings thanks to smart windows technology. Considering, the anodically colored NiO films, combinatorial synthesis based on a magnetron co-sputtering approach, allows in a single deposition the mapping of 76 samples, with a wide range of thicknesses (200 to 700 nm) and Li_xNi_yO compositions ($Li_{0.04}Ni_{0.96}O$ to $Li_{0.45}Ni_{0.55}O$), and enhanced optical contrast and durability. In this presentation, the thin film route will be highlighted as a versatile tool for the growth of oxide based materials with enhanced properties for better addressing efficient applications in the field of energy.

References:

1. Faceira et al., J. Phys. Chem (2022), Ad. Funct. Mat. 2023

KN-021

Proposing an Imprinted Poly(2-vinyl-4-nitroaniline) Modified Electrode for Differential Pulse Voltammetry Detection of Urinary Uric Acid

Mei-Jywan Syu*, Hsiao-Yu Cheng

Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan

***Corresponding author e-mail:** syumj@mail.ncku.edu.tw syumei.carbon@gmail.com

ABSTRACT

Uric acid is the end product of purine metabolism. Abnormal uric acid level is closely associated with metabolic disorders such as gout and kidney diseases. Consequently, to measure uric acid concentration is essential for early diagnosis of these diseases. In this work, we developed a molecularly imprinted polymer (MIP) sensor to determine the uric acid concentration in urine. 2-Vinyl-4-nitroaniline (VNA) as the functional monomer, Ethylene glycol dimethacrylate (EGDMA) in a large proportion as the crosslinker, and the uric acid template were added to achieve the interactions among all. Thermo-polymerization was then initiated in the presence of an initiator, 2,2-azobis-isobutyronitrile (AIBN). Via which, the uric acid imprinted poly(2-vinyl-4-nitroaniline) (PVNA) film, was fabricated onto the Au electrode. Afterwards, the imbedded uric acid templates were washed out so that the cavities with specific binding sites for uric acid molecules were developed. The cavities could then uptake uric acid molecules. Differential pulse voltammetry (DPV) was utilized as the mode for electrochemical detection of uric acid. An imprinting factor of 10.1 to evaluate the specificity of the MIP sensor towards uric acid with respect to the nonimprinted polymer (NIP) sensor was achieved. The sensor thus prepared shows good linearity in the uric acid concentration range of 0~80 mg/dL. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were analysed for understanding the electrochemical characteristics of the MIP electrode. Selectivity and storage stability of the MIP electrode were also evaluated. Further, the urine specimens received from NCKU hospital with IRB approved (B-ER-110-510) were used to test the precision of the MIP sensor. In summary, the results confirm feasibility of the MIP sensor on clinical detection of uric acid concentration.

References:

1. D Lakshmi, MJ Whitcombe, F Davis, PS Sharma, BB Prasad. Electroanalysis 23 (2011) 305−320.
2. MJ Syu, TJ Hsu, ZK Lin. Anal Chem 82 (2010) 8821−8829.

KN-022

Comparative Studies on Some Novel Quantum Systems at Extreme Pressures and Magnetic Fields

Awadhesh Mani

Condensed Matter Physics Division, Materials Science group,
Indira Gandhi Centre for Atomic Research, Homi Bhbha National Institute,
Kalpakkam – 603102, Tamil Nadu

***Corresponding author e-mail:** mani@igcar.gov.in

ABSTRACT

In this presentation, comparative studies on the evolution of physical properties of a few novel quantum systems, (viz., Topological Insulators (TI), FeAs-based superconductors and d-electron based Kondo Insulators) under extreme pressures and magnetic fields at low temperatures will be elucidated. Topological insulators (TIs) belong to a novel class of materials which host concomitantly insulating bulk states along with metallic edge/surface states. The Bi-based chalcogenides (Bi_2Se_3 and Bi_2Te_3) are the simplest 3-dimensional (3D) TIs wherein the 2D surface states culminate into a single Dirac cone. The high pressure studies reveal the profound effect of pressure on the physical properties of $Bi_2Se_{3-x}Te_x$ systems [1]. The application of external pressure on Te-doped samples leads to the occurrence of multiple electronic phase transitions such as an insulator-to-metal transition (MIT) followed by pressure-induced superconducting transition at higher pressures. The detailed analysis of the experimental data reveals that the pressure-induced superconductivity observed in these systems is of conventional (BCS) type. System $BaFe_2As_2$ belongs to FeAs family of compounds which exhibits Spin Density Wave (SDW) ordering of Fe spins in concomitance with the structural transition from the tetragonal to an orthorhombic phase below 132–140K. The importance of external pressure and chemical substitution in inducing superconductivity in $Ba(Fe_{1-x}Ru_x)_2As_2$ system and its correlation will be brought out in this talk. Our detailed studies revealed that the compositional and pressure dependence of T_c for various values of x can be unified, if viewed in terms of the underlying strength of the spin-fluctuations, which has been obtained from the analysis of normal state resistivity [2-3]. FeSi and $FeSb_2$ are rarest d-electron based Kondo Insulator (KI) which possesses intriguing magnetic, thermal and transport properties. The evolution of the ground state properties of this system under pressure as well as chemical substitution leading to interesting insulator to metal transition on account on delocalization of localised states and its underlying physics will be also be discussed [4-6].

References

1. Devidas, T. R.; Abhirami, S.; Sharma, S.; Amaladas, E. P.; Mani, A. *EPL* 2018, *121*, 67001.
2. Mani, A.; Ghosh, N.; Paulraj, S.; Bharathi, A.; Sundar, C. S. *Europhys. Lett.* 2009, *87*, 17004.
3. Devidas, T. R.; Mani, A.; Sharma, S.; Vinod, K.; Bharathi, A.; Sundar, C. S. *Solid State Commun.* 2014, *185*, 62–.
4. Mani, A.; Janaki, J.; Satya, A. T.; Kumary, T. G.; Bharathi, A. *J. Phys.: Condens. Matter* 2012, *24*, 075601.

KN-023

A Dual Bioceramic Strategy for Integrated Bone and Wound Regeneration Using Hydroxyapatite and Bioactive Glass Systems

Balakumar Subramanian*

National Centre for Nanoscience and Nanotechnology, University of Madras

Guindy Campus, Chennai -25, TamilNadu, India

***Corresponding author e-mail:** balasuga@yahoo.com

ABSTRACT

The rational design of multifunctional biomaterials that combine mechanical robustness, biological responsiveness, and clinical adaptability remains a major challenge in tissue engineering. Bioceramics such as hydroxyapatite (HAp) and bioactive glass (BG) are particularly attractive due to their osteoconductive, angiogenic, and biointeractive properties, as well as their long-term chemical stability. In this study, a modular and scalable bioceramic-based platform is proposed, integrating bone-regenerative scaffolds and soft tissue wound patches to address the diverse structural and biological requirements of cortical and cancellous bone repair alongside accelerated wound healing. Porous bovine bone derived hydroxyapatite (BNHAp) scaffolds were fabricated using a polyurethane foam replica technique and biofunctionalized with collagen-gelatin to enhance cell–matrix interactions and extracellular matrix mimicry. The scaffolds exhibited phase-pure HAp with interconnected porosity and tunable compressive strengths ranging from 0.11 MPa (spongy bone) to 0.43 MPa (cortical bone), enabling structural customization according to defect type. In vitro assessments confirmed excellent blood compatibility, high protein adsorption capacity, and sustained fibroblast proliferation. Degradation behavior was controllable through pore architecture, while mineralization assays demonstrated rapid apatite nucleation. Importantly, *in vivo* angiogenesis analysis highlighted enhanced vascular network formation, indicating strong pro-angiogenic potential.

Complementarily, flexible wound healing patches were developed using hydroxypropyl methylcellulose, polycaprolactone, and 59S bioactive glass through combined spin coating and electrospinning, forming hierarchically stacked fibrous layers. These patches displayed mechanical resilience (tensile strength 6.14 MPa), conformability, and moisture-retentive behavior favorable for wound environments. Controlled biodegradation, ultra-low hemolysis (0.28%), and sustained metformin release over three days supported therapeutic efficacy. Cellular, biochemical, and microbiological evaluations revealed >90% cell proliferation, significant anti-inflammatory activity, angiogenic stimulation, and broad-spectrum antibacterial performance. In vivo wound healing studies demonstrated complete closure within 14 days, accompanied by rapid re-epithelialization, organized collagen deposition, and dense vascularization. Overall, this study highlights a versatile, cost-effective, and clinically translatable bioceramic composite strategy, where architecture-driven bone scaffolds and drug-eluting wound patches operate synergistically to promote integrated hard and soft tissue regeneration.

Keywords: Bioceramics, Bovine bone derived hydroxyapatite, Bioactive glass, Cortical bone regeneration, Tissue engineering scaffolds, Wound healing patches

Topological Data Analysis for Materials Informatics

Kazushi Ikeda[1], Yuki Ura[1], Hiroya Ikeda[2]

[1]*Nara Institute of Science and Technology, Ikoma, Nara, Japan, 6300192*

[2]*Shizuoka University, Hamamatsu, Shizuoka, Japan, 4328561*

***Corresponding author e-mail:** kazushi@is.naist.jp

ABSTRACT

ZnO-nanorods synthesized on conductive fabrics are a strong candidate for high-efficiency flexible thermoelectric devices, however, the optimal synthesis conditions required to maximize the thermoelectromotive force are not yet fully understood. Since SEM images of the nanorods are relatively easier to obtain than thermoelectric properties through experiments, it is beneficial to estimate the properties from the images. A topological data analysis (TDA) called Persistent Homology (PH) is shown to effectively extract features from SEM images of ZnO-nanorods and to be correlated to synthesis conditions. In this talk, I introduce TDA methods and show their effectiveness in materials informatics.

References:

1. Yuki Ura, et al., Proc. AFMD 2024, 153.
2. Hiroya Ikeda, et al., 122 (2022), SDM2022-15.
3. Yuki Ura, et al., Proc. ISBE 2025.

KN-025

Engineering Halide Perovskites for Photonic and Optoelectronic Applications

Sudakar Chandran*

Department of Physics, Multifunctional Materials Laboratory, Indian Instittue of Technology Madras, Chennai 600036

*Corresponding author e-mail: csudakar@iitm.ac.in

ABSTRACT

Halide perovskites have emerged as a versatile materials platform for next-generation photonic and optoelectronic devices owing to their exceptional optical gain, bandgap tunability, high absorption coefficients, and defect tolerance. This talk will highlight recent advances from our group on tailoring both lead-based and lead-free halide perovskites for microcavity lasing, optoelectronics, and multifunctional electro-optical applications. Whispering gallery mode (WGM) lasing is demonstrated in perovskite quantum dots (QDs) integrated with TiO_2 spherical microcavities, where strong coupling between the QD gain medium and optical resonator enables low-threshold stimulated emission, high quality (Q) factors, and robust room-temperature operation. $CsPbI_3$ and Rb-substituted $CsPbBr_3$ QDs exhibit enhanced photostability and tunable WGM microlasing, while coupled microcavity architectures allow controlled modulation of resonance behavior. Beyond lasing, post-synthetic halide mixing in $CsPbI_3$–xBrx nanocrystals reveals distinct ion-exchange pathways governed by nanocrystal aging and surface chemistry, providing insights into composition control and optical tunability. The development of lead-free photonic systems is further advanced through core–shell TiO_2@$Cs_2AgBiBr_6$ microspherical resonators exhibiting amplified spontaneous emission mediated by WGMs, as well as porous single crystals of $Cs_2AgBiBr_6$ that enhance charge transport and photovoltaic performance. Additionally, dopant-engineered layered double perovskites display sharp zero-phonon-line and near-infrared emissions, while controlled ion migration enables fully reversible electrochromism in several lead-free perovskite families. This talk will demonstrate how compositional engineering, defect control, and photonic structuring can be synergistically exploited to realize stable, tunable, and environmentally benign halide perovskite–based photonic and optoelectronic devices.

KN-026

Designing Advanced Quantum Dots/Graphene Broadband Photodetectors

Judy Wu*[1]

[1]*Department of Physics and Astronomy, University of Kansas, Lawrence, United States of America*

***Corresponding author e-mail**: jwu@ku.edu

ABSTRACT

Photodetectors based on colloidal quantum dots (QD)/graphene nanohybrids are quantum sensors due to strong quantum confinement in QD and graphene. The optoelectronic properties of QD/graphene nanohybrids are affected by the quantum physics that predicts a high photoconductive gain and hence photoresponsivity (R^*) depending on the pixel length (L) as $R^* \propto L^{-2}$. Experimental confirmation of the effect of the pixel geometric parameters on the optoelectronic properties of the QD/graphene photodetector is therefore important to elucidate the underlying quantum physics but presents a challenge in atomic-scale control of the device microstructure to allow the geometric effect to be extracted precisely. Motivated by this, an array of QDs/graphene nanohybrid photodetectors were designed with variable QD/graphene pixel length L and width W in the range of 10-150 μm for a study of R^*, noise, and D^*. Intriguingly, R^* exhibits a monotonic decreasing trend of $1/L^2$ while being independent of W, confirming experimentally the theoretical prediction. Furthermore, a few examples will be highlighted on designs of high-performance QD/graphene photodetectors for broadband photodetection within and beyond the limit of semiconductor bandgaps in ultraviolet, visible, infrared, and x-ray.

References:

1. Gong, Maogang, Liu, Bo, Shultz, Andrew, Schmitz, Russell C., Vargas, Hugo Barragan, Alzahrani, Saad, Robles Hernandez, Francisco C., Olson, Austin, Wu, Judy Z., "Decoupling of Photocurrent and Dark Current for Extraordinary Detectivity in Uncooled Middle-Wavelength Infrared Nanohybrid Photodetectors". ACS Nano 19(9): p. 8520-8538 (2025).
2. Andrew Shultz, Bo Liu, Maogang Gong, Francisco C. Robles Hernandez, and Judy Wu, "Pixel Geometry Effect on PbS Quantum Dot/Graphene Nanohybrid Broadband Photodetectors", Advanced Optical Materials. Vol. 12, issue 13, page 2302675 (2024).
3. M. G. Gong, D. Ewing, S. Sadeghi, J.Z. Wu, "Localized Surface Plasmon Resonance Enhanced Light Absorption in AuCu/CsPbCl3 Core/Shell Nanocrystals", Advanced Materials Page 2002163 (2020).

KN-027

Two-Dimensional Metal Chalcogenides: Exploring Exciting Opportunities for Neuromorphic Computing

Prof. Govind Gupta[1,2]

[1]*Sensor Devices & Metrology Group, CSIR-National Physical Laboratory (CSIR-NPL), Dr K. S. Krishnan Road, New Delhi 110012, India*

[2]*Academy of Scientific & Innovative Research (AcSIR), CSIR-HRDC Campus, Ghaziabad, Uttar Pradesh 201002, India*

Corresponding author's email: govindnpl@gmail.com, govind.nplindia@csir.res.in

ABSTRACT

Artificial Neural Networks are intriguing computer systems designed to simulate how the human brain processes information. While they offer significant advantages, they also present several challenges, including the need for large, high-quality datasets, substantial computational resources, a tendency to overfit, and a "black box" nature that makes it difficult to understand their inner workings. Recently, neuromorphic devices have gained importance as technology advances. These devices play a crucial role in supporting autonomous systems, robotics, healthcare, and edge AI, all of which rely on brain-inspired, low-power processing. Efforts worldwide are underway to develop neuromorphic technologies that replicate the structure and functions of the human brain to address increasing demands. Moreover, the rise of the Internet of Things (IoT) is driving the development of more powerful computing and data processing capabilities, accelerating the adoption of these innovative devices. In this exciting context, I would like to share insights into designing and developing a scalable, multifunctional neuromorphic device based on monolayer MoS2 grown by chemical vapour deposition, with a particular focus on defect engineering. I will explain how this system exhibits neuromorphic behavior, particularly its ability to emulate synaptic plasticity—an essential feature of biological neural networks. This remarkable capability allows the system to perform complex cognitive tasks even in challenging environments. The fusion of material science and neuromorphic computing marks the beginning of a new and exciting era in electronics. Additionally, I will briefly discuss recent advancements in gas sensor technologies as well.

KN-028

Modulating Physical Properties and Enhancing stability of Catanionic Vesicles Using Fatty Acid Additives

Wen-Ching Lee, Hsiu-Ju Chang, Sonali Mondal, Chien-Hsiang Chang*

Department of Chemical Engineering, National Cheng Kung University, Tainan 701, Taiwan

***Corresponding author e-mail:** changch@mail.ncku.edu.tw

ABSTRACT

Ion pair amphiphiles prepared from mixed cationic/anionic surfactants can form catanionic vesicles with a bilayer structure in an aqueous phase through a forced formation process, and can be used for drug delivery. However, the prepared catanionic vesicles are not thermodynamically stable systems. Therefore, methods such as using the repulsion effect provided by charge additives and adjusting the bilayer rigidity by introducing bilayer stabilizers are commonly used to prepare catanionic vesicles. This study utilizes the advantages of fatty acids in regulating bilayer rigidity and imparting charge properties to vesicles as additives to regulate the formation and stability of catanionic vesicles. Specifically, ion pair amphiphiles were used as raw materials, and fatty acids with different structures were selected as additives to prepare catanionic vesicles. To investigate the role of fatty acid structure in regulating vesicular properties, this study explored the effects of fatty acid addition on the formation and stability of catanionic vesicles by analyzing vesicle size, zeta potential, stability, and bilayer rigidity. The results show that adding fatty acids as additives can prepare highly stable vesicles, which will promote the application of catanionic vesicles.

Layered Boron Nitride and its III-Nitride Heterostructures

Suresh Sundaram[1,2,3]*, Phuong Vuong[1,2,3], May Tran Thi[2], Ali Kassem[2], Ashuthosh Srivastava[1,2,3], Tarik Moudakir[4], Simon Gautier[4], Paul L. Voss[1,2], Jean Paul Salvestrini[1,2,3], Abdallah Ougazzaden[1,2].

[1]*Georgia Institute of Technology, School of Electrical and Computer Engineering, GT Europe, 57070 Metz, France.*

[2]*CNRS, IRL 2958, G T - CNRS, 2 rue Marconi, 57070 Metz, France.*

[3] *GT Europe, 2 rue Marconi, 57070 Metz, France.*

[4] *Institut Lafayette, 2 rue Marconi, 57070 Metz, France.*

***Corresponding author e-mail:** ssundara@georgiatech-metz.fr

ABSTRACT

Two dimensional (2D) materials have recently attracted lots of interest as it offers exotic functionalities and dramatic performances. Specifically, h-BN, a 2D futuristic wide bandgap nitride semiconductor has several advantages, one of them being that it can be grown in the same MOVPE reactor as other III- nitrides, leading to facile integration in the III-nitride device structures in active regions avoiding contamination and reproduciblity issues [1, 2, 3]. Here we report, MOVPE van der Waals eptaxial growth of h-BN and successful demonstration of its integration with other III-nitride devices. This material growth by MOVPE has been successfully scaled up to 6" diameter [4]. Further, we present the characteristics of the light emitting diodes grown on h-BN/sapphire which can be lifted off from the sapphire susbtrates,preserving the phyical properties of the device structures and transfered to any arbitrary templates. Vertical integration of these LEDs on BN grown by van der Waals epitaxy with red color LEDs grown on graphene by remote epitaxy for realization of full color micro-LEDs display will be discussed [1]. Controllable growth of this 2D materials on dielectric patterned substrates leading to selective area growth of III-nitride based device arrays has been employed for realizing transferrable and individually-addressable micro-LEDs with smooth side walls [5]. In-addition, we will discuss its integration with UVLEDs structures as active layers. These growth experiments on scaling up and heterointegration gives a very important insight on the possible commercialization of use of 2D materials integration in novel device structures, especially h-BN which will be discussed as a path forward to solve the critical issues in free standing/indivually addressable, thin flexible LEDs and other novel device structures.

References:

1. J. Shin, H. Kim, S. Sundaram, et. al., *Nature*, 2023, 614, 81-87.
2. Han et al., Science, 2024, 384, 312–317.
3. Kang et al., Nature Materials, 2023, 22, 1470–1477.
4. P.Vuong, T. Moudakir, R. Gujrati, et. al., *Adv. Mater. Technol.,* 2023, 2300600, 1–7.
5. R. Gujrati, A. Srivastava, P. Vuong, et. al., Adv. Mater. Technol., 2023, 2300147, 1–10

KN-032

Designing Greener Energy Conversion System for A Sustainable Future

Tharamani C. Nagaiah

Department of Chemistry, IIT Ropar, Rupnagar, Punjab-140 001

***Corresponding author e-mail:** tharamani@iitrpr.ac.in

ABSTRACT

Global energy requirements are touching new meridians with the gradual advancement in the living standards and the day-by-day growing world population. This necessitates the exploration to seek for greener and sustainable energy reservoir systems which ought to be environmentally agreeable for such an intriguing purpose. Electrochemical energy conversion and storage devices offer some most alluring aptitudes for providing clean energy. To name a few of these include fuel cells, rechargeable metal-air/peroxide batteries and HCl/ H2S electrolysis and likewise.[1,2] Oxygen being central to the processes in these devices, a lot of attention has been focused upon the study of oxygen chemistry in terms of oxygen reduction reaction (ORR) and also Hydrogen evolution reaction (HER) and thence to the melioration of the associated electrocatalysts. In the past decade research has depicted tremendous improvement towards the betterment of fuel cells/Zn based batteries/hydrogen production in its legions of shortcomings or corrigible features.[3,4] But still an infinite pursuit towards the exploration of effective, sturdy and energy efficient catalysts continues. The talk addresses,

• several strategies pursued to replace noble-metal free electrocatalysts for ORR/HER.

• Zn based battereis

• visualization of local electrocatalyic activity by SECM.

Keywords: ORR, HER, electrocatalyst, Zn based batteries, SECM

References

1. M. Zhang et al., Energy Environ. Sci., 2020, 13, 119–126.
2. M. Kumar and C. Nagaiah Tharamani, J. Mater. Chem. A, 2022, 10, 7048–7057.
3. S. Mehta et al., Adv. Energy Mater., 2024, 14, 2401515.
4. M. Kumar and C. Nagaiah Tharamani, Energy Storage Mater., 2022, 49, 390–400.

Impact of Carbon Doping and Device Structure on the X-ray Response of GaN Detectors

Toru Aoki[1], Kagemitsu Inaba[1], Tomoya Imakawa[1], Katsuyuki Takagi[1], Hiroki Kase[1], Fumimasa Horikiri[2], Hyun-Jar Lee[3], Joung-Hun Shin[1,3]

[1]*Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan*

[2] *Research Center of Ion Beam Technology, Housei University, Tokyo, Japan*

[3]*BTOZ, Republic of Korea*

***Corresponding author e-mail:** aoki.toru@shizuoka.ac.jp

ABSTRACT

Gallium nitride (GaN) has attracted increasing attention as a promising semiconductor material for low-energy X-ray detection owing to its wide bandgap, high radiation tolerance, and favorable attenuation characteristics in the mammography energy range. In this study, the fundamental detector properties of GaN-based X-ray detectors were systematically evaluated with a particular focus on the influence of carbon doping and device structure.

Two types of carbon-doped semi-insulating GaN (GaN:C) detectors with different carbon concentrations were fabricated in a metal–semiconductor–metal configuration. Their fundamental electrical and X-ray response characteristics were evaluated. Current–voltage measurements demonstrated that higher carbon doping effectively suppresses leakage current, achieving resistivities on the order of 10^{14} Ω·cm, comparable to or exceeding those of conventional direct-conversion detector materials. Under X-ray irradiation (40 kVp), both GaN:C devices exhibited clear photocurrent responses proportional to dose rate, confirming direct-conversion operation. However, pronounced differences in temporal response were observed: detectors with lower carbon concentration showed extremely slow transient responses, exceeding 10^3 s, attributed to carrier trapping by carbon-related deep levels.

To overcome these limitations, pin-type GaN detectors with well-defined intrinsic layers-designed to suppress deep-level trapping-were also investigated. Electrical and capacitance–voltage measurements confirmed stable depletion behavior, while X-ray response measurements demonstrated faster and more stable signal formation compared with GaN:C devices. These results indicate that defect control and appropriate device architecture are critical for achieving practical response speed in GaN-based X-ray detectors.

The present study demonstrates the trade-off between high resistivity and temporal response in carbon-doped GaN and highlights the advantages of pin-type GaN structures. The findings provide important design guidelines for developing next-generation low-energy X-ray detectors targeting high spatial resolution and low-dose imaging applications.

Keywords: X-ray detector, GaN, doping, device structure

References:

1. L. Zhow, X. Lu, J. Wu, H. Jiang, L. Chen, X. Ouyang, and K. M. Lau, IEEE. Electron Dvice. Lett., **40** (2019) 1044

KN-034

Broadband miniaturized spectrometers with van der Waals junctions

Lipsanen Harri*[1]

[1]Department of Electronics and Nanoengineering, Aalto University, FIN-02150 Espoo, Finland

*Corresponding author harri.lipsanen@aalto.fi

ABSTRACT

Miniaturized spectrometers are crucial for applications in on-chip and implantable devices, requiring high spectral resolution in limited spaces. Here, we present our van der Waals heterojunction-based spectrometers that achieve tunable spectral responses through band structure engineering, offering sub-nanometer wavelength resolution and a broad operational bandwidth of ~500 to 1600 nanometers.[1-3]

References:

1. H.H. Yoon, H.A. Fernandez, F. Nigmatulin, W. Cai, Z. Yang, H. Cui, F. Ahmed, X. Cui, M.G. Uddin, E.D. Minot, H. Lipsanen, K. Kim, P. Hakonen, T. Hasan, Z. Sun, Science, 378 (2022), P.296-299.
2. M.G. Uddin, S. Das, A.M. Shafi, L Wang, X. Cui, F. Nigmatulin, F. Ahmed, A.C. Liapis, W. Cai, Z. Yang, H. Lipsanen, T. Hasan, H.H. Yoon, Z. Sun, Nat. Commun., 15 (2024), p. 571.
3. Xiaoqi Cui, Fedor Nigmatulin, Lei Wang, Igor Reduto, Andreas C. Liapis, Mingde Du, Md Gius Uddin, Shafi Mayeen Abde, Faisal Ahmed, Yi Zhang, Hoon Hahn Yoon, Harri Lipsanen, Seppo Honkanen, Timo Aalto, Zongyin Yang, Tawfique Hasan, Weiwei Cai and Zhipei Sun, "Miniaturized Optical Spectroscopy with a Tunable Optoelectronic Interface", Science Advances 11, eado6886 (2025).

Live Cell Imaging and Cell Stimulations with Direct Electron-Beam Excitation Assisted Microscoopy

Yoshimasa Kawata[1,2]*, Yu Masuda[2], Maciej Kretkowski[2]*, Wataru Inami[1,2]

[1]*Research Institute of Electronics, Shizuoka University, Hamamatsu 432-8561, Japan*

[2]*Faculty of Engineering, Shizuoka University, Hamamatsu 432-8561, Japan*

***Corresponding author e-mail:** kawata@shizuoka.ac.jp

ABSTRACT

Nanoimaging techniques capable of visualizing dynamic specimens in aqueous environments are in high demand in the life sciences, as they enable detailed investigation of molecular interactions and functional mechanisms within living cells. To address this need, we have developed a Direct Electron-Beam Excitation Assisted Optical (D-EXA) microscope, which achieves lateral spatial resolution on the order of several tens of nanometers in liquid environments. Figure 1(a) shows the basic configuration of D-EXA and Fig. 1(b) shows the high spatial resolution translation stage with piezo system[1,2]. The D-EXA system integrates a scanning electron microscope with an optical fluorescence microscope, allowing for high-resolution imaging under diverse conditions, including ambient air and aqueous solutions. We also present a novel method for targeted cellular stimulation using a focused electron beam to probe subcellular functions in living cells. We demonstrated that electron beam stimulation induces intracellular Ca^{2+} elevation in neuronal cells, suggesting the feasibility of precise functional modulation.

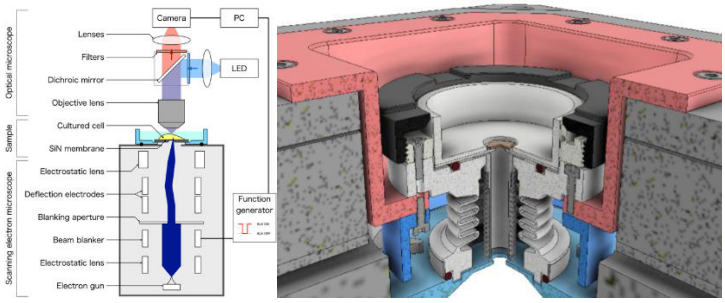


Fig. 1 (a) Basic configuration of D-EXA microscope, (b) high spatial resolution translation stage with piezo system

Keywords: Bio imaging, optical microscopy, scanning electron microscopy, calcium ion

References:

1. K. Hosomi, W. Inami, and Y. Kawata, Jpn. J. Appl. Phys. 64 062005 (2025).
2. K. P. Khakurel, K. Hosomi, et al, J. Appl. Cryst. 57, 1907–1912 (2024).

KN-036

Tetrapods based Advanced Materials for Advanced Technologies

Yogendra Kumar Mishra*

Professor Mads Clausen Institute, NanoSYD, Smart Materials

University of Southern Denmark, Alsion 2, 6400, Sønderborg, DENMARK

***Corresponding author e-mail:** mishra@mci.sdu.dk

ABSTRACT

Considering the size dependent utilization complexities of nanoscopic dimensions tin real technologies, the focus of nanomaterials community is converging to three-dimensional (3D) smart nanomaterials which are built out of interconnected nanostructures building blocks. This talk will briefly introduce the importance of tetrapod nanostructures towards smart 3D ceramic nanostructuring via a simple and single step flame-based approach for synthesis of zinc oxide tetrapods. These ceramic tetrapods have already demonstrated their potential roles in many different technologies. These zinc oxide tetrapods can be used as solid backbone or sacrificial templates to design hybrid or new tetrapods as smart materials. These smart 3D nanomaterials offer many applications in engineering and advanced technologies. Application examples of 3D ceramic tetrapods in nanosensing, optical sensing, whispering gallery mode resonances, light trapping and guiding, composite engineering, antiviral candidates, water purification, piezotronics, agriculture, and in several other applications will be demonstrated [1-10]. The integration of tetrapods in electrospun fibers offer many advantages in biomedical engineering and few examples about nano-engineered electrospun fibers will be presented as recent developments.

Keywords: Zinc Oxide Tetrapods, Smart Materials, Advanced Technologies

References:

1. Small 21, 2408414, **2025**
2. Materials Today Electronics 8, 100102, **2024**
3. Chemical Engineering Journal 462, 141984, **2023**
4. Progress in Materials Science 139, 101169, 2023
5. Progress in Polymer Science 101516, **2022**
6. Materials Today 50, 533-569, **2021**
7. Materials Today 48, 7-17, **2021**
8. Advanced Functional Materials 31, 20007555, **2021**
9. Materials Today 32, 108 -130, **2020**
10. Materials Today 6, 631-651, **2018**

An Innovative Printed Device for Sensing of Exhaled Gas

Naveen Balaji[1,2], Dieu Linh Nguyen[1,3], Delli Babu[2] Thi Thu Vu[3], Jean-Christophe Lourme[4], Caroline Abreu[1], Sumangala T.P. [2], Benoît Piro*[1]

[1] *ITODYS, CNRS, Université Paris Cité, 75006 Paris, France*

[2] *Department of Physics, School of Advanced Sciences, Vellore Institute of Technology Vellore, Tamil Nadu, India - 632014*

[3] *University of Science and Technology of Hanoi, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, 100000 Hanoi, Vietnam.*

[4] *ValoTec, 1 mail du Professeur Georges Mathé, 94800 Villejuif, France*

***Corresponding author e-mail:** piro@u-paris.fr

ABSTRACT

Small Intestinal Bacterial Overgrowth (SIBO) and other food-related intolerances are increasingly diagnosed using breath tests that quantify hydrogen (H_2) and methane (CH_4) produced by bacterial fermentation. Although widely used in medical practice, current breath analysers exhibit significant limitations. Many systems cannot detect multiple gases simultaneously, some rely on reusable mouthpieces incorporating sensors that raise hygiene concerns, and others require large exhaled volumes due to remote sensor placement, making testing challenging for children and elderly patients. These constraints highlight the need for compact, low-cost, and highly sensitive sensing platforms suitable for point-of-care diagnostics.

In this work, we propose a fully printed gas sensor based on an original organic field-effect transistor (OFET) architecture functionalized with catalytic nanomaterials for hydrogen detection at room temperature. While conventional resistive gas sensors operate through changes in material resistivity upon gas exposure, transistor-based sensors offer intrinsic signal amplification via modulation of charge transport within the semiconducting channel. This architecture enables enhanced sensitivity while maintaining low power operation.

We demonstrate that the transistor configuration improves hydrogen sensitivity by approximately one order of magnitude compared to an equivalent resistive sensor fabricated from the same active material. Importantly, the device operates at room temperature, eliminating the need for integrated heaters and significantly reducing power consumption. The fully printed design further supports scalable and low-cost manufacturing, with the potential for disposable implementations to address hygiene requirements in clinical settings.

Overall, this work establishes organic transistor-based sensing as a promising strategy for next-generation breath analyzers, combining sensitivity, low power consumption, and patient-friendly design. The proposed approach opens new perspectives for reliable, non-invasive screening tools targeting SIBO and other gastrointestinal disorders.

KN-039

Improved Thermoelectric Figure of Merit in Cu_2Se Material

Ramesh Chandra Mallik

Thermoelectric Materials and Devices Laboratory, Department of Physics, Indian Institute of Science, Bangalore, India-560012

ABSTRACT

Copper Selenide (Cu_2Se) is recognised as a phonon liquid electron crystal (PLEC) material demonstrating excellent thermoelectric properties. This system has a crystal structure transition from monoclinic to cubic above 400 K. However, it is required to optimise it further for a device application. Here, we tune it by first introducing Cu deficiency with Te substitution and then double-substituting it with Gd and Te. Room-temperature and high-temperature X-ray diffraction have been performed to analyse the lattice evolution with temperature. We employed high-resolution transmission electron microscopy (HRTEM) to reveal the atomic-scale features for both Cu-deficient and Te-substituted Cu_2Se and Gd-Te double-substituted Cu_2Se. We carefully analysed the electron and phonon decoupling with density functional theory calculations and transport properties measurements. Our work demonstrates an excellent figure of merit zT of 1.98 at 977 K for $Cu_{1.96}Se_{0.80}Te_{0.20}$ and zT of 2.02 at 977 K for $Cu_{1.97}Gd_{0.03}Se_{0.97}Te_{0.03}$ sample. The fabricated device modules show a power output of 52 mW for $Cu_{1.96}Se_{0.80}Te_{0.20}$ and 83 mW for $Cu_{1.97}Gd_{0.03}Se_{0.97}Te_{0.03}$ under a temperature gradient of 670 K.

Reference:

1. R. Saini et al., J. Mater. Chem. C, 2025, 13, 18690–18701.

KN-040

Dimension Controlled Ferroelectricity and Bulk Photovoltaic Effect in $CsPbBr_3$ Perovskite Nanocrystals

Somobrata Acharya

School of Applied & Interdisciplinary Sciences

Indian Association for the Cultivation of Science

Jadavpur, Kolkata-700 032

*Corresponding author e-mail: camsa2@iacs.res.in

ABSTRACT

Ferroelectric perovskite nanocrystals with both spontaneous polarization and visible light absorption are promising candidates for designing ferroelectric photovoltaic applications (1). Here we report on the ferroelectricity in the dimension controlled $CsPbBr_3$ nanocrystals. We show that the key ferroelectric parameters change with the dimensions of $CsPbBr_3$ nanocrystals. Furthermore, we show that $CsPbBr_3$, exhibits a ferroelectricity-driven photovoltaic effect under visible light in the absence of an external electric field. Pristine three-dimensional $CsPbBr_3$ nanocrystals exhibit intrinsic ferroelectric key properties with a notable saturated polarization of ~0.15 μC/cm2 and a high Curie temperature of 462 K, driven by the stereochemical activity of the Pb (II) lone pair (2). Furthermore, application of an external electric field allows the photovoltaic effect to be enhanced and the spontaneous polarization to be switched with the direction of the electric field. $CsPbBr_3$ nanocrystals exhibit a robust fatigue performance and a prolonged photoresponse under continuous illumination in the absence of an external electric field. These findings establish all-inorganic halide perovskite nanocrystals as potential candidates for designing photoferroelectric devices by coupling optical functionalities and ferroelectric responses.

References:

1. Yang, S. Y.; Seidel, J.; Byrnes, S. J.; Shafer, P.; Yang, C.-H.; Rossell, M. D.; Yu, P.; Chu, Y.-H.; Scott, J. F.; Ager, J. W.; Martin, L. W.; Ramesh, R.* Nat. Nanotechnol. 2010, 5 (2), 143−147.
2. Ghosh, A.; Paul, S.; Das, M; Sarkar, P. K.; Bhardwaj, P.; Sheet, G.; Das, S.; Kalimuddin, S.; Datta, A; Acharya, S.* ACS Nano 2024, 18, 23310-23319.

KN-041

Functionalized Carbon-based Materials for Rechargeable Zinc-Air Batteries

M. Sathish

Scientist-F, Electrochemical Power Sources Division,

CSIR-Central Electrochemical Research Institute, Karaikudi -630 003, Tamilnadu, INDIA

***Corresponding author e-mail:** marappan.sathish@gmail.com; msathish.cecri@csir.res.in

ABSTRACT

The transition toward sustainable energy technologies demand electrochemical storage systems that are simultaneously high-energy-density, safe, and economically viable. Metal–air batteries have emerged as promising next-generation energy storage systems owing to their high theoretical energy density, environmental compatibility, and potential for sustainable energy applications [1]. Among them, zinc–air batteries (ZABs) have attracted significant attention due to the natural abundance, safety, and low cost of zinc. However, the practical deployment of rechargeable ZABs is largely limited by sluggish oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) kinetics at the air cathode, necessitating the development of highly active and durable bifunctional electrocatalysts [2]. Here, we present recent advances in carbon-based electrocatalysts for high-performance zinc–air batteries, with particular emphasis on rationally designed heterostructured catalytic systems aimed at overcoming these kinetic limitations. By integrating transition-metal active centres within electronically conductive carbon frameworks, we develop catalytic architectures that simultaneously enhance activity, stability, and mass transport. Two complementary catalyst strategies will be highlighted. First, a layered double hydroxide (LDH) supported over a MOF-derived carbon hybrid catalyst is developed to create highly accessible active sites and improved charge transfer pathways for enhanced bifunctional oxygen electrocatalysis [3]. Second, an ionic-liquid-derived dual-phase carbon support system incorporating cobalt species within a ternary heteroatom-doped carbon framework (B, N, F) is engineered to stabilize active centres and promote synergistic catalytic activity. The unique biphasic carbon architecture effectively anchors metal nanoparticles, suppresses agglomeration, and enhances catalytic durability during prolonged battery operation [4]. These engineered catalysts demonstrate remarkable bifunctional oxygen electrocatalysis and deliver promising performance in rechargeable zinc–air batteries. Beyond device performance, the work provides mechanistic insights into the structure–activity relationships governing oxygen electrocatalysis, offering guiding principles for the next generation of cost-effective air cathode materials for advanced metal–air energy systems.

References

1. Zhou, Y., Mao, Y., Chang, M., Wang, Z., Xie, W., Ye, C., & Waterhouse, G. I. Adv. Funct. Mater., 2026, e19133.
2. Tu, W. B., Song, L. N., Liang, S., Wang, Y., Sun, Y., Wang, H. F., & Xu, J. J. Adv. Energy Mater., 2025, 15(24), 2404946.
3. Allwyn, N., Gokulnath, S., & Sathish, M. ACS Appl. Mater. Interfaces, 2024, 16(16), 20360.
4. Allwyn, N., Chandran, M. K. N., Maithreyan, V., Shalom, M. A., & Sathish, M. J. Mater. Chem. A, 2025, 13(19), 13935.

KN-042

Supramolecular Assembly of Donor-Acceptor (Macro)Molecular Systems for Low-Power Energy Harvesting

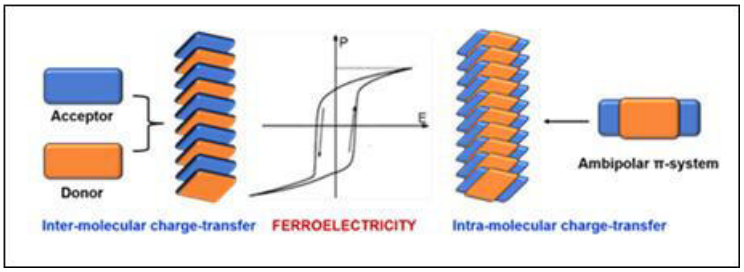
Anurag Mukherjee,[1] Shubhankar Barman,[1] Swadesh Paul,[2] Supriya Bandyopadhyay,[1] Anuja Datta, * [1, 2] and Suhrit Ghosh*[1]

[1]*School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Kolkata, India-700032,*

[2]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, India-603203)*

ABSTRACT

Electroactive materials (ferroelectric and piezoelectric) are of great value for sensors, photonics, energy-efficient memories, and other applications. Organic soft-ferroelectrics are of emerging interest as they promise to offer distinct advantages for robust, lightweight, inexpensive, easily processed, environment-friendly devices.[1] We have recently introduced supramolecular polymers/ foldable polymers of donor-acceptor charge-transfer complexes, [2-4] intrinsically polarizable ambipolar chromophoric systems, [5-6] and chromophore-appended helical polymer [7] exhibiting excellent FE-property at ambient temperatures. By definition, all FE-materials exhibit piezoelectricity, suitable for PE micropower energy harvesting from electromechanical behaviour. We have recently shown prominent piezoelectricity in chiral supramolecular polymers of ambipolar π-systems with adequate understanding about structural effects.[8] This presentation will highlight our recent work in this area [9] with particular emphasis on the impact of the molecular structure, supramolecular assembly with long range order and chirality on ferroelectricity/ piezoelectricity of purely organic donor-acceptor systems.



References

1. C. Park et al., *Adv. Mater.*, 2020, e2004999.
2. S. Barman et al., *Chem. Commun.*, 2022, **58**, 10508.
3. A. Mukherjee et al., *Angew. Chem. Int. Ed.*, 2022, e202203817.
4. S. Bandyopadhyay et al., *ACS Macro Lett.*, 2026, D5CC06572K.
5. A. Mukherjee et al., *Chem. Sci.*, 2022, **13**, 781.
6. S. Barman et al., *J. Phys. Chem. C*, 2023, **127**, 7852.
7. S. Bandyopadhyay et al., *Chem. Commun.*, 2025, **61**, 937.
8. S. Paul et al., *Chem. Mater.*, 2023, **35**, 6463.
9. S. Barman et al., *Chem. Eur. J.*, 2023, e202303120.

KN-043

Crystal-Engineered MOFs and Interfacial Chemistry for Next-Generation Ammonium-Ion Sustainable Energy Storage Devices

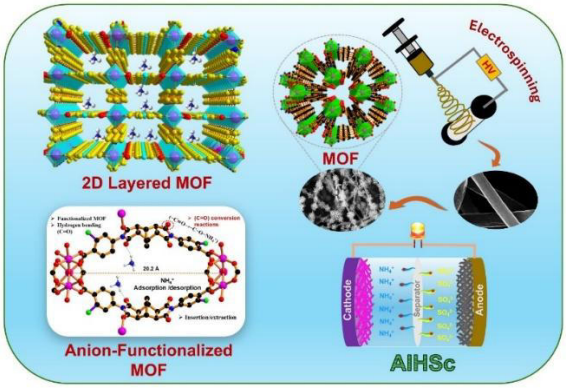
Nissar Hussain, Zahir Abbas and Shaikh M. Mobin*

Department of Chemistry, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore 453552, India.

***Corresponding athor e-mail:** xray@iiti.ac.in

ABSTRACT

Ammonium ions (NH_4^+) are emerging as a compelling alternative to conventional alkali-metal charge carriers for sustainable electrochemical energy storage, owing to their natural abundance, environmental benignity, and distinctive hydrogen-bonding interactions with host frameworks. Unlocking their full potential demands the development of advanced electrode architectures with precisely defined crystallographic frameworks, tailored surface functionalities, and highly accessible ion-transport pathways to address intrinsic limitations in diffusion kinetics and cycling stability. The rational design of such electrodes begins with crystal engineering of redox-active metal–organic frameworks (MOFs) to produce ordered porous architectures with high stability, uniform and size-matched ion channels, and densely populated electrochemically active sites for reversible NH_4^+ intercalation.[1-2] To address the challenge of electrical conductivity, MOFs are integrated with conductive scaffolds, particularly MXene-derived carbonized nanofibers, yielding hierarchical heterostructures that combine high surface area with interconnected ion–electron pathways (Scheme1).[3] Such hybridization not only accelerates charge propagation but also provides mechanical robustness and structural integrity during prolonged cycling. These strategies establish a generalizable blueprint for the targeted synthesis of next-generation green energy storage devices, positioning ammonium-ion systems as safe, cost-effective, and environmentally sustainable alternatives to conventional alkali-ion technologies.



Scheme 1

References:

1. Sun, Y.; Yin, B.; Yang, J.; Ding, Y.; Li, M.; Li, H.; Li, J.; Jia, B.; Zhang, S.; Ma, T. Energy Environ. Sci. 2023, 16, 5568.
2. Gao, M.; Wang, Z.; Liu, Z.; Huang, Y.; Wang, F.; Wang, M.; Yang, S.; Li, J.; Liu, J.; Qi, H.; Zhang, P.; Lu, X.; Feng, X. Adv. Mater. 2023, 35, 2305575.
3. Hussain, N. and Shaikh, M. M. Chem. Sci. 2025, 16, 8460.

KN-046

Nanostructured Carbons for Bottling and Utilizing Sunlight for Sustainable Energy and Environemental Applications

Chandramouli Subramaniam

Department of Chemistry & Centre for Defence Technologies Innovations and Strategies, Indian Institute of Technology Bombay

ABSTRACT

The total volume of water on earth is constant at 10^{21} liters. India has 4% of the global fresh-water resources with ~20% of the global population. Therefore, majority of Indian sub-continent is suffering from acute water stress. Equitable access to clean potable water is both a direct, important target of United National Sustainable Development Goals (SDG 6) and simultaneously carries significance to several other SDGs (SDG 3,7,13,15). Therefore, sustainable, cost-effective and affordable recovery of freshwater from contaminated water feedstock is the need of the hour to ensure it equitable access. Solar-thermal interfacial evaporation offers immense and hitherto untapped potential for energy-efficient, sustainable freshwater production. However, fundamental challenges in materials and system-design result in low water evaporation rates (Rw < 1-2 $kgm^{-2}h^{-1}$) and even lower solar-freshwater productivity (SWP). Further, the lack of thermally and chemically stable materials that can operate in extreme salinities such as seawater without fouling or degrading is a major bottleneck that limits the wider adaptation of the technology. This talk would describe an ultra-thin, porosity-engineered polymeric scaffold (poly-HIPE, PH) that is anisotropically coated with nanostructured carbon florets (NCF) to deliver high solar-thermal conversion efficiency (η-STC = 84%), excellent Rw (6.5 $kgm^{-2}h^{-1}$) and exceptional SWP (3.5 $Lm^{-2}h^{-1}$) from sea-water. A few salient features of the material are

(a) Thinnest such membrane with no-signs of fouling over 30 days in sea-water, achieving
(b) Salt-rejection of ~95% with facile reusability for over 30 days,
(c) Producing freshwater of ~20 liters per m^2 area per day at
(d) Lowest CO_2 footprint (< 3 W/L, ~3 g /L)

Fundamental insights of materials-design to address the exothermic water-evaporation step that are synergized with systems-design approaches to achieve these key performance indices would be discussed in the talk.

References

1. Adv. Energy Mater., 2021, 11, 2003626
2. Small, 2020, 16, 1903334 ACS Appl. Mater. Interfaces, 2022, 14, 13271
3. ACS Sus. Chem. Eng. 2021, 9, 7792
4. ACS Appl. Mater. Interfaces, 2020, 12, 42669
5. ACS Appl. Nano Mater. 2019, 3, 468
6. Chem. Eng. J., 2024, 500, 156617
7. ACS Sustainable Chem. Eng., 2024, 12, 14638.
8. npj clean water, 2023, 6, 75
9. ACS Appl. Mater. Interface, 2023, 15, 43810

KN-047

Optical Laser Ceramics Y_2O_3 Doped with Tm^{3+}, Ho^{3+} for Solid-State Lasers in the Two-Micron Spectral Range

Ryabochkina P.A.[1], Ariskin A.O.[1], Alekseeva A.S.[1], Balashov V.V.[2],
Maksimov R. N.[3], Osipov V.V[3]

[1-]*National Research Mordovia State University, Russia*

[2-]*Fryazino branch of V.A. Kotelnikov Institute of Radio Engineering and Electronics. Russian Academy of Sciences, Russia*

[3-]*Institute of Electrophysics of the Ural Branch of the Russian Academy of Sciences, Russia*

ABSTRACT

Cubic sesquioxide crystals (Y_2O_3, Lu_2O_3, Sc_2O_3) doped with Tm^{3+}, Ho^{3+} ions are characterized by high peak absorption cross-sections and high thermal conductivity making them attractive for active media in two-micron solid-state lasers. However, due to their high melting temperatures (~2400 °C), there are limitations in growing large-sized single crystals of these materials. In this regard, RE-doped sesquioxide laser ceramics have been actively used as an alternative for solid-state laser gain media in recent years [1-4]. This paper presents the results of a study of the spectral and luminescent characteristics of Tm^{3+} and Ho^{3+} ions in Y_2O_3:Tm and Y_2O_3:Ho optical laser ceramics. A comparative analysis is performed with similar characteristics for $Y_3Al_5O_{12}$:Ho and $Y_3Al_5O_{12}$:Tm ceramics. The nonradiative energy transfer processes from the $^3H_4$ level of Tm^{3+} ions to the $^5I_7$ level of Ho^{3+} ions upon excitation of the $^3H_4$ level of Tm^{3+} ions in Y_2O_3:Tm,Ho ceramics are investigated. The structure and spectral and luminescent characteristics of Y_2O_3:Tm and Y_2O_3:Ho nanopowders obtained by coprecipitation and microwave-assisted hydrothermal synthesis, which serve as the initial precursors for producing optical laser ceramics, are also studied. This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation, Grant No. FZRS-2025-0001.

References:

1. P.A. Ryabochkina, A.N. Chabushkin, Yu.L. Kopylov, V.V. Balashov and K.V. Lopukhin. Two-micron lasing in diode-pumped Y_2O_3:Tm ceramics. Quantum Electronic. Vol. 46. P. 597–600. 2016.
2. Artemov S.A, Balashov V.V., Chabushkin A.N., Dmitriev O.A., Khrushchalina S.A., Kopylov, Larina, N.A, Lyapin A.A., Ryabochkina P.A., Volkova T.V., Zakharov N.G. Nonradiative energy transfer of electronic excitation between Tm^{3+} ions in Y_2O_3:Tm laser ceramics// Optical Materials. Vol.101, №3, 2020.
3. Yue, Fangxin, Jambunathan, Venkatesan, David, Samuel Paul at. al. Diode-pumped master oscillator power amplifier system based on cryogenically cooled Tm:Y_2O_3 transparent ceramics// Optical Materials Express. 2021. DOI: 10.1364/OME.422603.

KN-048

Impact of Intermediate Diradical Character on Optical and Magnetic Properties in Croconaine Dyes

Takeshi Maeda*

Graduate School of Engineering, Osaka Metropolitan University, Sakai, Osaka 599-8531, Japan

***Corresponding author e-mail:** tmaeda@omu.ac.jp

ABSTRACT

Molecules with intermediate diradical character exhibit a unique electronic structure in which two electrons with antiparallel spins are not completely paired but are instead partially bonded in the ground state. This electronic state is associated with properties such as nonlinear optical responses and semiconducting behaviour, making these molecules attractive candidates for functional materials. In this study, we focus on short-wavelength infrared (SWIR)-absorbing croconaine dyes incorporating five-membered oxocarbon and chalcogenopyrylium skeletons.[1,2] These dyes exhibit intermediate diradical character, which contributes to their optical and magnetic properties. They show pronounced two-photon absorption in the SWIR region. This behaviour is related to the intermediate diradical character, which makes the electron distribution along the π-conjugated system more susceptible to distortion by the optical field generated by intense laser.[3] Furthermore, we examine the electron spin resonance (ESR) behaviour originating from unpaired electrons in the diradical structures and investigate how phase transitions in the solid state and molecular assembly structures influence the magnetic response.[4] This presentation discusses the relationship between molecular structure, intermediate diradical character, and optical and magnetic properties, and provides insights relevant to the design of optoelectronic and magnetic materials.



Figure. *Molecular structures and resonance forms of chalcogenopyrylium-based croconaine dyes with intermediate diradical character, and schematic illustrations of their one- and two-photon absorption in the SWIR region.*

References:

1. T. Maeda, T. Oka, D. Sakamaki, H. Fujiwara, N. Suzuki, S. Yagi, T. Konishi, K. Kamada, Chem. Sci., 2023, 14, 1978.
2. T. Oka, T. Maeda, D. Sakamaki, N. Suzuki, S. Yagi, S. Kodama, H. Fujiwara, Org. Chem. Front., 2025, Advance Article (doi: 10.1039/D4QO01722F).
3. Oka, T.; Maeda, T.; Sakamaki, D.; Fujiwara, H.; Suzuki, N.; Yagi, S.; Mauric, L.; Kamada, K. 2025, 13, 11970.
4. T. Maeda, K. Ono, T. Ohno, D. Sakamaki, H. Fujiwara, N. Suzuki, S, Kodama, S. Yagi, in preparation.

KN-049

Materials Development and Characterization for Redox Flow Technologies

Mathieu Etienne

LCPME, CNRS, Université de Lorraine, 54000, Nancy, FRANCE

***Corresponding author e-mail:** Mathieu.etienne@cnrs.fr

ABSTRACT

Redox flow technology is a broad concept that encompasses not only redox flow batteries but also related technologies for remediation, waste valorization and water electrolysis for the production of green hydrogen. Materials to be considered in the development of such technologies include soluble redox mediators, electrodes, membranes and catalysts.

This communication will highlight developments realized in material optimization, including electroanalytical methods that can be used for screening their reactivity.

Acknowledgment

This work was supported by a French government grant from the Agence Nationale de la Recherche (ANR) under the France 2030 program (references ANR-23-PEBA-0005 and ANR-22-PEBB-0005). The authors also acknowledge financial support from the REDHY project. This project has received funding from Clean Hydrogen Partnership Joint Undertaking under Grant Agreement No 101137893. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation programme, Hydrogen Europe and Hydrogen Europe Research.

Unraveling Interface Physics of Ferromagnet/Nonmagnet Heterostructures For Development of Efficient Spin Orbit Torque Applications

Dr. Indranil Sarkar

Institute of Nano Science and Technology, Mohali

Abstract

Interfaces of ferromagnet (FM)/nonmagnet (NM) presents a fascinating playground for realizing spin dynamics and spin transport phenomena that controls the underlying physics of spin orbit torque required for next generation low power and high efficiency MRAM applications. In this talk, I shall present our research work based on the quintessential FM/NM heterostructures namely, CoFeB/NM and CoFe/Ta for unraveling the underlying role of electronic and physical structure necessary for engineering the spin transfer characteristics and spin dynamic effects across these interfaces. Through this results we shall demonstrate the role of non-magnetic underlayer in tuning the lectronic structure of the ferromagnetic layer that controls spin transfer properties across the interface. Furthermore I shall present results on quantization induced thickness dependent oscillations in spintronic properties.

KN-051

Interaction between Universities and Industry: The Case of National Research Mordovia State University

Dr. ANATOLY LYSYAKOV

National Research Mordovia State University Russia

ABSTRACT

The study reflects successful project implementation experiences, from research to technology implementation in production. Models of interaction between the university and enterprises are analyzed. Particular attention is paid to the production of new materials both in Russia and internationally. The potential for collaboration with international companies is analyzed.

Characterization of Complex Dynamics in A Chain of Plasmonic Nanoparticles

Majid Taki

PhLAM, Université de Lille Sciences et Technologies −59655 Villeneuve d'Ascq cedex

ABSTRACT

We investigate theoretically and numerically the non-linear plasmonic behavior of finite unidimensional chains of silver nanoparticles (AgNPs) embedded in a silica matrix. The NPs have a diameter of 20nm for a period of 60nm, and are illuminated normally by a monochromatic pump of frequency close to the localized plasmon resonance. The non-linearity arises from Kerr susceptibility in the silver dielectric constant [1], and the optical response of the metal NPs is described in the dipolar approximation by their polarizability, including retardation corrections. Particles are coupled together through the homogeneous Green's tensor, which leads to a modified discrete Lugiato-Lefever equation describing a global non-local interaction where one AgNP interacts with all plasmonic nanoparticles. Several behaviors have been evidenced, as: modulational instability (figure (a)-ii), kinks, dark solitons, and oscillons [2]. However much less investigations have been carried out on the complex spatio-temporal dynamics (figure (b)-i).

In this work, we focus on the quantitative characterization of the spatio-temporal chaos as a function of the detuning and the intensity of the longitudinally-polarized beam, using a numerical method developed in [3]. Based on the calculation of the chaotic trajectories (i.e. the time evolution of each particle's dipole amplitude), Lyapunov spectra are computed as a function of the length of the chain, see figure (b), allowing to determine the Yorke-Kaplan dimension (figure (b), inset) and finally the correlation length characteristic of the spatio-temporal chaos [4]. We will show how our approach allows characterizing the stability of the complex dynamics and evidenced the occurrence of a turbulent regime in the plasmonic nanoparticles devices [5].

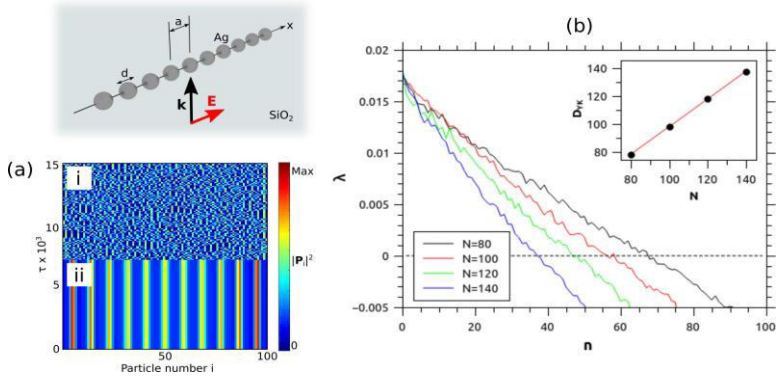


Figure: (a) Trajectories in case of modulational instability, (ii), and spatio-temporal chaos, (i); (b) Typical Lyapunov spectra and associated Yorke-Kaplan dimensions characterizing the fully developed spatio-temporal chaos (turbulence) appearing in the system for different lengths of chains (chaotic trajectories).

References

1. Drachev, V. P., Buin, A. K., Nakotte, H. & Shalaev, V. M. Size Dependent χ (3) for Conduction Electrons in Ag Nanoparticles. **Nano Lett. 4, 1535–1539 (2004).**
2. Noskov, R. E., Belov, P. A. & Kivshar, Y. S. Subwavelength Modulational Instability and Plasmon Oscillons in Nanoparticle Arrays. **Phys. Rev. Lett. 108, (2012).**
3. Clerc, M. G., Ferré, M. A., Coulibaly, S., Rojas, R. G. & Tlidi, M. Chimera-like states in an array of coupled-waveguide resonators. **Opt. Lett. 42, 2906 (2017).**
4. Investigating Route to Chaos in Nonlinear Plasmonic Dimer, Z. Ziani, G. Lévêque, S. Coulibaly, A. Taki, and A. Akjouj;
5. **Ann. Phys. (Berlin) 2020, 2000240**
6. Characterization of spatiotemporal chaos in arrays of nonlinear plasmonic nanoparticles, Z. Ziani, G. Lévêque, S. Coulibaly, M. Taki, and A. Akjoujy, **Phys. Rev. B 100, 165423 (2019)**

KN-053

Heteroepitaxial Structures and High Growth Rate of Semi-Insulating InP for Buried Heterostructure Quantum Cascade Lasers by Hydride Vapour Phase Epitaxy

Sebastian Lourdudoss[1]*, Manavaimaran Balaji[2], Axel Strömberg[1], Sakthivel Raja[3], Sridharan Moorthy Babu[4] and Yan-Ting Sun[1]

[1]*KTH-Royal Institute of Technology, Stockholm, Sweden*

[2]*University of Madras, Chennai, India*

[3]*SRM TRP Engineering College, Trichy, India*

[4]*Anna University, Chennai, India*

***Corresponding author e-mail:** slo@kth.se

ABSTRACT

Hydride vapour phase epitaxy (HVPE) has been exploited for growing a) potential heterostructures and b) buried heterostructures quantum cascade lasers (BH-QCL) through regrowth of semi-insulating (SI) InP:Fe. (a) include: (i) III-V on Si for light sources and tandem solar cells , (ii) quasi phase matched orientation patterned (OP) GaP on OP-GaAs - and OP-GaAsP on OP-GaAs structures for non-linear applications and (iii) GaP on Ga2O3 for heterojunction diode . b) Owing to the inherent large growth rate of HVPE, its short time regrowth of SI-InP:Fe is extensively exploited for realizing BH-QCL for high power - , large thermal dissipation , good beam quality and optical free space communication . In extreme cases where etched QCL mesa depths can reach down to 14 µm, the regrowth took place only in ~45 minutes and that too without mask encroachment and voids .

Keywords: HVPE, III-V on Si, GaP on Ga2O3, OP-GaP, Buried heterostructures, Quantum cascade lasers

References

1. Giriprasanth Omanakuttan et al., Optical Materials Express Vol. 10(7), pp. 1714-1723 (2020).
2. Chengru Wang et al., Journal of Applied Physics, Vol. 128, 055308 (2020).
3. Vladimir L. Tassev et al, Optical Materials Express, Vol. 6(5) 1724-1737 (2016).
4. Manavaimaran Balaji et al., Crystals, Vol. 13, 168 (2023).
5. Vladirmir L. Tassev et al., Journal of Crystal Growth Vol. 486, 155–161(2018)
6. Dhandapani Dhanabalan et al., Phys. Status Solidi A 2025, 2500234.
7. Wondwosen Metaferia et al., Optical Engineering, Vol. 53(8), 087104, 2014.
8. Zhixin Wang, Optics Express, Vol. 27(16), 22708 (2019).
9. G. M. de Naurois et al., AIP Advances 1, 032165 (2011).
10. J. H. Ryu et al., IEEE Photonics Journal 14(3), 1522706 (2022).
11. Mengyao Han, Journal of Lightwave Technology, 41(20), 6514-6520 (2023).
12. Wondwosen Metaferia et al., ECS Transactions, 64 (17) 61-68 (2014).

IT-001

Polarized Halide Perovskite Materials for Photoelectrochemical Water Splitting

Aravind Kumar Chandiran

ABSTRACT

Electric or magnetic polarization affects the properties of catalysts for enhancing the water splitting reaction. The enhancement arises because of multiple factors including the modification of bulk charge transport properties in the absorber, reduction in the barrier for catalytic reaction, and recombination properties. In this talk, the role of electric/magnetic polarization on these properties and their relationship to water splitting performance will be discussed.

Probing Magnetic Order and Spin–Charge–Lattice Coupling in van der Waals Magnets Using Femtosecond Time-Resolved Reflectivity

N. Kamaraju

Professor

Department of Physical Sciences,

Indian Institute of Science Education and Research (IISER) Kolkata

Abstract:

Understanding magnetic ordering and its coupling to electronic and lattice degrees of freedom is central to low-dimensional quantum magnetism. In this talk, I will present femtosecond time-resolved nondegenerate reflectivity studies of two van der Waals magnetic systems, $NiPS_3$ [1] and $CrSiTe_3$ [2]. In the antiferromagnet $NiPS_3$ [1], we investigate spin–orbit entangled excitons and reveal coupled excitonic and spin relaxation dynamics exhibiting strong temperature evolution across both the exciton dissociation and Néel transitions, including signatures of critical slowing down and persistent short- range magnetic correlations above magnetic ordering. In $CrSiTe_3$ [2], picosecond acoustic strain pulses generated by ultrafast excitation enable real-time probing of magnetic dimensional crossover through distinct modifications of carrier relaxation and spin–lattice coupling pathways. Together, these results demonstrate that ultrafast optical reflectivity provides a sensitive nonequilibrium probe of magnetic correlations and spin–charge–lattice interactions in layered quantum magnets.

References:

1. S. Sahu *et al.*, arXiv:2509.04900 (2025), under review.
2. A. Kumar *et al.*, *Phys. Rev. B* **111**, L140414 (2025).

IT-003

Excess Water Vapor Absorption and Structure Deformation of Cage-Structured Crystal $12CaO{\cdot}7Al_2O_3$

Naonori Sakamoto[1, 2, 3]*, Soma Ishibashi[2], Takuma Yonemura[2], Ryota Maruyama[2], Takahiko Kawaguchi[2], and Naoki Wakiya[1, 2, 3]

[1] *Research Institute of Electronics, Shizuoka University, 3-5-1 Johoku, Naka-ku, Hamamatsu-shi, 432-8561, Japan*

[2] *Department of Engineering, Graduate School of Integrated Science and Technology, Shizuoka University, 3-5-1 Johoku, Naka-ku, Hamamatsu-shi, 432-8561, Japan*

[3] *Graduate School of Science and Technology, Shizuoka University, 3-5-1 Johoku, Naka-ku, Hamamatsu-shi, 432-8561, Japan*

***Corresponding author e-mail:** sakamoto.naonori@shizuoka.ac.jp

ABSTRACT

$12CaO{\cdot}7Al_2O_3$ (abbreviated as C12A7) is composed of a positively charged cage framework structure and anions encapsulated within the cage. It has been reported that the oxygen ions in the cages can be replaced with other anionic species by appropriate treatment, and that various unique characteristics are exhibited depending on the anion species [1]. When C12A7 synthesized in air is heated in air, it loses weight in the range of 200 to 400°C [2]. This phenomenon is presumed to be due to a reaction with water vapor in the air, but the details are not clear, and the effect of this phenomenon on the physical properties of C12A7 is also not clear. In this study, we investigated the effect of this reaction on C12A7.

C12A7 powder without excess water vapor was first prepared by post annealing the C12A7 powder at 600 °C for 3 hours in an Ar atmosphere and cooled down to room temperature. The powder was then heat treated in a precisely controlled humidity atmosphere at a sample temperature of 220 °C for 3 to 24 hours. The amount of water vapor in the atmospheres was also varied from the saturated water vapor of 20 to 80 ºCs. The samples before and after absorption were evaluated by gravimetric measurements, XRD, and Raman scattering. XRD patterns of C12A7 synthesized in air and maintained at 220 °C in saturated water vapor at 80 °C showed no formation of impurity phase. Detailed observation of the XRD pattern showed that the original C12A7 peak shifted to the lower angle side with increasing the heating time. The peak shift to the low-angle side was confirmed for all of the C12A7 peaks, indicating that C12A7 has an increased lattice constant while maintaining its basic crystal symmetry. This result suggests that the reaction with water vapor is not due to simple surface adsorption but to inclusion in the cage. Similar water vapor absorption occurred in a deuterium oxide (D_2O) atmosphere, and it showed desorption of DHO molecules during heating up again at about 300 °C. This result shows an exchange of hydrogen ions occurring among the water vapor in the C12A7 crystals. This also implies that the C12A7 has a potential for high proton conductivity below 300 °C.

Keywords: cage structure; crystal structure; proton conduction; encapsulation; ubiquitous elements

References:

1. H. Hosono, Sci.Tech. adv. Master., 5, (2004), 409-416.
2. A. S. Tolkacheva et al, Russ. J. Inorg, 57, 2012, 1014-1018.

IT-004

Stability of Hydrogen-bonded Semiconductors for Organic Electronic Devices

Mihai Irimia-Vladu[1]

[1] *Johannes Kepler University Linz, Institute for Physical Chemistry, Linz Institute for Organic Solar Cells (LIOS), Linz, Austria.*

***Corresponding author e-mail:** mihai.irimia-vladu@jku.at

ABSTRACT

Nature represents an immense reservoir of inspiration for scientists looking to select materials that are biodegradable and biocompatible. In nature, many pigments are hydrogen-bonded small molecules as opposed to larger, van der Waals bonded synthetic molecules like pentacene, phthalocyanines or oligothiophenes. These molecules demonstrate H-bonding as well as π-stacking, producing highly-ordered thin films with crystalline textures unlike the typical herringbone pattern found in many molecular semiconductors. H-bonded, natural or nature-inspired semiconductor materials have been recently implemented in organic field effect transistors and inverter circuits, and afforded performances on par with state-of-the-art synthetic organic materials. Among the materials we have exploited are naturally-occurring indigo and Tyrian purple together with a large family of synthetically produced indigoids, anthraquinones and acridones. Most of these pigments are ambipolar semiconductors with balanced electron and hole mobilities in the range of 0.01 to 0.5 cm^2/Vs, coupled with air stability of both electron and hole channels. Field effect mobilities as high as 1.5 cm^2/Vs have been recorded in air stable epindolidione and Quinacridone. No degradation in OFET performance has been observed for samples stored and measured in air over a period exceeding 5 months. Nature inspires us to choose among a wide range of cheap and extensively available materials for creating new electronic functionalities, coming closer to a vision of a sustainable electronics world.

Tuning Multiferroic Properties in Y-Type Hexaferrite through Doping

A. K. Singh, G. Palai

Department of Physics and Astronomy, National Institute of Technology Rourkela, Odisha 769008, INDIA

***Corresponding author e-mail**: singhanil@nitrkl.ac.in

ABSTRACT

In the last few decades, multiferroic (MF) materials have attracted interesting attention due to their mutual control of electric and magnetic properties termed as magnetoelectric (ME) effect. This area of research is important in terms of potential technological applications such as spintronic devices, electronic devices, medical drug delivery, and ME sensors. Most MF materials exhibit high field control ME coupling below liquid nitrogen temperature, which is not appropriate for effective devices based on the ME effect. To realize useful devices based on the ME effect, a low-field control of the ME effect at room temperature (RT) is required. Direct measurement of ME coupling is not an easy task, as most MF materials are poor insulators. Hence, an alternative route to investigate ME coupling is to measure the influence of dielectric properties with the application of a magnetic field, termed the magnetodielectric (MD) effect. Interestingly, Y-type hexaferrite possesses a significantly low field control ME effect at RT, which has an advantage over several other single-phase MF materials. The Y-type $Ba_2Mg_2Fe_{12}O_{22}$ (BMF) hexaferrite has drawn significant attention recently due to its tunable magnetic and ME properties upon suitable substitution at magnetic and non-magnetic sites. This work investigates different synthesis routes, electrical, magnetic, and magnetodielectric coupling of pure BMF, its substituted samples, and BMF-based composites.

IT-006

High-Strength Poly(Vinyl Alcohol) Physical Eutectogels: Effects of Polymer Molecular Weight, DES Composition, and Heat Treatment

Ruei-Min Chuang[1], Trung Hieu Vo[1], Heng-Kwong Tsao[1,*], Yu-Jane Sheng[2]

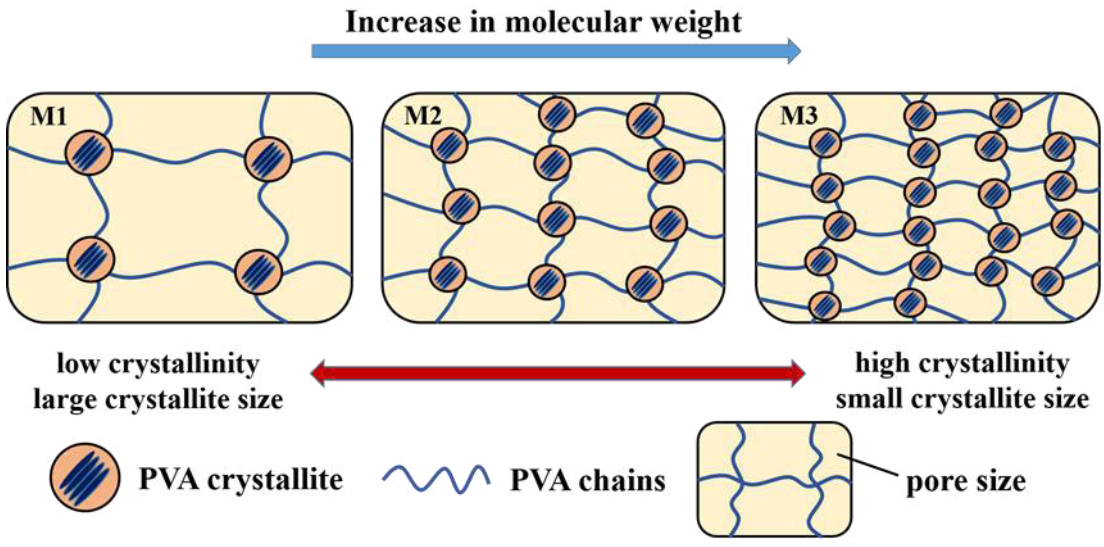
[1] *Department of Chemical and Materials Engineering, National Central University, Taoyuan 32001, Taiwan, ROC*

[2] *Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan, ROC*

***Corresponding author e-mail**: hktsao@cc.ncu.edu.tw

ABSTRACT

A one-step manufacturing process is employed to fabricate stretchable physical eutectogels. It involves directly mixing polyvinyl alcohol (PVA) with choline chloride as a hydrogen bond acceptor and either ethylene glycol or glycerol (Gly) as a hydrogen bond donor. This process results in the formation of numerous crystallite domains of PVA within the deep eutectic solvent (DES), which act as physical crosslinking points in the eutectogel. The study systematically investigates the effects of PVA molecular weight, DES composition, and various heat treatments on the mechanical properties of eutectogels. The stress-strain curves demonstrate that a higher PVA molecular weight, the addition of Gly to the DES, and repeated freeze-thaw cycles can enhance the mechanical properties of the PVA physical eutectogel. Finally, scanning electron microscopy and X-ray diffraction are used to examine and analyze the polymer networks and crystallite domains in terms of pore size, crystallinity, and crystallite domain size.



IT-007

Facile Synthesis of High-Performance CuS-Coated CuI Cathode for Seawater-Activated Magnesium Batteries

Vikum Premalal

Indian Institute of Technology Madras, Chennai

ABSTRACT

High-performance electrode materials for seawater-activated batteries are increasingly critical for expanding marine energy applications. These systems typically employ reactive metals and their alloys as anodes, while the cathode typically comprises composite materials. However, the search for efficient and economical cathode materials remains a key research challenge. This study presents a high-performance cathode material, CuS-coated CuI, synthesized via a facile and scalable method. The electrochemical performance of this novel cathode was systematically evaluated in a non-rechargeable seawater battery configuration, paired with an AZ31B Mg alloy anode with natural seawater. The fabricated cell exhibited a stable discharge voltage plateau between ~1.17 V and 1.0 V at a current density of 100 mAg-1 of active material, achieving a specific capacity of 277.42 mAh g-1, specific energy of 244.98 mWhg-1, and a specific power of 88.31 mWg-1. Cyclic voltammetry (CV) analysis revealed well-defined redox behavior, while electrochemical impedance spectroscopy (EIS) confirmed favorable charge transfer kinetics and low internal resistance. Although AgCl is widely recognized as a high-performance cathode benchmark,its prohibitive cost limits widespread adoption. The synthesized CuS-coated CuI cathode demonstrates strong potential as a viable, high-performance, and cost-effective alternative,paving the way for its application in next-generation, marine-oriented, seawater-activated battery technologies.

Keywords: Seawater, Primary battery, AZ31B Mg alloy, CuS-coated CuI, Marine energy

IT-008

Laser-Structured Stainless Steel for Low-Temperature Friction Reduction

Pavels Onufrijevs[*1], Ernests Jansons[2], Janis Lungevics[2], Jevgenijs Kaupuzs[1], Armands Leitans[2], Raimonds Sirants[2]

[1]*Institute of Physics and Material Sciences, Faculty of Natural Sciences and Technology, Riga Technical University, Latvia*

[2]*Institute of Mechanical and Biomedical Engineering, Faculty of Civil and Mechanical Engineering, Riga Technical University, Latvia*

*Corresponding author e-mail: pavels.onufrijevs@rtu.lv

ABSTRACT

Laser processing allows precise control of surface morphology and chemical composition to adjust the functional properties of materials [1]. Laser-induced periodic surface structures (LIPSS) can effectively optimize interfacial interactions, wettability, and tribological characteristics [2]. These properties are essential for components operating under demanding and harsh environmental conditions.

The aim of this study is to investigate the sliding performance of LIPSS formed on stainless steel Uddeholm Ramax HH using a nanosecond-pulsed laser under ice-sliding conditions. The samples before and after Nd:YAG laser (λ=*1064nm,* τ=*6ns*) processing were characterized using surface texture 3D profilometry, FESEM, contact angle measurements, Raman spectroscopy, and X-ray diffraction. Surface analysis revealed the formation of low spatial frequency LIPSS with period around 1µm. Ice friction experiments demonstrated an approximately threefold reduction in the coefficient of friction for laser-irradiated surfaces over a sliding velocity range of 0.05 to 0.38 m/s, with stable behavior observed under applied normal loads ranging from 20 to 80 N. The observed friction reduction is attributed to the combined effects of optimized micro- and nanoscale surface morphology and the formation of Fe_2O_3/Fe_3O_4 oxide layers, which suppress adhesion at the ice–surface interface. These experimental results demonstrate the potential of laser technologies as an efficient, durable, and environmentally friendly approach for improving the performance of metallic components operating in cold environments.

Acknowledgment: This study was supported by the Fundamental and Applied Research project “Innovative Multifunctional Laser-Textured Surfaces with Improved Tribological Performance and Icephobicity” (LZP-2023/1-0060).

References:

1. M. Ahmed Obeidi, E. McCarthy, D. Brabazon, *Surf. Coat. Technol.*, **307** (2016) 702–712.
2. J. Bonse, S. Gräf, *Laser Photonics Rev.*, **14** (2020) 1–25.

Bioconjugation on Nanopatterned Surfaces for Biosensing: Experimental Insights and Firs tPrinciples DFT

Shikha Varma

Inter University Accelerator Center, (IUAC), N. Delhi Institute of Physics (IOP), Bhubaneswar

ABSTRACT

Bioconjugation of nucleotides with surfaces forms the fundamental basis for numerous biotechnological and biosensing applications. The enhanced role of nanostructured surface in the bioconjugation process with DNA is explored here. Creation of specific states and charge transfer profiles highlight the pronounced influence of nanostructured patterning, induced via Ion beam sputtering, for improved bioconjugation. Due to the lowered free energy nature, nanostructured surfaces enable stronger linkages, thereby offering broader applications in the field of biotechnology.

IT-010

Degradation Customization of Degradable Metallic Biomaterials

Satyabrata N Sahoo[1], Santanu Mandal[1], Samit Kumar Nandi[3]*, and Mangal Roy[1]*

[1]*Department of Metallurgical and Materials Engineering, Indian Institute of Technology-Kharagpur, Kharagpur-721302, India*

[2]*School of Minerals, Metallurgical and Materials Engineering, Indian Institute of Technology-Bhubaneswar, Khorda 752050, India*

[3]*Department of Veterinary Surgery & Radiology, West Bengal University of Animal & Fishery Sciences, Kolkata 700037, India*

ABSTRACT

Degradable metallic biomaterials have shifted the established paradigm of metallic biomaterials from being corrosion-resistant to having controlled degradation. Degradable implants have been considered promising candidates for treating bone fractures as they eliminate the requirement of secondary surgery and help in pediatric bone growth. Fe, Mg, and Zn-based alloys have been extensively studied due to their low density and favorable mechanical and biological properties. However, Mg's strength, ductility, degradation rate, and hydrogen gas evolution are still a concern. Pure Fe-bearing implants provide good mechanical support, but a lower degradation rate is an issue. This presentation will focus on the degradation rate of both Mg and Fe-based systems. We will discuss the improvement in corrosion resistance of Mg-based systems as well as improving the corrosion rate of Fe-based systems. The effects of corrosion and alloy composition on in vitro cytocompatibility and in vivo biocompatibility will also be discussed.

Keywords: Degradable biomaterial, Fe-Mn alloy; Mg based alloys; In vivo.

References:

1. M. Roy et al., Acta Biomater., 2023, **168**, 650–669.
2. M. Roy et al., ACS Biomater. Sci. Eng., 2023, **9**, 2495Splitter->2513.
3. M. Roy et al., J. Magnesium Alloys, 2025.

Gas-phase Electrophoresis-based Characterization for Real-time Quantifying Synthesis of Advanced Nanomaterials

De-Hao Tsai*[1]

[1] *Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30044, Taiwan, ROC*

***Corresponding author e-mail:** dhtsai@mx.nthu.edu.tw

ABSTRACT

This study presents a novel approach for controlled synthesis and real-time characterization of advanced nanomaterials (metal-organic framework and derived material, crosslinked hydrogel, graphene oxide, nanoparticle cluster) by utilizing electrospray-differential mobility analysis (ES-DMA), a gas-phase electrophoresis-based approach. By precisely controlling key synthesis parameters, we successfully synthesized the material by design with tailored size, composition, and properties. The integrated ES-DMA system provides rapid, in-line analysis of physical size and distribution, enabling real-time monitoring and optimization of the synthesis process. The evolution of the number-based particle size distribution revealed a strong correlation with the synthesis conditions, demonstrating the high degree of controllability achieved by this integrated approach. This novel methodology offers a promising platform for the high-throughput synthesis of uniform and well-defined nanostructured materials with enhanced traceability, paving the way for advancements in various emerging applications.

References:

1. P-Y Lai, D. Senthil Raja, J-W Chang, J-H Huang, D-H Tsai, J. Colloid Interface Sci.,2025, 684, 1, 201-212.
2. D. Senthil Raja, D-H Tsai, Chem. Commun., 2024, 60, 8497-8515.
3. Y.-H. Sung, D. Senthil Raja, J.-H. Huang, D-H Tsai, Small Methods. 2024, 8(5) 2301435.
4. Y.-H. Sung, C.-L. Wu, J.-H. Huang, D-H Tsai, Analytical Chemistry, 2023, 95, 9, 4513-452
5. D. Senthil Raja, C-H Lee, P-Y Lai, Y-H Wang, D-H Tsai, Talanta, 2025, 294, 128254.

IT-012

Domain Structure and Magnetic Reversal by Electric Field in Cobalt-substituted Bismuth Ferrite Thin Films and Nanodots

Kei Shigematsu[1,2]

[1]*Institute of Science Tokyo, Yokohama, Japan*

[2]*Kanagawa Institute of Industrial Science and Technology, Yokohama, Japan*

***Corresponding author e-mail:** kshigematsu@msl.iir.isct.ac.jp

ABSTRACT

Magnetization reversal induced by an electric field in multiferroic materials is keenly investigated because it can be utilized for an ultra-low-consumption voltage-write magnetic-read-out memory device. Co-substitution in $BiFeO_3$ ($BiFe_{0.9}Co_{0.1}O_3$; BFCO) destabilizes the cycloidal modulation of spins and generates a canted collinear spin state with non-zero saturation magnetization[1]. We have investigated the magnetization reversal induced by electric field by observing magnetic and ferroelectric domain before/after electric poling in BFCO thin films by scanning probe microscopy. We demonstrated the direction of magnetization reversal depended to polarization switching pathways, so-called 71, 109 and 180 deg. switching. For example, we have recently demonstrated the correlation of ferroelectric and magnetic domain structures after applying an electric field in the in-plane $[1\text{-}10]_{pc}$ direction to $(110)_{pc}$-oriented BFCO/$SrTiO_3$ (110) thin film (Fig. 1)[2]. We also observed the magnetic/ferroelectric domain in BFCO nanodots fabricated by deposition with an anodized porous alumina mask. The various ferroelectric and ferromagnetic domain structure depending on the nanodot size were observed, and the strong magnetoelectric coupling in BFCO nanodots was confirmed[3].

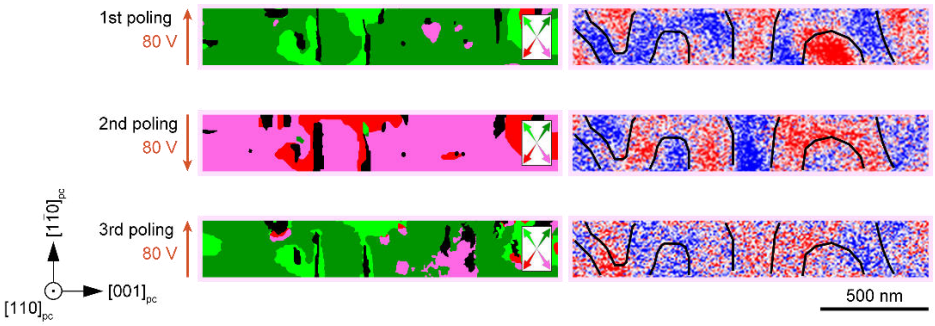


Fig. 1 3D-PFM images and MFM phase images from BFCO/$SrTiO_3$(110) thin films in polings at 80 V via a Pt coplanar electrode. The polarization direction in each variant on the $(110)_{pc}$ plane is indicated in greenish or reddish colors shown inset of PFM images.

Keywords: perovskite oxide; bismuth ferrite; multiferroic; scanning probe microscopy

References:

1. H. Hojo *et al.*, Adv. Mater., **29**, 160313 (2017).
2. T. Itoh, K. Shigematsu *et al.*, Adv. Mater. 2419580 (2025).
3. K. Ozawa, K. Shigematsu *et al.*, ACS Appl. Mater. Interfaces **16**, 20930 (2024).

IT-013

Molecularly Engineered Semiconducting Polymers for Solar-Driven Hydrogen Evolution and Circular Waste Upcycling via Photoreforming

Ho-Hsiu Chou

National Tsing Hua University, No. 101, Sec. 2, Kuang-Fu Rd, Hsinchu 300044, Taiwan

ABSTRACT

By mimicking natural photosynthesis, artificial photosynthesis using polymer photocatalysts for the visible-light-driven hydrogen generation through water splitting is an almost ideal process for converting abundant solar energy into useable fuel in an environmentally friendly and high-energy-density manner. Solar-driven photocatalytic hydrogen evolution has gained significant attention due to the inexhaustible supply of solar energy. Extensive efforts have been made to develop highly efficient photocatalytic materials, with organic semiconductors being a prime focus due to their low-cost production, adjustable molecular structures, and tunable bandgaps, which offer distinct advantages over inorganic counterparts. Since the successful use of graphitic carbon nitride in photocatalytic hydrogen evolution systems in 2009, research on polymeric photocatalysts—including linear conjugated polymers, conjugated microporous polymers, polymer dots, covalent triazine frameworks, and covalent organic frameworks—has steadily increased. In this presentation, we discuss the development of new conjugated polymers and polymer dots (Pdots) as photocatalysts for hydrogen evolution, exploring their molecular design, photophysical properties, mechanisms, and applications. This talk will present a clear strategy for the design and recent advancements in polymer photocatalysts for artificial photosynthesis.

IT-014

Beyond the Monolayer: Translating Langmuir-Blodgett WO_3 Assembly into Solar Cell Metrics

Vibha Saxena

Technical Physics Division,

Bhabha Atomic Research Centre, Mumbai, India

***Corresponding author e-mail**: vibhas@barc.gov.in

ABSTRACT

In a high-performance dye- sensitized (DSCs) and perovskite (PSCs) solar cells, the electron transport layer (ETL) serves as a critical interfacial component between fluorine-doped tin oxide (FTO) and mesoporous TiO_2 (m-TiO_2) layer. Its main role is to selectively block the hole transfer to reduce recombination while simultaneously facilitating fast electron transport. Most commonly used solution-processed spin-coated anatase TiO_2 ETLs face several shortcomings due to low electron mobility, presence of surface defects and UV light instability, thereby restricting the efficiency and stability of solar cells. To overcome these issues, several alternative materials as well as surface modification strategies for ETLs have emerged. Despite having multiple polymorphs, higher electron mobility and affinity, better chemical stability, WO3 has seldom been used as ETL in DSCs and PSCs. The key challenges in employing WO3 ETL in DSCs and PSCs is to produce uniform, crystalline and controlledthickness films so as to obtain improved interfacial properties such as charge extraction and transport. Moreover, preparation of thin crystalline WO3 (>50nm) prepared using conventional deposition methods, such as sputtering, e-beam evaporation require substrate temperature >300°C, thereby restricting their use for flexible devices. Unlike conventional vacuum-based deposition methods, Langmuir-Blodgett (LB) technique is highly versatile, environmental-friendly, and simpler technique to prepare ordered crystalline thin films of precise thickness on all kind of substrates. In recent years at BARC, we have developed a methodology to prepare monolayer of WO3-octadecyl amine complex (WO_3,ODA) at the air-water interface. Surface properties of the monolayer were investigated thoroughly to achieve compact and uniform multilayer deposition (WO_3,ODA multilayer) on various substrates. By manipulating, the decomposition of the WO_3,ODA multilayers, several phases of stochiometric crystalline WO_3 films could be obtained. In this talk, a comprehensive review of WO_3 ETL developed for high-performance DSCs and PSCs, will be presented. Based on the research experience gained from results, future directions for other applications will also be discussed.

References:

1. Vibha Saxena et al, Materials Advances, 5 (2024) 7659-7670., Sol. RRL (2022) 2200222. Electrochim. Acta 318 (2019) 405-412., Appl. Phys. Lett., 100(13), 133303, (2012), Org. Electron., 14 (2013) 3098-3108, J. Phys. Chem. C, 117 (2013) 21096-21104.

IT-015

From Functionalization to Functionality: Physicochemical Design Principles of Sp^2-Carbon Nanoallotropes Across Dimensions

Slawomir Boncel*[1,2]

[1] *NanoCarbon Group, Faculty of Chemistry, Silesian University of Technology, Gliwice, PL*

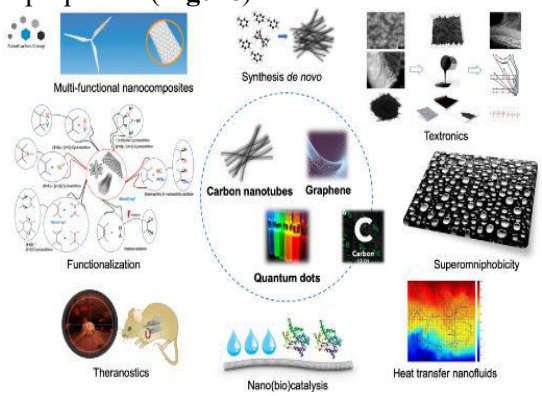
[2] *Centre of Organic & Nanohybrid Electronics (CONE), Silesian University of Technology, Gliwice, PL*

***Corresponding author e-mail:** slawomir.boncel@polsl.pl

ABSTRACT

The transfer of extraordinary properties of sp^2-nanocarbons (NCs) from nano- to macro-scale is challenging due to the non-trivial control over their morphology and surface physicochemistry (1). The fundamental properties of NCs as a function of dimensionality from 0D to 3D remain incompletely understood, often with contradictory reports about their affinities and reactivities, hindering potential applications (2). Physicochemical modifications of 0D quantum dots (CQDs), 1D carbon nanotubes (CNTs), and 2D graphene/graphenoids enabling their individualization, frequently requiring development of functional 3D networks based on non-compromised morphology, are essential for their enhanced electrical, thermal, mechanical, catalytic, and biological characteristics of superior properties (**Figure**).

We have designed and synthesized and/or manufactured: textronics for Holter electrocardiography (3), conductive (4) and super-hydrophobic (5) coatings, high-performance heat transfer fluids (6), phase change materials (7), magnetic drug delivery systems (8), superlubricants (9), only-carbon 1D and 2D emulsifiers (10), and hybrid catalytic systems.



References

1. Z. Amjad et al., Nanoscale 2024, 16, 9197;
2. M. Małecka et al., Adv. Coll. Interface Sci. 2024, 334, 103311;
3. S. Boncel, et al., ACS Appl. Nano Mater. 2022, 5, 15762;
4. A.W. Kuziel et al., ACS Sus. Chem. Eng. 2022, 10, 6596;
5. E. Korczeniewski et al., Chem. Eng. J. 2024, 482, 148777;
6. M. Dzida, et al., ACS Appl. Mater. Interfaces 2022, 14, 50836;
7. A.W. Kuziel, et al., J. Energy Storage 2021, 36, 102396;
8. S. Boncel et al., ACS Biomater. Sci. Eng. 2016, 2, 1273;
9. Ł. Wojciechowski et al., Tribol. Int. 2024, 191, 109203;
10. Kuziel, et al., Adv. Mater. 2020, 32, 2000608.

IT-016

Integrated Photonic Devices and AI-Driven On-Chip Spectroscopy for Rapid Biomedical Diagnostics

Senthil Murugan Ganapathy

Optoelectronics Research Centre, University of Southampton, Southampton SO17 1BJ, United Kingdom

***Corresponding author e-mail:** smg@orc.soton.ac.uk

ABSTRACT

Fast and reliable diagnostics are increasingly needed in healthcare, particularly in settings where access to centralized laboratories is limited or time is critical. Vibrational spectroscopy, through infrared (IR) and Raman techniques, offers a powerful way to probe molecular composition without labels or complex sample preparation. Yet despite its promise, clinical adoption has been slow. Traditional spectroscopic systems are often bulky, expensive, and difficult to deploy outside the laboratory, creating a clear need for compact, user-friendly technologies that can operate at the point of care. In this plenary, I will discuss how recent advances in integrated photonics are enabling a shift from laboratory-based spectroscopy to miniaturised, on-chip diagnostic platforms. By combining IR and Raman measurements on a single platform and coupling them with data-driven analysis, it becomes possible to extract meaningful molecular information from small sample volumes with high sensitivity. This multimodal approach provides a more complete biochemical picture than either technique alone and opens new opportunities for rapid, quantitative diagnostics. Central to this work is a silicon-based attenuated total reflectance (ATR) spectroscopy chip designed for scalability and real-world use. Metasurface-enhanced ATR structures strengthen light–matter interactions, significantly improving detection sensitivity while maintaining a compact footprint. In parallel, adaptive correction algorithms suppress atmospheric interference from water vapour and CO_2, removing the need for nitrogen purging and simplifying operation. The platform's clinical relevance is demonstrated through applications including early detection of neonatal respiratory distress syndrome and the analysis of cancer-related biomarkers and DNA fragment length in biofluids. Together, these advances bring vibrational spectroscopy closer to routine clinical use, transforming rich spectral information into practical diagnostic insight and helping bridge the gap between the laboratory and the bedside.

IS-017

Magnetic Properties of $GdMnO_3$ Films on Epitaxial and Non-Epitaxial Substrates

Venkateswaran C

University of Madras, Chennai

ABSTRACT

The structural, topographical and magnetic properties of orthorhombic $GdMnO_3$ (GMO) thin films deposited on $SrTiO_3$ (110) and Quartz substrates by RF Magnetron Sputtering are studied. Uniform plane growth of orthorhombic GMO is seen in the (100) direction of STO, whereas a polycrystalline feature with an island growth is observed on the Quartz substrate. GMO deposited on both the substrates show canted antiferromagnetism at ~ 25 K and a paramagnetic-antiferromagnetic transition at T_N ~ 47 K. But the GMO coated on Quartz substrate shows a cusp, representing spin glass transition at low temperature ZFC measurements. The results will be discussed.

IT-018

Deep Learning–Based Screening for Sarcopenic Dysphagia to Support Clinical Decision Making

Yuki Maruno[1], Yumi Ikeguchi[2], Kokona Koyano[3], Fuka Sono[3], Hiroe Seto[3], Nobuo Sakata[4], *Kotomi Sakai[4], Kuniyoshi Hayashi*[3]*

[1]*Kansai University, Osaka, Japan*

[2]*PKUTECH Co., Ltd., Tokyo, Japan*

[3]*Kyoto Women's University, Kyoto, Japan*

[4]*Heisei Medical Welfare Group Research Institute, Tokyo, Japan*

***Corresponding author e-mail:** hayashikuni@kyoto-wu.ac.jp

ABSTRACT

Dysphagia is characterized by impaired swallowing that interferes with the safe intake of food and liquids. Sarcopenic dysphagia, resulting from systemic muscle loss, is common in older adults and may lead to malnutrition and aspiration pneumonia [1,2]. The concept and diagnostic framework of sarcopenic dysphagia have been established in recent consensus statements and guidelines [3,4], highlighting the importance of early identification and appropriate management [5]. This study aimed to develop a clinically applicable, non-contact screening method for sarcopenic dysphagia using deep learning–based image analysis.

In this cross-sectional study, anterior neck photographs were obtained from older patients. Image features associated with sarcopenic dysphagia, particularly clavicular prominence, were analyzed. A screening model was constructed using EfficientNetV2, and neck regions were automatically detected and cropped using YOLO. Fine-tuning and data augmentation were applied to optimize model performance.

The optimal model achieved an accuracy of 0.96, demonstrating high predictive performance in identifying sarcopenic dysphagia from neck appearance alone.

This deep learning–based screening approach may support early identification of at-risk patients and facilitate referral for comprehensive swallowing evaluation and intervention before the onset of complications such as malnutrition or aspiration pneumonia.

References:

1. Wakabayashi H, Sakuma K. Rehabilitation nutrition for sarcopenia with disability: a combination of both rehabilitation and nutrition care management. J Cachexia Sarcopenia Muscle. 2014.
2. Mori T, et al. Development of a diagnostic algorithm for sarcopenic dysphagia. JCSM Clinical Reports. 2017.
3. Fujishima I, et al. Sarcopenia and dysphagia: Position paper by four professional organizations. Geriatr Gerontol Int. 2019.
4. Cruz-Jentoft AJ, et al. Sarcopenia: revised European consensus on definition and diagnosis (EWGSOP2). Age Ageing. 2019.
5. Cichero JAY, et al. Standardisation of terminology and definitions for texture-modified foods and thickened liquids (IDDSI). Dysphagia. 2017.

Cobalt-Free High-Energy Ni-Rich Cathodes Enabled by Structural and Interface Engineering

Partha Saha

Department of Ceramic Engineering, NIT Rourkela-769008, Odisha, India

***Corresponding author e-mail:** sahap@nitrkl.ac.in

ABSTRACT

The growing demand for high-energy-density lithium-ion batteries (LIBs), particularly for electric vehicles and portable electronics, has intensified research on Ni-rich layered oxide cathodes such as $Li_xNi_yMn_zCo_{1-y-z}O_2$ (NMC). However, conventional Ni-rich NMC materials suffer from Li^+/Ni^{2+} cation disorder, irreversible H2→H3 phase transitions, oxygen instability, and rapid capacity and voltage fading, while reliance on cobalt and manganese raises cost and supply concerns. To overcome these limitations, a systematic materials-design strategy is developed combining site - specific dopant engineering, cobalt/manganese elimination, and interface optimization. Mg^{2+} and Zr^{4+} co-doping in NMC cathodes effectively suppresses cation mixing, strengthens the transition-metal–oxygen framework, enlarges interlayer spacing, and mitigates oxygen migration, leading to improved cycling stability and reduced voltage decay. Building on this concept, cobalt-free and Co/Mn-free ultrahigh Ni cathodes are designed with enhanced thermal and electrochemical stability. Furthermore, integration with a polarized β-phase PVDF-HFP nanofiber-coated separator stabilizes the cathode–electrolyte interface, enabling high capacity, long- term cycling stability, and low voltage fading.

IT-020

Magneto-Functional Effects in Magnetic Metal–Ceramic Nano-Granular Thin Films

Hiroshi Masumoto[1]*

[1]*Frontier Research Institute for Interdisciplinary Sciences (FRIS)*
Tohoku University, Sendai, Japan

***Corresponding author e-mail:** hiromasu@fris.tohoku.ac.jp

ABSTRACT

Magnetic metal–ceramic nano-granular thin films, in which nanometer-sized magnetic metal granules are dispersed in a ceramic matrix, have attracted considerable attention due to their tunable functional properties achieved through compositional control. When the magnetic metal content is high (generally above 60%), high-frequency magnetic properties are exhibited, whereas at moderate magnetic metal contents (approximately 60–30%), tunnel magnetoresistance (TMR) properties appear. These properties have been extensively studied for several decades and are now widely utilized in electromagnetic applications.

In nanocomposite thin films with lower magnetic metal contents (approximately 40–10%), our research group has discovered a novel magneto-dielectric phenomenon, which we term the tunnel magneto-dielectric (TMD) effect. TMD nanocomposites consist of sparsely dispersed magnetic granules with sizes of several nanometers embedded in an insulating matrix, where the tunnel barriers are sufficiently thin to allow quantum tunneling. When an alternating electric field and a magnetic field (H) are applied, the oscillation rate—determined by the tunnel barrier height and the relative magnetization orientation of the granules—can coincide with the frequency of the applied AC field, resulting in a pronounced peak in the dielectric change, $\Delta\varepsilon'/\varepsilon'_0$, at a specific frequency. This dielectric response is theoretically understood to originate from spin-dependent polarized charges formed through spin-dependent tunneling processes, providing insight into the physical mechanism underlying the TMD effect.

This presentation will introduce the research background, the TMD effect, thin-film fabrication methods, performance enhancement, and newly identified functionalities in magnetic metal–ceramic nano-granular thin films.

Keywords: Magnetic metal–ceramic nanocomposites, Nano-granular thin films, Spin-dependent tunneling, Magneto-functional effects

References:

1. N. Kobayashi, H. Masumoto, et al. : Nature Communications 5, 4417 (2014).

IT-021

Phase Separation and Metal-Insulator Transition in TiO_2-VO_2 Thin Films Using Dynamic Aurora PLD

Naoki Wakiya[1,2*], Takahiko Kawaguchi[2], Naonori Sakamoto[1,2]

[1]*Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan*

[2]*Department of Engineering, Shizuoka University, Hamamatsu, Japan*

***Corresponding author e-mail:** wakiya.naoki@shizuoka.ac.jp

ABSTRACT

VO_2 has a metal-insulator transition temperature (T_c) at 68 °C. Below T_c, it transmits infrared radiation in its monoclinic (insulating phase) state, whereas above T_c, it reflects infrared radiation in its tetragonal (metallic phase) state. Therefore, window glass coated with VO_2 thin films is expected to be a smart window. However, because VO_2 has a high transition temperature of 68 °C, T_c must be lowered to near room temperature to realize smart windows. One method to lower T_c is to induce spinodal decomposition of TiO_2-VO_2 thin films by prolonged annealing, thereby applying stress to the interface. We have previously found that spinodal decomposition can be accelerated by applying a magnetic field during deposition of cobalt ferrite thin films using the dynamic aurora PLD method.[1)] The purpose of this study is to clarify the effect of stress on the T_c of spinodally decomposed TiO_2-VO_2 thin films by two methods: (A) long-term deposition and (B) deposition under a high magnetic field. The thin films were deposited on rutile TiO_2(001) substrates. Fig. 1 shows a graph with lattice distortion (c/a) on the horizontal axis and transition temperature on the vertical axis. (A) Long-term deposition and (B) deposition under a high magnetic field both show trends similar to those of previous studies, demonstrating a positive correlation. This suggests that, regardless of the spinodal decomposition method, only the amount of distortion is necessary to control the transition temperature. Therefore, by optimizing the oxygen pressure while applying a high magnetic field during deposition, it is expected that it will be possible to create superlattice structures in a short time and control T_c.

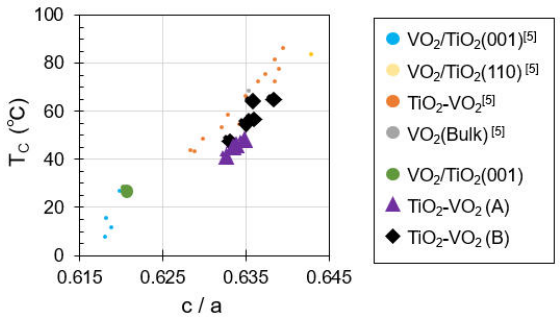


Fig. 1 (a) Strain and transition temperature

Keywords: Smart window, Metal-insulator transition, TiO_2-VO_2, Spinodal decomposition

References:

1. N. Wakiya et al., J. Magn. Mater., **432**, (2017) 391

In vitro formation of 3D cell structures using magnetic nanomaterials

Ekaterina Brodovskaya, Denis Yakobson, Mikhail Zharkov, Nikolay Pyataev

National Research Mordovia State University, Saransk, Republic of Mordovia, Russia, 430005

ABSTRACT

The aim of the work: to investigate possibility of 3D cell structure formation using magnetic nanomaterials.

Results: The possibility of forming structures using magnetic nanomaterials such as magnetic nanoparticles (MNPs) and microcapsules with MNPs has been demonstrated. With the help of optical influences, it is possible to selectively kill cells without disrupting the viability of neighboring ones.

This study outlines the findings on a method for constructing tissue structures using MNPs (nanorods) and microcapsules with MNP and chlorin E6 subjected to magnetic fields and light irradiation. The cytotoxicity of the iron oxide nanorods and microcapsules was assessed using the MTT assay on cells, revealing low cytotoxicity. Double staining with fluorescent dyes (acridine orange and ethidium bromide) indicated that necrosis was the primary mechanism of cell death following laser exposure (808 nm) for magnetic nanorods and red light (660 nm) for microcapsules with chlorin E6. The study demonstrated the potential to form 3D cellular structures by exposing cells to a magnetic field with magnetic nanorods and microcapsules. Our synthesized magnetic nanomaterials exhibit significant promise for use in optical hyperthermia and the magnetic formation of tissue structures.

X-ray Photoelectron Spectroscopy and Critical Exponent Study of Nanocrystalline $Pr_{0.7-x}Y_xBa_{0.3}MnO_3$(x = 0, 0.05 and 0.1)

Rabindra Nath Mahato

School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India

ABSTRACT

X-ray photoelectron spectroscopy (XPS) analysis and magnetic critical exponent studies have been carried out on nanocrystalline A-site Yttrium-doped Pr–Ba manganite samples, Pr0.7-xYxBa0.3MnO3 (x = 0 and 0.1) which exhibit a second-order ferromagnetic to paramagnetic phase transition. The XPS survey spectra along with high-resolution core-level spectra of the constituent elements were analyzed to investigate the surface chemical composition and electronic states as a function of Y substitution at the A-site. Furthermore, the critical behavior near the magnetic phase transition was systematically examined using various techniques such as critical isotherm analysis, modified Arrott plots, and the Kouvel–Fisher method. Determination of the universality class of the magnetic phase transition is essential, as it provides insight into the nature and range of magnetic interactions present in the system. The extracted critical exponents β, γ, and δ do not correspond to any of the standard theoretical universality classes, indicating the presence of complex magnetic interactions and possible effects of structural disorder and finite-size scaling.To validate the reliability of the obtained critical exponents, the scaling equation of state was constructed, and the magnetization isotherms were found to collapse onto two distinct universal branches above and below the Curie temperature *T*!. This confirms the self-consistency and robustness of the evaluated critical parameters and demonstrates that the magnetic interactions are properly renormalized in the critical regime, satisfying both the scaling hypothesis and the scaling equation of state.

IT-024

Thin Film Electrodes for Photo-degradation of pollutants and Power Generation in Microbial Fuel Cells – Doping and Coating Strategies

D. Paul Joseph

Department of Physics, National Institute of Technology Warangal,

Telangana State, Warangal, 506004, India.

***Corresponding author e-mail:** paul@nitw.ac.in

ABSTRACT

Persistently growing need for energy and growing environmental pollution have accelerated the exploration of sustainable and environmentally benign solutions for power generation, pollutant remediation, and wastewater treatment. Conventional approaches involve powder and particulate thick coatings, which holds multiple drawbacks, like stability, re-use complexity, and secondary contamination. To combat these issues, thin film-based photocatalysis has emerged as a promising technique for the effective degradation of organic contaminants in wastewater, taking advantage of the increased surface area, higher light interaction, and ease of recovery/cleaning/reuse compared to typical powder or particulate photocatalysts.

This presentation will cover the aspects of spray coating of transparent conducting doped SnO_2 thin film electrodes. The applicability of these electrodes with a focus on doping and coating strategies making them viable for photo-degradation of dye pollutants/antibiotic (as an immobilized photocatalytic electrode, minimizing secondary contamination) and for power generation in a microbial fuel cell (MFC) are tested.

These electrodes offer low material loading with durability and stability in pollutant degradation using cost-effective white LED light utilizing the defect states of the material. Concurrently, these electrodes also offer a sustainable approach in MFCs to remediate wastewater whilst generating bioelectricity. Thus, the results of the electrodes demonstrating effective pollutant degradation, water remediation, and power generation, indicating its potential as a multifunctional system for a sustainable environment will be elucidated in sufficient detail.

IT-025

Surface Structure Engineering of Highly Active and Durable Oxygen Evolution Catalysts

Shigeto Hirai*

School of Earth, Energy and Environmental Engineering,

Kitami Institute of Technology, Kitami, Japan, 090-8507

***Corresponding author e-mail**: hirai@mail.kitami-it.ac.jp

ABSTRACT

The oxygen evolution reaction (OER) is an important reaction of electrochemical water splitting[1] and rechargeable metal-air batteries[2]. However, the kinetics of OER are sluggish, and it is difficult to lower the overpotential even with the OER electrocatalysts. More importantly, even the acid stable iridium metal oxide-based catalysts suffer from lattice collapse that gives birth to the trade-off relationship of activity and durability[3] , and it is a big challenge to develop highly electrocatalysts. Firstly in this talk, $Ca_{1-x}Sr_xRuO_3$ ($0 \le x \le 0.1$) will be introduced, which is a series of excellent OER catalysts under alkaline conditions with both high activity and durability[4] . The close relationship between electron correlation and the OER activity in this system suggests that the coexistence of metallic conductivity and strong electron correlation is the key to develop OER electrocatalysts with highly durable and active surface structure [4] . Secondly, $BaIr_{1-x}Mn_xO_3$ ($0.1 \le x \le 0.3$) will be introduced, which is a series of excellent OER catalysts under acidic conditions with both high activity and durability[5] . Specifically, the substitution of the Ir-site with Mn for $BaIrO_3$ prevents the lattice collapse after repeated OER cycling, leading to a remarkable activity enhancement by a factor of 28 and an overall improvement in durability (Fig. 1). This dual enhancement of OER performance was accomplished by the novel strategy of balancing the elemental dissolution of the electrocatalyst to obtain highly durable and active surface structure after repeated OER cycling[5]

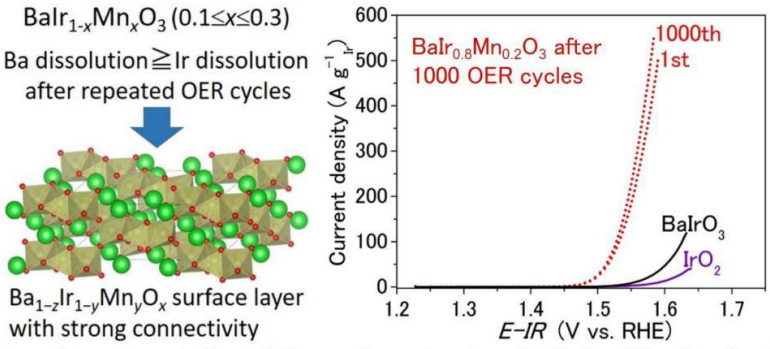


Fig. 1 Schematic representation of the surface structure in $BaIr_{1-x}Mn_xO_3$ after 1000 OER cycles, and its cycle dependence of the linear sweep voltammograms for $BaIr_{0.8}Mn_{0.2}O_3$.

Keywords: oxygen evolution reaction; electron correlation; lattice collapse; surface structure

References:

1. T. E. Mallouk, Nat. Chem., 5 (2013) 362-363.
2. Y. C. Lu et al., J. Am. Chem. Soc., 132 (2010) 12170-12171.
3. C. W. Song et al., Energy Environ. Sci., 13 (2020) 4178-4188.
4. S. Hirai et al., J. Mater. Chem. A, 7 (2019) 15387-15394.

IT-026

Metal Oxide Semiconductor Nanostructures for Energy Conversion and Energy storage Applications

Koteswara Rao Peta

Department of Electronic Science, University of Delhi South Campus, New Delhi, India

***Corresponding author e-mail:** krao@south.du.ac.in

ABSTRACT

Recently, Metal oxide semiconductor nano structures have gained much attention compared to conventional inorganic nano semiconductors with respect to excellent electronic structure, defect states, material processing, high optical transmittance, environmental stability and tunable shapes, thereby enabling conventional and new functions. Recently, remarkable advances in metal oxides for various electronic devices have been achieved, including transparent conducting oxides, successful p-type doping and can be manufactured on large scale with low cost vacuum free techniques at low temperature ambience. In this talk, firstly we focus on synthesis approaches for various nano structures of metal oxides for energy conversion applications. Particularly, ZnO nano-rods studied for polymer LED applications. When ZnO nanorods were integrated in MEHPPV light emitting diode (PLED) there is an enhancement in the luminance. It was observed that, luminance of ZnO nanorod/MEH-PPV LED increased compared to PLED without rods due to single waveguide effect in ZnO nano-rods. Further, successfully green synthesized Sm^{3+} ions doped ZnO nanoparticles (NPs). It was found that, the crystallite size of NPs decreases as the concentration of Sm^{3+} ions in NPs increases along with formation of ZnO/SmO core-shell hetero structure. The nano junction formation at the hetero structured interface help to reduce recombination of carriers and is used as electron transport layer in polymer based liquid junction Photovoltaic cell. Lastly, physical, optical and magnetic properties of cost effective, eco-friendly synthesised ZFO, C-ZFO, CFO and BFO spinel nano-structures and their prospective applications in the field of energy storage.

IT-027

Toward Explainable Breath Analysis Using Semiconductor Sensor Arrays

Yuichi Sakumura[1], Momo Shikata[1], Kenta T. Suzuki[1], Woosuck Shin[2]

[1] *Nara Institute of Science and Technology, Japan*

[2] *National Institute of Advanced Industrial Science and Technology, Japan*

ABSTRACT

Breath analysis has emerged as a promising non-invasive approach for disease diagnosis because volatile organic compounds (VOCs) in human breath reflect metabolic processes, inflammation, and microbial activity. Our previous studies demonstrated that quantitative VOC profiling using mass spectrometry enables discrimination among healthy subjects and patients with lung cancer, metabolic dysfunction-associated steatohepatitis (MASH), liver cancer, and periodontal disease. However, the widespread clinical implementation of breath diagnostics remains limited due to the intrinsic drawbacks of mass spectrometry, including high cost, large system size, operational complexity, and time-consuming analysis.

To address these challenges, this talk presents our recent efforts toward semiconductor sensor–based breath diagnostics aimed at replacing conventional analytical instrumentation while preserving biochemical interpretability. Unlike existing approaches that directly classify diseases from sensor resistance signals using black-box models, our strategy reconstructs chemically meaningful VOC concentrations prior to diagnostic inference, thereby maintaining biological and medical validity.

Artificial breath gases were generated by precisely mixing multiple VOC species at controlled concentrations to emulate realistic breath compositions. The gas mixtures were introduced into an eight-channel semiconductor sensor array, and resistance time-series responses were recorded. Using regression analysis, VOC concentrations were estimated from multidimensional sensor responses. The results demonstrate that quantitative reconstruction of VOC concentrations is achievable with practical accuracy, indicating that sensor arrays can function as compact chemical encoders analogous to a low-dimensional spectroscopic system. This framework bridges high-precision analytical chemistry and practical healthcare sensing, providing a pathway toward portable, explainable, and clinically acceptable breath diagnostics. Future directions toward real-breath validation and continuous health monitoring using semiconductor sensing platforms will also be discussed.

IT-028

Resource Recovery from Seawater Reverse Osmosis (SWRO) Desalination Brine

Wen Yi Chia [1,*], Wei Liang Tan [1], Vinh-Hien Truong [1], Tzyy Haur Chong [1, 2]

[1]*Nanyang Environment & Water Research Institute, Singapore Membrane Technology Centre, Nanyang Technological University, Singapore*

[2]*School of Civil and Environmental Engineering, Nanyang Technological University, Singapore*

***Corresponding author e-mail:** wenyi.chia@ntu.edu.sg

ABSTRACT

Seawater reverse osmosis (SWRO) is essential for producing drinking water in regions with limited freshwater sources, but it generates significant volumes of high-salinity brine. Discharge of this brine into marine environments can lead to ecological harm. With the growing focus on circular economic principles, there is increasing interest in converting this waste stream into a resource. One promising avenue is the recovery of sodium chloride from brine for reuse in the chemical industry. This research transforms this waste stream into a high-purity sodium chloride suitable for the chlor-alkali industry, specifically for disinfectant production. The proposed multi-stage process integrates an oxidation and air stripping stage for bromide elimination, followed by nanofiltration (NF) and ion exchange (IX) for the effective removal of impurities. Laboratory-scale experiments using real SWRO brine have demonstrated the system's efficacy. Optimized oxidation conditions successfully removed bromide to a low concentration which meets the stringent target of <10 mg/L required for high-quality disinfectant synthesis. The NF and IX pre-treatments consistently achieved over 90% removal of interfering ions, reducing final concentrations of calcium, magnesium, and sulfate to below 5 mg/L, respectively. This crucial step prevents scaling and ensures the purity of the final product. A key finding was the successful production of a 0.75% sodium hypochlorite solution directly from the treated brine. By turning waste into a resource, this work supports the broader goals of industrial circularity and environmental sustainability.

Keywords: SWRO brine, resource recovery, sodium chloride, nanofiltration, chloro-alkali

Engineering Metal Anodes for High-rate Solid-state Batteries

M. M. Shaijumon[1,2]

[1]*School of Physics, Indian Institute of Science Education & Research Thiruvananthapuram, Maruthamala P. O., Kerala, India, 695551*

[2]*Centre for Advanced Materials Research with International Engagement (CAMRIE), Indian Institute of Science Education & Research Thiruvananthapuram, Maruthamala P. O., Kerala, India, 695551*

***Corresponding author e-mail:** shaiju@iisertvm.ac.in

ABSTRACT

Lithium/Sodium metal batteries offer great promise towards realizing high energy density devices. However, challenges such as lithium/sodium metal degradation and dendrite growth remain critical, especially when using lean metal anodes. We present some of our recent effrots in exploring efficient strategies toward modifying the current collectors for stable anode-less Li/Na metal batteries. For example, a thin layer of copper selenide grown on commercial Cu foil via chemical vapor deposition and subsequently lithiated to form a Li_2Se matrix with interspersed Cu particles serves an efficient current colletor. During lithium plating, the electroplated lithium is encapsulated within the Cu-Li_2Se matrix in a protective configuration, contrasting the exposed and dendritic lithium deposition observed on bare copper current collectors. This beneficial interface layer facilitates the guided migration of lithium ions toward the base Cu substrate, driven by its negative potential, thereby minimizing direct lithium metal exposure to the corrosive electrolyte. Full cell studies carried out using LFP cathodes, and carbonate-based electrolytes (without additives) demonstrate superior cycling stability. We further address similar issues in sodium metal batteries through a simple yet effective surface modification using an indium oxychloride coating on the current collector. Formation of an artificial SEI hybrid layer composed of NaIn and sodium oxychloride (Na3OCl) results in enhanced ion diffusion, improved interfacial stability, and space charge regulation to enable uniform dendrite-free sodium deposition. These studies provide insights into interfacial engineering strategies for future solid-state battery designs.

References

1. D. Lin et al., *Nat. Nanotechnol.*, 2017, **12**,196– 206.
2. B. Liu et al, *Joule*, 2018, **2**, 833–845.
3. N. Rajasekharan et al., *Adv. Funct. Mater.*, 2025, 2502473.

IT-030

Probing Dopant-Induced Quantum Structures by Tunneling Spectroscopy in Silicon Nanodevices

Daniel Moraru[*1,2,3], Daris Alfafa[2,3], Marius Dobromir[4], and Arief Udhiarto[3]

[1]*Research Institute of Electronics, Shizuoka Univ., Japan*

[2]*Graduate School of Science and Technology, Shizuoka Univ., Japan*

[3] *Institute for Interdisciplinary Research, "Alexandru Ioan Cuza" Univ. Iasi, Romania*

[4]*Dept. of Electrical Engineering, Faculty of Engineering, Universitas Indonesia*

***Corresponding author e-mail:** moraru.daniel@shizuoka.ac.jp

ABSTRACT

Quantum tunneling provides a powerful transport mechanism that can be exploited not only for device operation, but also as a spectroscopic probe of nanoscale electronic structure [1,2]. In our ultra-thin silicon-on-insulator (SOI) devices, fabricated using our Cleanroom facilities, quantum tunneling can be explored either as single-electron tunneling (SET) in transistors[3,4] or as band-to-band tunneling (BTBT) in diodes[5,6]. Such mechanisms are highly sensitive to potential fluctuations induced by inherent dopant randomness. Here, we present an investigation of various methods for spectroscopy analysis of thin SOI highly-doped films, including devices, revealing the possibility of probing dopantinduced quantum structures. First, we show the macroscopic properties of SOI films from techniques such as XPS [7], which set the ground for a deeper understanding of the impact of dopants on crystalline films of silicon. Second, we discuss the role of dopant clusters as quantum dots (QDs) and the possibility of detailed SET-based spectroscopy of such QDs, when embedded into nanoscale channels of transistors [8,9]. Third, we address the impact of dopant-induced perturbation of potential in nanoscale depletion regions of highly-doped pn diodes [4,10,11], especially on the electron waves during BTBT transport. Overall, our results establish tunneling-based spectroscopy as a sensitive probe of atomic-scale disorder, providing further insights when combined with materialcharacterization techniques for the engineering of future atomic-level electronics.

Keywords: silicon-on-insulator, dopant-induced quantum dots, quantum tunneling

References:

1. D. Moraru et al., Nanoscale Res. Lett. 6, 479-1-9 (2011).
2. D. Moraru et al., Nanoscale Res. Lett. 10, 372-1-10 (2015).
3. M. Tabe et al., Phys. Rev. Lett. 105, 016803 (2010).
4. A. Udhiarto, D. Moraru, T. Mizuno, and M. Tabe, Appl. Phys. Lett. 99, 113108 (2011).
5. M. Tabe et al., Appl. Phys. Lett. 108, 093502 (2016).
6. A. Udhiarto et al., Jpn. J. Appl. Phys. 60, 024001 (2021).
7. T. T. Jupalli, D. Alfafa, M. Dobromir, and D. Moraru, Phys. Stat. Sol. A (online, 2026).
8. A. Afiff et al., and D. Moraru, Applied Physics Express 12, 085004_1-5 (2019).
9. T. T. Jupalli et al., and D. Moraru, Applied Physics Express 15, 065003 (2022).

IT-031

Cost-Effective Reference Materials Development using Spark Plasma Sintering for Thermoelectric Applications

Saravanan Muthiah[1,2]*

[1]*CSIR-National Physical Laboratory, Dr K.S. Krishnan Marg, New Delhi-110012, India*

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India*

***Corresponding author e-mail:** msaravanan04@gmail.com,saravanan.nplindia@csir.res.in

ABSTRACT

Thermal diffusivity measurement via flash analysis techniques has become popular among other thermal-conductivity measurements in homogeneous solid materials, such as metals, alloys, ceramics, semiconducting compounds, and thermoelectric materials. Also, the small disc specimen requirement and fast measurements make the flash analyser more competitive in continuous, mass, and inline quality manufacturing units in the thermal management sector.

The thermal analyser includes a flash source, thermal couples, and a detector for rear-face temperature rise and specimen thickness to estimate the specimen's thermal diffusivity. All sources involved in the measurement have associated sub-measurements with uncertainties. Combining all uncertainties and ensuring that the specimen's thermal diffusivity is measured at every measurement point is a cumbersome exercise. Though the direct method of error analysis in thermal diffusivity measurement emphasises accurate calibration and standardisation of the measurement, complexity arises from the consideration of several independent parameters. Here, the pure alumina material, synthesised by rapid compaction spark plasma sintering, was used to validate the thermal diffusivity measurement. The indirect validation technique, with its computed thermal diffusivity values, is compared with an independent flash analyser at multiple locations to verify the results. The proposed SPS-sintered Alumina reference material, which validates thermal diffusivity values by an indirect method, provides a low-cost solution for fast testing at the production line.

IT-032

Detector Grade CdZnTe Single Crystals for Room Temperature Gamma-ray Detector Applications

S.Ganesamoorthy

Radiological Applications and Development Division, SQRMG, IGCAR, Kalpakkam

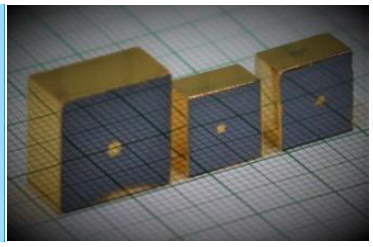
***Corresponding author e-mail:** sgm@igcar.gov.in

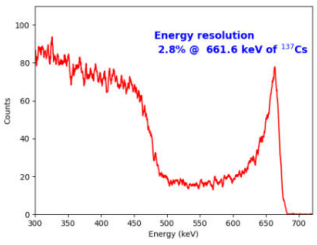
ABSTRACT

Radiation detections and radio isotope identification are of paramount importance in DAE. Cadmium Zinc Telluride (CZT) with its wide band gap (1.56 eV) and high electron density is an apt material for compact radiation detectors to be used at room temperature in comparison to HpGe which requires cryo cooling. CZT single crystals are grown using travelling heater method by a modified high temperature solution growth in excess of Tellurium. The growth process yields 20 mm diameter and 100 mm long single crystal boules from which useful elements of dimensions 10 mm X 10 mm X 5 mm are harvested after identifying regions with Te inclusion size less than 5 microns with uniform distribution using IR transmission microscopy. Subsequently, the surface states of these elements are modified by chemical etching and gold electrodes are deposited in a quasi-hemispherical (QH) geometry to maximise the electron collection efficiency. Using these gold-electroded CZT elements, along with a preamplifier, shaping amplifier and multichannel analyser battery powered portable gamma-ray spectrometers have been demonstrated with energy resolution of 2.8 % at 662 keV gamma-ray from 137Cs source.

Portable gamma spectrometer, QH electrode CZT elements and Gamma ray spectrum of 137Cs photo peak showing 2.8% energy resolution







Development of Plastic Scintillators Having Fast Response Using Perovskite Quantum Dots

Masanori Koshimizu[1]*

[1]Research Institute of Electronics, Shizuoka University, Hamamatsu, Shizuoka 432-8011, Japan

*Corresponding author e-mail:koshimizu.masanori@shizuoka.ac.jp

ABSTRACT

Scintillators are a kind of phosphor that can be used for real-time radiation detection. Among scintillators based on various inorganic and organic compounds, plastic scintillators are widely used owing to their low cost, scalability, and fast scintillation decay. They are composed of host polymers and organic luminescent molecules. One of the drawbacks of plastic scintillators for X-ray and gamma-ray detection is their low interaction efficiency due to the low atomic numbers of the constituent elements. An effective method to enhance the interaction efficiency is the loading of nanoparticles containing heavy elements [1–3]. The interaction efficiency has successfully enhanced by the loading of the nanoparticles, whose scintillation emission efficiency and the absorption probability of the scintillation emission of the plastic scintillators are negligible. To enhance interaction efficiency by loading nanoparticles, an alternative method is the loading of emissive nanoparticles. An effective candidate is semiconductor quantum dots having high photoluminescence quantum yields and fast photoluminescence decay. Among them, perovskite quantum dots based on lead halide have fast photoluminescence decay [4,5]; hence, the loading of the perovskite quantum dots is preferable to achieve fast scintillation decay. In this talk, I will briefly discuss the recent results on the development of plastic scintillators

References:

1. Masanori Koshimizu, Funct. Mater. Lett. 13 (2020) 2030003.
2. Masanori Koshimizu, Jpn. J. Appl. Phys. 62 (2023) 010503.
3. Masanori Koshimizu, J. Lumin. 278 (2025) 121008.
4. Arisa Magi, Masanori Koshimizu, Atsushi Sato, Yutaka Fujimoto, Shunji Kishimoto, Takayuki Yanagida, Keisuke Asai, Jpn. J. Appl. Phys. 62 (2022) SB1036.
5. Atsushi Sato, Yutaka Fujimoto, Keisuke Asai, Masanori Koshimizu, Jpn. J. Appl. Phys. 63 (2024) 01SP06.

IT-034

Finite-Difference Steepest Descent (FDSD) Method for Modeling Light Propagation in Structures with Metal Nanoparticles

Jevgenijs Kaupužs*[1], Svitlana Bugaychuk[2], Majid Taki[2], Pavels Onufrijevs[1], Oleksandra Gridyakina[3], Tomasz Wolinski[3], Janusz Parka[4]

[1]*Institute of Physics and Materials Science, Riga Technical University, Riga, Latvia, LV-1048*

[2]*PhLAN, University of Lille, Lille, France, 59655*

[3]*Faculty of Physics, Warsaw University of Technology, Warsaw, Poland, 00-665*

[4]*Faculty of Advanced Technologies & Chemistry, Military University of Technology, Warsaw, Poland, 00908*

***Corresponding author e-mail:** jevgenijs.kaupuzs@rtu.lv

ABSTRACT

We investigate light propagation in structures with regularly arranged metal nanoparticles based on Maxwell's equations for electromagnetic waves. Recently, we proposed a numerical method for solving such problems [1], which has now been substantially improved. Unlike the finite-difference time-domain (FDTD) method, which solves time-dependent wave equations, our approach directly computes stationary electromagnetic field amplitudes from a system of linear algebraic equations, offering enhanced numerical stability.

In this work, we present a new and significantly more efficient solution strategy compared with the Gaussian elimination method used previously. The proposed algorithm is based on an iterative steepest descent method combined with several optimization procedures, leading to a major improvement in computational efficiency. This advancement enables the effective treatment of data-intensive problems involving reflection, scattering, and absorption of electromagnetic waves in complex structures, including solar cells and hybrid liquid-crystal devices [2]. The method is validated by demonstrating convergence to the analytical Mie solution for a spherical particle. In this benchmark test, our approach shows substantially better performance than standard FDTD simulation software.

The authors acknowledging support from the ERA-NET Co-fund M-Era.NET 3 project under Horizon Europe: "Optically Addressed Fast Inorganic-Organic Interface for Advanced Optics and Terahertz Photonics" (INORIN).

References:

1. J. Kaupužs, et.al., Coatings, 14 (2024) 1612.
2. S. Bugaychuk, et.al., Appl. Nanoscience, 10 (2022) 4965.

IT-035

Low-Temperature Sintering Copper Particle Technology - Figure Joining and Conductive Materials for Semiconductor Industry

Tetsu YONEZAWA*[1]

[1]*Divison of Materials Science and Engineering, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido 060-8628, Japan*

***Corresponding author e-mail:** tetsu@eng.hokudai.ac.jp

ABSTRACT

Low-temperature sintering copper particle technology has emerged as a promising alternative to conventional soldering and silver nanoparticle bonding for next-generation semiconductor packaging. With the rapid expansion of wide-bandgap power devices such as SiC and GaN, there is an increasing demand for joining and conductive materials that combine high thermal and electrical conductivity, mechanical reliability, and compatibility with low-temperature processing. Copper, owing to its low cost and excellent intrinsic properties, is an attractive candidate; however, its strong tendency toward oxidation has long hindered practical low-temperature sintering.

In this work, we present a comprehensive framework for low-temperature sintering copper particle technology, encompassing particle synthesis, surface chemistry control, paste formulation, and joining process optimization. Copper and sub-oxide copper particles with controlled surface reactivity are synthesized via wet-chemical routes, enabling the formation of highly active surfaces that promote sintering at temperatures below 200 °C. Particular emphasis is placed on the role of surface ligands, residual organics, and transient oxide species in governing particle–particle necking and densification behavior.

Sintering and joining experiments demonstrate that dense, conductive copper layers and Cu–Cu joints can be achieved under mild thermal conditions, with or without external pressure, depending on solvent systems and additive design. Microstructural analyses using SEM, TEM, and XRD reveal the evolution of grain growth, neck formation, and porosity reduction, while thermomechanical and electrical evaluations confirm suitability for semiconductor interconnect and die-attach applications.

The presented technology offers a scalable and environmentally benign pathway toward replacing high-cost silver-based materials and conventional solders. By integrating materials chemistry with process engineering, low-temperature sintering copper particle systems provide a versatile platform for advanced functional materials and reliable semiconductor packaging.

IT-036

Terahertz Spectroscopic and Imaging of Composite Materials

A.Mercy Latha

ABSTRACT

Terahertz (THz) spectroscopic and imaging techniques have emerged as a powerful characterization tool for advanced composite materials, owing to their sensitivity to molecular vibrations, dielectric contrast, and internal structural features. The composite materials are engineered by combining two or more distinct materials with different properties to achieve superior mechanical, thermal or electrical properties. THz spectroscopic analysis enables the extraction of frequency dependent material properties, namely, refractive index, absorption coefficient, etc., providing insights into material composition, fiber-matrix interactions, and moisture ingress. Complementary THz imaging facilitates the visualization of internal features, including structural inhomogeneities, interfacial defects, and damage progression, in a contact-less and non-ionizing manner, offering a valuable non-destructive evaluation (NDE) tool for composites. The NDE of composites is typically challenging as they are heterogenous, and anisotropic in nature, causing complex wave scattering, attenuation, and defect masking that makes flaw detection and characterization difficult with conventional techniques. In this invited talk, different use cases where THz spectroscopic and imaging techniques have been employed for the characterization and analysis of various composite materials including glass-fiber reinforced polymer, carbon-fiber reinforced polymer, ceramic matrix composite, sandwich materials, etc., will be presented.

Fluorescence Anisotropy and Chiroptical Luminescence: From Anisotropic Photoluminescence Probing to Cholesteric Liquid Crystal Control

Vincent K. S. Hsiao

Department of Applied Materials and Optoelectronic Engineering, National Chi Nan University, Nantou, 54561, Taiwan

***Corresponding author e-mail:** kshsiao@ncnu.edu.tw

ABSTRACT

Fluorescence anisotropy and chiroptical luminescence provide powerful optical probes for revealing molecular chirality, orientation, and excited-state dynamics in complex photonic systems. In this keynote, I will first introduce our recent work on probing molecular chirality and optical activity through the anisotropic photoluminescence of porous silicon. By exploiting the intrinsic anisotropic emission of porous silicon, we demonstrate a polarization-resolved fluorescence approach capable of distinguishing enantiomeric organic molecules and monitoring photoinduced molecular transformations with enhanced sensitivity. This method offers a solid-state platform for fluorescence anisotropy measurements beyond conventional solution-based techniques.

Building on this concept of anisotropic and polarization-controlled emission, the second part of the talk extends to chiroptical luminescence control using cholesteric liquid crystals. Cholesteric liquid crystals provide a self-organized helical photonic environment that can strongly couple with chiral luminescent molecules, enabling amplification, modulation, and even switching of circularly polarized luminescence through external stimuli such as electric fields and temperature. By comparing these two material systems, this talk highlights how fluorescence anisotropy and chiral photonic structures can be synergistically utilized to control and enhance chiroptical emission. The insights presented here offer new perspectives for designing advanced optical sensing platforms and tunable chiral photonic devices.

IT-039

Structure-Function Modulation in Semiconductor Heterostructures for Efficient Solar Fuel Production

Srabanti Ghosh*, Dipendu Sarkar, Jishu Pramanik

[1]*Energy Materials & Devices Division (EMDD), CSIR - Central Glass and Ceramic Research Institute, Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, India*

[2]*Academy of Scientific & Innovative Research (AcSIR), 201 002, Ghaziabad, India*

***Corresponding author e-mail:** srabanti.cgcri@csir.res.in

ABSTRACT

Structure–Function modulation in semiconductor heterostructures, through the deliberate tuning of structural features at the atomic and nanoscales, enhances the photocatalytic efficiency of coupled semiconductor systems capable of driving multi-electron solar-to-chemical transformations, including water splitting for H_2 production, CO_2 reduction to value-added fuels, and N_2 fixation to NH_3 [1]. Engineering parameters, such as crystal phase, interface bonding, defect density, and heterostructures, enable precise control of electronic structure, band alignment, and interfacial charge dynamics. Strategic construction of type-II, Z-scheme, or S-scheme heterojunctions further allows selective retention of strong redox potentials while suppressing charge recombination. A wide range of representative systems, metal oxides, conducting polymers, bismuth oxyhalides (BiOX; X = Cl, Br, I), metal chalcogenides, oxide perovskites, and their heterostructures have been extensively investigated to clarify how these parameters influence light harvesting, charge carrier generation, and charge separation dynamics [2]. For example, layered BiOCl, owing to its intrinsic internal electric field derived from its unique crystal structure, exhibits markedly improved charge separation. When integrated into a heterostructure with Cu_2SnS_3, atomic-scale interfacial Bi–S bonds are formed, acting as effective charge-transfer channels between the two semiconductors and significantly boosting H_2 production efficiency [3]. More recently, atomic-level interface engineering and the establishment of built-in electric fields in S-scheme $Bi_2WO_6/ZnIn_2S_4$ heterojunctions have demonstrated pronounced improvements in water splitting [4]. A new class of $Sr_3FeCoO_{6.72}$ (SFC)-based composites have been introduced as catalysts for nitrogen reduction, where enhanced interfacial charge transfer and increased exposure of active sites improve the efficiency of NH_3 synthesis [5]. Parallel efforts toward practical implementation have led to the development of an indigenous prototype device for scalable applications. Collectively, structure–function modulation in semiconductor heterostructures establishes a powerful design paradigm for optimizing multifunctional performance in photocatalysis, enabling efficient solar energy conversion and stability, and selectivity for solar-driven fuel production.

References:

1. Song, H.; Luo, S.; Huang, H.; Deng, B.; Ye, J. ACS Energy Lett. 2022, 7, 1043–1065.
2. Ghosh, S.; Natalie, K. A.; Ramos, L.; Remita, S.; Dazzi, A.; Besseau, A. D.; Goubard, F.; Aubert, P.-H.; Remita, H. Nat. Mater. 2015, 14, 505–511.

MEMS Microcantilever Sensors Functionalized with ZnO Nanorods for High-Sensitivity Gas Detection

Ratno Nuryadi*[1], Lia Aprilia[2]

[1,2]Research Organization for Nanotechnology and Materials, National Research and Innovation Agency (BRIN), South Tangerang, Banten 15314, Indonesia

*Corresponding author e-mail: ratno.nuryadi@brin.go.id

ABSTRACT

The increasing demand for real-time and high-sensitivity monitoring of environmental parameters has accelerated the development of micro- and nanoscale sensing technologies. Microelectromechanical systems (MEMS) sensors offer attractive features, including miniaturization, low power consumption, and compatibility with various sensing modalities. In parallel, nanostructured materials such as zinc oxide (ZnO) nanorods have emerged as promising functional layers due to their excellent electronic, mechanical, and surface properties. In this study, MEMS-based microcantilever sensors functionalized with ZnO nanorods are investigated for gas-sensing applications.

ZnO nanorods were synthesized directly on the microcantilever surface via a hydrothermal method, resulting in a high surface-to-volume ratio that enhances molecular adsorption. To further improve gas sensitivity and selectivity, the ZnO nanorods were decorated with aluminum (Al) and platinum (Pt) nanoparticles. The sensing performance was evaluated under dynamic mode operation, where resonance frequency shifts were employed as the primary sensing metric.

The experimental results demonstrate that the functionalized MEMS microcantilever exhibits excellent gas-sensing performance, achieving ultrahigh sensitivity down to the picogram-level mass loading. Al-decorated ZnO nanorods showed enhanced sensitivity toward carbon monoxide (CO) at room temperature. The sensor also responded to carbon dioxide (CO_2) and methane (CH_4) with comparatively lower sensitivity, while Pt decoration significantly enhanced the response to CH_4, indicating the contribution of catalytic effects in gas adsorption. Repeated measurements confirmed good reproducibility and operational stability. Overall, this work highlights the strong potential of ZnO-nanorod-functionalized MEMS microcantilever sensors as versatile and reliable platforms for advanced gas and environmental monitoring applications.

References:

1. L. Aprilia, R. Nuryadi, M. Hosoda, M. A. Barique, A. Udhiarto, D. Hartanto, Y. Neo, H. Mimura, Jpn. J. Appl. Phys., 59 (2020) 077003.
2. R. Nuryadi, L. Aprilia, M. Hosoda, M. A. Barique, A. Udhiarto, D. Hartanto, M. B. Setiawan, Y. Neo, H. Mimura, Sensors, 20 (2020) 2013.
3. L. Aprilia, R. Nuryadi, A. G. Saputro, S. A. Wella, I. M. Isa, S. A. Bakar, Y. Neo, H. Mimura, IEEE Sensors J., 24 (2024) 29806–29813.
4. F. Dzulfiqar, L. Aprilia, A. Udhiarto, R. Nuryadi, IEEE Trans. Instrum. Meas., 74 (2025) 2009110.

IT-041

Non-collinear antiferromagnets for spintronic applications

Binoy K. Hazra

Department of Physics, Indian Institute of Technology Guwahati, 781039, Assam, India

ABSTRACT

Antiferromagnetic materials are considered a promising alternative to conventional ferromagnets for spintronic applications. They are resistant to external magnetic interference, have very fast spin dynamics, produce minimal magnetic stray fields, and exhibit unique magneto-optical and magneto-transport properties. However, these inherent characteristics also pose challenges for their manipulation and for reading their magnetic states, which need to be addressed in order to make antiferromagnets a practical choice for spintronic applications. In the first part of my talk, I will discuss a new mechanism to manipulate the magnetic states of a non-collinear antiferromagnet that goes beyond a simple spin-orbit-torque mechanism1. In the second part, I will discuss generating robust spin currents in epitaxial thin films of a noncollinear antiferromagnet.

References:

1. B. Pal et al. *Sci. Adv.* **8**, eabo5930 (2022).
2. B. K. Hazra *et al. Nat. Commun.* **14**, 4549 (2023).

IT-043

Reactive Glass–Metal Interaction under Ambient Conditions Enables Surface Modification of Gold Nano-islands

Amarnath R. Allu [1,2]

[1]CSIR-Central Glass and Ceramic Research Institute, Kolkata, 700032, India

[2]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India

ABSTRACT

Stabilizing gold nanoparticles with controllable surface composition through reactive metal–support interactions under ambient conditions is highly challenging. In this work, we introduce reactive glass–metal interaction (RGMI) as a robust route to engineer thermally stable gold nano-islands (GNIs) with tunable surface chemistry. By systematically varying the composition of sodium aluminophosphosilicate (NAPS) glass, we demonstrate that the glass matrix actively governs interfacial reactions, leading to enhanced stability of gold nanostructures at moderate temperatures (550 °C) under ambient conditions. Detailed structural and spectroscopic analyses reveal that the adsorption and intercalation of Na and P species at the GNI surface induce lattice distortions in the Au(111) planes and generate additional electronic states near the Fermi level. Notably, this method eliminates the need for chemical precursors, reducing agents, high-temperature processing, or prolonged synthesis durations, thereby providing a sustainable and straightforward fabrication approach. Furthermore, the engineered GNI–glass interface modulates hot-carrier dynamics by prolonging electron lifetimes, which is advantageous for catalytic activity. Overall, RGMI emerges as a versatile platform for designing thermally robust, multi-element nanostructures with significant potential in catalysis, sensing, and optoelectronic applications.

References:

1. Haque, S.; et al. *Adv. Funct. Mater.* **2025**, e27669.

IT-044

From Earth to Mars: Pioneering Metal-Carbon Dioxide (Metal-CO_2) Battery Solutions for a Greener Tomorrow

Chandra Shekhar Sharma

Department of Chemical Engineering, Indian Institute of Technology, Hyderabad, India.

***Corresponding author e-mail**: cssharma@che.iith.ac.in

ABSTRACT

As climate change intensifies, energy solutions for Earth have become crucial towards a sustainable future. Metal-carbon dioxide (CO_2) batteries offer a transformative approach, converting CO_2 into usable energy while addressing carbon management and reducing emissions. Beyond Earth, these batteries hold significant potential for Mars, where CO_2 is abundant (95 %) providing essential power for future colonies, supporting habitats and life support systems. By harnessing the in-situ resources of Mars, metal-CO_2 batteries could enable sustainable living on the Red Planet. However, its practical implementation faces challenges, including low cyclability, high overpotentials, and poor reversibility due to the thermodynamic stability of discharge products like Li_2CO_3 and amorphous carbon.[1–4] Our work addresses these challenges by developing unique catalysts including carbon, transition metals, composite nanoparticles. These catalysts enhance the CO_2 reduction and therefore the cyclability of the system. Their bifunctional catalytic behavior helps reduce the activation energy required for the decomposition of the Li_2CO_3 and amorphous carbon, resulting in enhanced reversibility. Benefitting from this, we were able to achieve a cycle life of ~200 cycles at the current density of 500 mA g-1 for a limited capacity of 500 mAh g-1 along with an operational time exceeding 600 hours. Additionally, we explored translating the system from lithium to the more abundant sodium and potassium metals, paving the way for future sustainable energy solutions.[5–9].

References:

1. K. Chourasia, M. Shavez, K. M. Naik, C. Bongu, C. S. Sharma, ACS Appl. Energy Mater. 2023, 6, 378.
2. K. Chourasia, K. M. Naik, C. S. Sharma, Batter. Supercaps 2023, n/a, e202300328.
3. K. Chourasia, A. D. Pathak, C. Bongu, K. Manikandan, S. Praneeth, K. M. Naik, C. S. Sharma, Small Methods 2022, 6, 2200930.
4. K. Chourasia, K. M. Naik, N. K. Apparla, Surya Babu S., A. Mall, Srijina M., C. S. Sharma, in (Ed: J.B.T.-E. of E.P.S. (Second E. Garche), Elsevier, Oxford, 2025, pp. 347–357.
5. K. M. Naik, A. Kumar Chourasia, C. S. Sharma, Chem. Eng. J. 2024, 490, 151729.
6. K. M. Naik, A. K. Chourasia, M. Shavez, C. S. Sharma, ChemSusChem 2023, 16, e202300734.
7. A.K. Chourasia, K. M. Naik, C. S. Sharma, Carbon N. Y. 2024, 218, 118754.
8. K. M. Naik, A. K. Chourasia, C. S. Sharma, J. Power Sources 2024, 608, 234623.
9. A.D. Pathak, A. K. Chourasia, C. S. Sharma, J. Power Sources 2024, 616, 235131.

Nanomechanical Metamaterials and Multifunctional Metalenses

Bruce(Jun-Yu) Ou

School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom

ABSTRACT

We first overview the recent advances in plasmonic or dielectric nanomechanical metamaterials fabricated on elastic nanomembranes of silica or silicon nitride. Such metamaterials allow nanometric displacement of their building blocks under external forces and can be reconfigured with external stimuli to achieve optical modu-lation at high frequencies. Mechanical and optical resonances enhance the magnitude of actuation and opti-cal response within these nanostructures, which can be driven by electric signals of only a few volts, micro-watt optical, or acoustic signals. These approaches allow a range of functionalities to be achieved through optical elements of sub-micron thickness, including sensing, light modulation, and nonlinear effects.

In the second part of the talk, we will showcase a few multifunctional microscopes based on flat optics and engineered metalens. Our results could open new applications in biomedical imaging, machine vision, and semiconductor inspection.

IT-046

Water-based Solid Battery using 3D-Slime Interface quasi-Solid Electrolyte (3D-SLISE)

Yosuke Shiratori[1], Shintaro Yasui[1,2,*]

[1]*Laboratory for Zero-Carbon Energy, Institute of Science Tokyo, Tokyo, Japan*

[2]*Materials and Structures Laboratory, Institute of Science Tokyo, Yokohama, Japan*

***Corresponding author e-mail:** yasui.s.6818@m.isct.ac.jp

ABSTRACT

The development of sulfide-type solid electrolytes has been investigated for the practical application of all-solid-state batteries with high energy density. However, sulfide-type solid electrolytes are known to react with moisture in the atmosphere to generate hydrogen sulfide. On the other hand, atmospherically stable oxide-type solid electrolytes are investigated for safer use. In addition, completely new high ionic conductivity electrolytes have been proposed, such as hydrate melts and silica-ionic liquid composites, which have attracted much attention due to their aqueous processes, low-temperature operation, and rapidly expanding process/application windows. More recently, flexible oxide-polymer composite solid electrolytes with excellent electrochemical properties have been reported. We have developed a series of oxide-based composite solid electrolytes with superior ionic conductivity in the order of several mS/cm and handling properties into the air to realize environmentally benign and formable solid-state lithium-ion batteries. Although "water-prohibition" is common in the battery world, we dared to use water processing to consider environmental harmonization and cost performance. As long as water is used, control of water electrolysis is very important, but this can be cleared by precise control. Our prepared batteries showed promising room-temperature charge-discharge properties under a stack pressure of 30 MPa, with over 2,000 cycleability at 3C operation and no discharge capacity reduction compared to the first cycle. We will provide detailed information of completely new solid-state batteries.[1,2)]

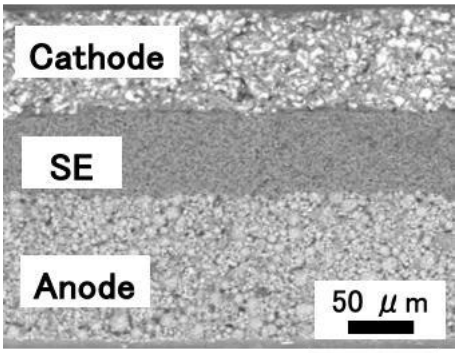


Fig. 1 (a) Cross-sectional SEM image of battery cell

Keywords: Solid-state battery, Water-based, Safe, Low-cost, Air-handling, Direct-recyclable

References:

1. Y. Shiratori et al., Adv. Mater., 37 (2025) 2505649.
2. Y. Shiratori et al., Adv. Energy Mater., under review.

Utilizing CO_2 for Synthesis of Organic Carbonates via Direct Carbonylation of Glycerol

Wan-I Chen, Ya-Chen Yu, Bing-Hung Chen*

Department of Chemical Engineering, National Cheng Kung University, Tainan, 70101, Taiwan

*Corresponding author e-mail: bkchen@ncku.edu.tw

ABSTRACT

This study investigates the CO_2 utilization to produce glycerol carbonates via the direct carbonylation of glycerol with CO_2 over ZnO-based catalysts. Owing to the high stability of both glycerol and CO_2, the direct carbonylation reaction is difficult to proceed, requiring high-temperature and high-pressure conditions, which significantly increase equipment and operational costs [1, 2]. Several factors influence the reaction outcome, including reaction temperature, pressure, solvent ratio, and catalyst dosage. Typically, the carbonylation reactions in this work were carried out at 5 MPa CO_2 at 180°C with 2-cyanopyridine and ethanol as dehydrating agents. ZnO/ZrO_2 catalysts were synthesized with the incipient wetness impregnation method to facilitate the reaction (Figure 1). Specifically, $Zn(NO_3)_2 \cdot 6H_2O$ was used as the precursor, while ZrO_2 served as the support. ZnO was loaded onto ZrO_2 via the wet impregnation method, forming a ZnO/ZrO_2 catalyst. The catalyst was characterized using various analytical techniques, including XRD, SEM, EDS, Nitrogen physisorption analyzer, CO_2-TPD, and ICP-OES. The yield of glycerol carbonate was adopted as the response variable, while the optimal reaction condition was sought via the response surface methodology (RSM) with a central composite design (CCD) [3]. Explicitly, a quadratic polynomial equation to describe the yield of glycerol carbonate was obtained by fitting the experimental data. The optimal condition was thus extracted from the established further verified with independent sets of experiments performed in the proximity to the optimal condition.

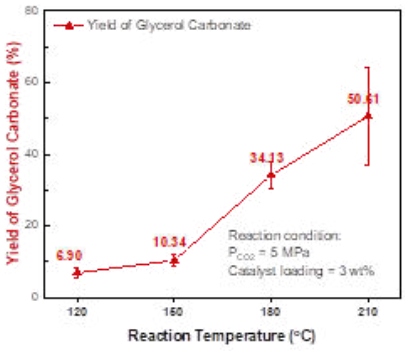


Figure 1. Effect of reaction temperature on the yield of glycerol carbonate via the direct carbonylation of glycerol with CO_2.

References:

1. J. Liu, D. He, Transformation of CO_2 with glycerol to glycerol carbonate by a novel $ZnWO_4$-ZnO catalyst. Journal of CO_2 Utilization, 26, 370-379 (2018).
2. S. Lukato, G.N. Kasozi, B. Naziriwo, E. Tebandeke, Glycerol carbonylation with CO_2 to form glycerol carbonate: A review of recent developments and challenges. Current Research in Green and Sustainable Chemistry, 4, 100199 (2021).
3. D.C. Montgomery, Design and Analysis of Experiments, 10th ed. 2019: Wiley.

Microstructural dynamics of stretching nanofilm of hydrogels: effects of film thickness on mechanical properties

Chia-Yu Liao[1], Chih-Jung Lin[2], Yu-Jane Sheng[*,2], and Heng-Kwong Tsao[1]

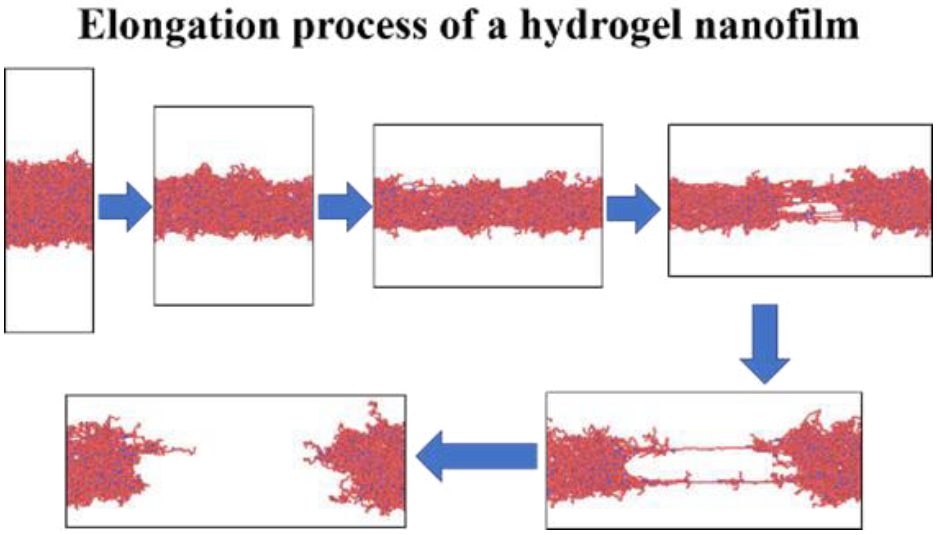
[1] Department of Chemical and Materials Engineering, National Central University, Taoyuan 32001, Taiwan, ROC

[2] Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan, ROC

*Corresponding author e-mail:yjsheng@ntu.edu.tw

ABSTRACT

While stretching hydrogel nanofilms enables the acquisition of stress-strain curves, deciphering the internal structure and mechanisms through experiments remains challenging. In this work, dissipative particle dynamics simulations are employed to observe microstructural changes in elongated hydrogel nanofilms. The morphological changes of the film, up to the point of fracture, are observed, and the corresponding stress-strain curve is obtained. Microscopic characteristics, including polymer size, strand size, and bond length, are systematically analyzed to understand the network's deformation. Additionally, the breakages of polymers, strands, and bonds are closely monitored. In a thin film, the microstructure of the interfacial region differs from that of the bulk region, with the latter enduring more forces during extension. Consequently, as film thickness increases, the contribution from the bulk region becomes more pronounced, leading to a further enhancement of mechanical properties.



IT-049

Modulation of the Interfacial Lithium-Ion Transport within Lithium Ion Batteries: Insights from Multi-Scale Simulations

Chi-Cheng Chiu*[1,2,3,4]

[1]*Department of Chemical Engineering, National Cheng Kung University, Tainan 701, Taiwan*

[2]*Center for Resilience and Intelligence on Sustainable Energy Research (RiSER), National Cheng Kung University, Tainan 701, Taiwan*

[3]*Program on Smart and Sustainable Manufacturing, Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University, Tainan 701, Taiwan*

[4] *Fire Protection and Safety Research Center, National Cheng Kung University, Tainan 711, Taiwan*

***Corresponding author e-mail:** ccchiu2@gs.ncku.edu.tw

ABSTRACT

Interfacial lithium-ion (Li^+) transport critically governs the rate capability, impedance, and long-term stability of lithium-ion batteries (LIBs), yet its molecular origins remain insufficiently understood due to the complex coupling between chemistry, electrostatics, and structure across multiple length scales. In this work, we utilize a multi-scale simulation framework that integrates molecular dynamics (MD) and kinetic Monte Carlo (kMC) methods to systematically elucidate Li^+ transport mechanisms at key battery interfaces, including electrolyte–cathode and polymer–ceramic boundaries in composite polymer electrolytes (CPEs), as well as electrode–binder–electrolyte systems. MD simulations were employed to resolve the interfacial structure, ion coordination, and electric double-layer behavior induced by different polymer binders, ranging from conventional poly(vinylidene difluoride) to Li^+-coordinating, negatively charged, and zwitterionic polymers. The results reveal that binder charge characteristics strongly regulate local ion distributions and electrostatic potential profiles, leading to pronounced differences in Li^+ mobility and interfacial resistance. Negatively charged binders enhance Li^+ accumulation near Li^+-depleted cathode surfaces, whereas zwitterionic binders suppress excessive ion polarization and mitigate interfacial bottlenecks. To bridge molecular insights with device-relevant transport, kMC simulations under non-equilibrium conditions were conducted using MD-derived descriptors. These simulations demonstrate how binder-induced electrostatic landscapes translate into distinct ion flux responses and impedance characteristics. In parallel, strategies for mitigating polymer–ceramic interfacial resistance in CPEs, such as ceramic surface functionalization and crystallinity modulation, are evaluated. Overall, this work highlights how targeted interfacial chemistry and charge engineering can be leveraged to rationally design next-generation LIB materials with improved ionic transport and performance.

References:

1. H.-S. Liu, Chen, K.-Y. Chen, C.-E. Fang, and C.-c. Chiu, Electrochimica Acta, 2021, 375, 137915
2. Tsao, C.-H. et al. ACS Applied Materials & Interfaces, 2021, 13, 9846–9855.
3. P.-Y. Wang, T.-H. Chiu, and C.-c. Chiu, Polymers, 2024, 16, 319.

IT-050

Telecom Band Silicon Based Optical Defects for Quantum Technologies

Zhiyenbayev[3] Kaushalya Jhuria[1,3], Wei Liu[2], Walid Redjem[3], Debanjan Polley [2,3], Arun Persaud2, Qing Ji[2], Yertay, Vsevolod Ivanov[4], Jacopo Simoni[4], Liang Z Tan[4], Jeffery Bokor[3], Boubacar Kanté[3], and Thomas Schenkel [2]

[1]*Department of Electrical Engineering, Indian Institute of technology, Delhi, Hauz-Khas 110016 2 Accelerator Technology and Applied Physics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

[3]*Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, CA 94720, USA*

[4]*Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

ABSTRACT

Silicon-based quantum emitters are candidates for large-scale qubit integration due to their single-photon emission properties and potential for spin-photon interfaces with long spin coherence times. Here, we demonstrate local writing and erasing of selected light-emitting defects using femtosecond laser pulses in combination with hydrogen-based defect activation and passivation at a single center level. By choosing forming gas (N2/H2) during thermal annealing of carbon-implanted silicon, we can select the formation of a series of hydrogen and carbon-related quantum emitters, including T and Ci centers while passivating the more common G-centers. The Ci center is a telecom S-band emitter with promising optical and spin properties that consists of a single interstitial carbon atom in the silicon lattice. Density functional theory calculations show that the Ci center brightness is enhanced by several orders of magnitude in the presence of hydrogen. Fs laser pulses locally affect the passivation or activation of quantum emitters with hydrogen for programmable formation of selected quantum emitters.

Development of an electron beam–pumped, localized surface plasmon–enhanced nanoscale light source for electron-beam–assisted optical microscopy

Atsushi Nakamura*, Shunpei Shiba, Kei Hosomi, Atsushi Ono, Yoshimasa Kawata, and Wataru Inami

Research Institute of Electronics, Shizuoka University, 3-5-1 Johoku, Hamamatsu, 432-8011 Shizuoka, Japan,

***Corresponding author e-mail:** nakamura.atsushi@shizuoka.ac.jp

ABSTRACT

We demonstrated LSP-enhanced cathodoluminescence (CL) from an ALD-grown $Al_2O_3/ZnO/Al_2O_3$ heterostructure incorporating Ag nanoparticles, aiming to develop a bright nanoscale light source for an EXA optical microscope. The observed luminescence enhancement is attributed to LSP–exciton coupling and the refractive-index gradient of the heterostructure, which improves light-extraction efficiency.

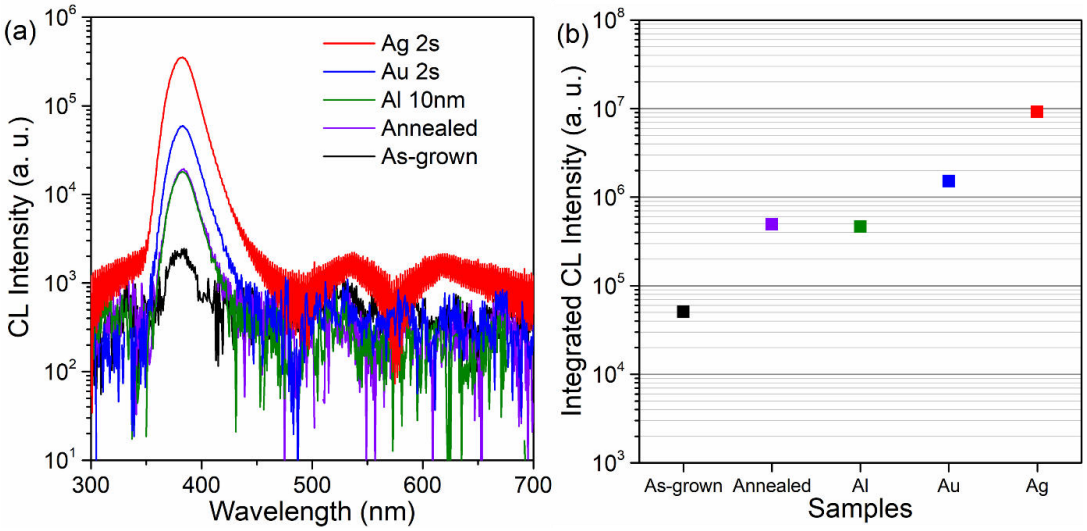


Fig. 1 (a) Comparison of CL spectra for $Al_2O_3/ZnO/Al_2O_3$ heterostructures at different stages of growth/annealing/encapsulation of metals. (b) Comparison of integrated CL intensity for $Al_2O_3/ZnO/Al_2O_3$ heterostructures at different stages of growth/annealing/encapsulation of metals. For the CL measurement, the acceleration voltage was 30 kV and the beam current was 300 nA.

Keywords: Localized surface plasmon; Cathodoluminescence; Atomic layer deposition

References:

1. Nakamura, S. Shiba, K. Hosomi, A. Ono, Y. Kawata, W. Inami, Development of a localized surface plasmon–enhanced electron beam–pumped nanoscale light source for electron beam excitation–assisted optical microscopy, Microscopy 74 (2025) 71–77. https://doi.org/10.1093/jmicro/dfae043.

IT-052

Surface-Induced Photorefractive Effect (SIPRE) In Liquid Crystal Nanocomposites for Applications in Fast Switchable Devices

Svitlana Bugaychuk*[1], Majid Taki[1], Pavels Onufrijevs[2], Jevgenijs Kaupužs[2], Oleksandra Gridyakina[3], Tomasz Wolinski[3], Janusz Parka[4]

[1]*PhLAN, University of Lille, Lille, France, 59655*

[2]*Institute of Physics and Material Science, Riga Technical University, Riga, Latvia, LV-1048*

[3]*Faculty of Physics, Warsaw University of Technology, Warsaw, Poland, 00-665*

[4]*Faculty of Advanced Technologies & Chemistry, Military University of Technology, Warsaw, Poland, 00908*

***Corresponding author e-mail:** svitlana.bugaychuk@univ-lille.fr

ABSTRACT

We present theoretical and experimental studies devoted to new developments of liquid crystals (LC) materials for state-of-the-art applications in photonics. For this purpose, hybrid liquid crystals (HLCs) are manufactured, containing an inorganic nanostructure (a gold nano-island film - Au-NIF) on the surface of one of the HLC cell substrates [1].

The theoretical model of the surface-induced photorefractive effect (SIPRE) [2] at the inorganic/organic interface elucidates the fast electro-optical response in HLC nanocomposites. The SIPRE model encompasses many physical processes, such as the creation of photoinduced unstable charges in LC cells, accompanied by the formation of an internal space-charge electric field; reorientation of LC molecules near the surface; confinement effects at the interface caused by the excitation of the localized plasmon resonance in metal nanoparticles [3]. Theoretical studies are closely linked to experimental achievements, which depend on the morphologies of the Au-NIFs used.

The overall goal of this research is to develop low-cost and efficient materials, with a broad range of applications in all-optical and electro-optical switches. In addition, recent scientific advances show that LCs can be effective materials for miniaturized elements in terahertz (THz) photonics. The authors acknowledging support from the ERA-NET Co-fund M-Era.NET 3 project under Horizon Europe: “Optically Addressed Fast Inorganic-Organic Interface for Advanced Optics and Terahertz Photonics” (INORIN).

References:

1. S. Bugaychuk, et.al., Appl. Nanoscience, 10 (2022) 4965.
2. F. Simoni, L. Lucchetti, Photorefractive Materials and Their Applications, Springer Series in Optical Sciences, 114 (2007) 571.
3. J. Kaupužs, et.al., Coatings, 14 (2024) 1612.

Application of Pulsed Electric Fields in Inorganic Materials Science

Tadachika Nakayama*

[1]*Nagaoka University of Technology,Nagaoka, Niigata, 940-2188, Japan*

***Corresponding author e-mail:** nky15@vos.nagaokaut.ac.jp

ABSTRACT

With the recent development of SiC semiconductor switching devices, nanosecond pulse power supplies are now available at low cost and high performance. Features of pulsed power supplies include the ability to apply an electric field at the timing when an electric field is required and to induce electrochemical reactions for a short period of time. Furthermore, in nanosecond pulse power supplies, the electric field can be reduced to zero before dielectric breakdown occurs. Therefore, nanosecond pulse power supplies can be used to apply voltages as high as 10 times or more than the breakdown voltage. We have used such nanosecond pulsed power supplies to expand into the fields of environmental remediation and energy conversion. Current water treatment is carried out by first precipitating large contamination, followed by microbial or chemical treatment. However, if the contamination is too severe, it cannot be precipitated sufficiently. In this study, the electrocoagulation method is used to quickly precipitate contaminants by electrically forming flocculant particles in the water. However, the problem with this method is that it consumes a large amount of electricity. In this study, however, a pulsed electric field is used to achieve water treatment with about half the power consumption of conventional methods. In terms of energy conversion, more electricity can be generated in pyroelectric power generation by priming the input of an external electric field. At this time, a DC electric field is generally used to realize the Olsen cycle, but by replacing this with a nanosecond pulsed electric field, the input power can be reduced.

IT-054

Complex Interactions Driven Assembly in the Multi-Component Colloids: Insights from Synchrotron SAXS

Jitendra Bahadur[1,2]

[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085, India*

[2]*Homi Bhabha National Institute, Mumbai, 400094, Mumbai, India*

***Corresponding author e-mail:** jbahadur@barc.gov.in

ABSTRACT

Understanding how matter organizes between molecular and mesoscopic length scales remains a central challenge across condensed matter and soft-matter physics. This intermediate mesoscopic length scale is where collective interactions, emergent order, and hierarchical structuring first appear which governs mechanical, optical, and transport properties in both advanced materials and biological systems. Synchrotron-based Small-Angle X-ray Scattering (SAXS) offers a uniquely powerful window into this regime, enabling in situ, in operando, and time-resolved characterization at nanometer length scale in wide range of research areas including soft-matter assemblies, biomolecular complexes, hybrid nanostructures, and functional materials. The talk will highlight the key features and capabilities of the SAXS beamline at Indus-2 synchrotron. It will be shown how the synchrotron SAXS allows us to unravel self-assembly pathways in multi-component colloids with a particular emphasis on the formation mechanisms of hierarchically structured colloidal assemblies directed by cooperative interactions resulting in cluster formation, coacervation, and mesoscale ordering. Self-assembly is a fundamental bottom-up route to constructing complex, hierarchical soft-matter structures, where subtle colloidal interactions dictate the emergent morphology of the resulting superstructures. In multi-component colloidal systems, intrinsic heterogeneity and interactions spanning multiple length scales generate rich physical behavior, dynamic self-organization, and pronounced sensitivity to small external stimuli driven by a delicate balance of enthalpic and entropic forces. Controlling the assembly of colloids into organized structures through electrostatic complexation with oppositely charged polyelectrolytes results in interesting phase diagrams and their tunable interactions and response to external stimuli enable controlled self-assembly into complex structures. Ultimately, these insights reveal why the nanoscale regime is not merely a structural bridge, but the origin of emergent physical properties central to materials science, soft matter, biophysics, and condensed matter research.

References:

1. S Mehta, J Bahadur et al, Langmuir 40, 21352 (2025)
2. S Mehta, J Bahadur et al, Soft Matter 20, 375 (2024

Spintronics using 2D materials

Pranaba Kishor Muduli[1]

[1]*Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India*

ABSTRACT

In this talk, I will explore the application of large-area van der Waals materials such as transition metal dichalcogenides (TMDs) to advance spin-orbit torque (SOT) based spintronic devices, addressing the limitations of conventional heavy metal systems, such as limited charge-to-spin efficiency. Key findings include the observation of large, spin-orbit coupling-dependent spin-to-charge conversion in monolayer TMDs, evidence of unconventional and giant damping-like spin torque conductivity in GeTe. Furthermore, a significant 63% enhancement in effective SOT efficiency was demonstrated in a PtSe2/NiFe heterostructure, with band structure calculations suggesting that a proximity magnetic field at the interface plays a crucial role in the strong charge-to-spin conversion, highlighting a new mechanism for achieving high-efficiency SOT for device commercialisation.

IT-056

Excitonic Signature of 2D Sliding/Interfacial/Moiré Ferroelectrics

Dr. Swarup Deb

Saha Institute of Nuclear Physics, Kolkata

ABSTRACT

Ferroelectricity is a property of certain materials that possess a permanent electric dipole, which can be reoriented by an external electric field - essentially an electrostatic counterpart to ferromagnetism. Since its discovery in the 1920s, ferroelectricity has enabled groundbreaking technologies, including ultrasound imaging (USG), ferroelectric RAM (FE RAM), infrared sensors, miniaturized actuators, etc.

In this talk, I will discuss the emergence of ferroelectricity in ultra-thin, six-atom-thick crystals- a class of two-dimensional (2D) van der Waals materials. Unlike conventional ferroelectrics, where polarization switching is driven by ionic displacement along the field direction, these materials rely on a unique mechanism called "SLIDE-TRONICS." Here, the LATERAL SLIDDING of atoms modulates the OUT-OF-PLANE electric polarization.[1]

Moreover, we find that, contrary to the conventional understanding of electrostatic screening- which suggests that mobile charge carriers should overshadow ferroelectricity - these 2D ferroelectrics retain polarization even under electrostatic doping, while simultaneously exhibiting high conductivity.[1 2]

By the end of this talk, I will highlight a specific class of 2D ferroelectric materials, such as transition metal dichalcogenides (TMDs), and briefly discuss how their properties can be explored using micro-spectroscopy and ultrafast spectroscopy, as well as their potential applications in field-effect optoelectronic devices.[3]

References:

1. Deb, S. et al. Cumulative polarization in conductive interfacial ferroelectrics. Nature 612, 465 (2022).
2. Cao, W. et al. Polarization Saturation in Multi-layered Interfacial Ferroelectrics. Adv. Materials, 2400750.
3. Deb, S. et al. Excitonic signatures of ferroelectric order in parallel-stacked MoS2. Nat Commun 15, 7595 (2024).

IT-057

InGaN LED Technology Trends for Agriculture and Bio-industry Applications: From Spectral Engineering to Van der Waals Epitaxy

Chang-Hee Hong

Department of Semiconductor Science and Technology, College of Science, LED Agri-bio Fusion Technology Research Center, Jeonbuk National University, Jeonju, 54896, Republic of Korea

ABSTRACT

Light-emitting diodes (LEDs) have emerged as an indispensable artificial light source in smart agriculture and bio-industries, transcending simple illumination to serve as a precise tool for biological control. It is because of the specific wavelengths of LEDs are utilized to optimize photosynthesis, photomorphogenesis, and photoperiodism. By tailoring the spectral power distribution, LEDs can enhance crop yields, nutritional quality, and secondary metabolite synthesis.

Despite these advantages, current agricultural LED systems—primarily relying on a combination of AlInGaP-based red and InGaN-based blue LEDs—face significant challenges, including disparate degradation rates, thermal instability, and complex driving circuitry due to inconsistent forward voltages. To address these issues, this paper highlights the potential of an all-InGaN-based single-material system, which offers a unified power platform and superior thermal robustness.

The realization of such a system, however, is hindered by the so-called "Green Gap" and "Red Gap"— the drastic decline in efficiency as indium (In) content increases for longer wavelengths during the growth of metalorganic chemical vapor deposition(MOCVD). We report recent MOCVD epitaxial breakthroughs and mechanical lift-off techniques aimed at overcoming these bottlenecks through high-In content growth strategies, such as strain-relaxed buffer layers and specialized nucleation techniques. Furthermore, we review the status of van der Waals epitaxy and remote epitaxy using 2D materials like graphene and h-BN. These techniques facilitate the growth of high-quality, strain-free InGaN membranes and enable non-destructive "copy-and-paste" transfer to high-thermal-conductivity substrates.

Finally, we discuss a comprehensive technical trend for the next generation of integrated LED solutions for sustainable and high-precision bio-environments.

IT-058

Solid Oxide Electrolysis of CO_2: Power to X

Chinmoy Ranjan[1]*

[1] *Indian Institute of Science, Bengaluru, 560012, India*

***Corresponding author e-mail:** ranjan@iisc.ac.in

ABSTRACT

CO_2 electro-reduction using solid oxide electrodes is one of the most promising technologies for converting CO_2 to fuels (Power to X). CO_2 reducing cathodes such as Ni-YSZ and $MCeO_{2-\delta}$ -YSZ have shown promise in converting CO_2 to CO. In the presence of H_2, these systems are prone to reverse water gas shift reactions and at 800 degrees both electrochemical and thermochemical reactions compete. Our operando studies will report on Ni-YSZ and Ceria -YSZ based electrodes. $CeO_{2-\delta}$ electrodes perform well in both CO_2 and CO_2 ($+H_2$) environments. The CO yield increases with increasing negative bias concomitant with increase in the number of Ce^{3+} sites. Our studies will uncouple production of CO by both thermochemical and electrochemical means and how they are correlated through similar active sites. The studies will highlight mechanistic aspects of both CO production and coking. Nature of the active site will be discussed. Unlike purely thermochemical systems, electrochemical systems present an opportunity to control CO and H2 ratios in syngas using simply bias.

Keywords: CO_2 electrolysis, solid oxide electrolysis, operando spectroscopy

References:

1. Enabling pure CO2 reduction on Ni {Cu} x-YSZ electrode via an oxide-mediated mechanism V Kamboj, S Raychowdhury, C Ranjan, Applied Catalysis B: Environment and Energy 344, 123631
2. Operando studies on solid oxide ceria electrodes during CO2 electroreduction V Kamboj, S Raychowdhury, C Ranjan, Applied Catalysis B: Environment and Energy 365, 124880
3. Cu infiltrated Ni-YSZ cathode in CO2 (+H2) stream: Reverse water gas shift vs. CO2 electrolysis V Kamboj, Chinmoy Ranjan, Journal of Power Sources 614 (15), 234985

IT-059

Quantum Beam Approaches to Advanced Functional Polymer Composites

Tomoki Maeda*

Research and Education Center for Atomic Sciences, Ibaraki University,

162-1 Shirakata, Tokai Village, Naka County, Ibaraki 319-1106, Japan

Institute of Quantum Beam Science, Graduate School of Science and Engineering, Ibaraki University,

162-1 Shirakata, Tokai Village, Naka County, Ibaraki 319-1106, Japan

***Corresponding author e-mail:** tomoki.maeda.polymer@vc.ibaraki.ac.jp

ABSTRACT

Quantum beams are high-intensity particle beams (electrons, neutrons, and muons) and electromagnetic radiation (X-rays and synchrotron radiation) generated by reactors and accelerators. Quantum beam science spans a wide range of scientific disciplines, including chemistry, materials science, biology, and engineering, and plays an important role in understanding structure–property relationships. In Japan, advanced large-scale research facilities such as SPring-8, NanoTerasu, and J-PARC have been established to promote quantum beam science.

This presentation highlights contrast variation methods in neutron scattering at J-PARC. Applications to thermoresponsive nanocomposite hydrogels for biomedical use will be introduced[1-6], followed by a newly developed contrast variation technique at BL20 iMATERIA[7-10]. Structural analyses of silica-filled rubber for automotive tires[8] and human hair[10] using this new technique will also be presented.

References:

1. Naho Oyama, Hiromasa Minami, Daichi Kawano, Makoto Miyazaki, Tomoki Maeda, Kazunori Toma, Atsushi Hotta, Koji Nagahama, Biomater. Sci., 2 (2014) 1057-1062.
2. Makoto Miyazaki, Tomoki Maeda, Kenji Hirashima, Naruki Kurokawa, Koji Nagahama, Atsushi Hotta, Polymer, 115 (2017) 246-254.
3. Midori Kitagawa, Tomoki Maeda, Atsushi Hotta, Polym. Degrad. Stab., 147 (2018) 222-228.
4. Tomoki Maeda, Midori Kitagawa, Atsushi Hotta, Satoshi Koizumi, Polymers, 11 (2019) 250.
5. Tomoki Maeda, Midori Kitagawa, Atsushi Hotta, Polym. Degrad. Stab., 187 (2021) 109535.
6. Tomoki Maeda, Keishi Tanimoto, Atsushi Hotta, Macromol. Chem. Phys., 223 (2022) 2100316.
7. Yohei Noda, Hideki Izunome, Tomoki Maeda, Takumi Inada, Satoru Ueda, Satoshi Koizumi, Quantum Beam Sci., 4 (2020) 32.
8. Yohei Noda, Tomoki Maeda, Takayuki Oku, Satoshi Koizumi, Tomomi Masui, Hiroyuki Kishimoto, Quantum Beam Sci., 4 (2020) 33.
9. Satoshi Koizumi, Yohei Noda, Tomoki Maeda, Takumi Inada, Satoru Ueda, Takako Fujisawa, Hideki Izunome, Robert A. Robinson, Henrich Frielinghaus, Quantum Beam Sci., 4 (2020) 42.

IT-060

Application of Probe Aberration Corrected STEM Techniques in Understanding Some Fascinating Features of Melt-Cast $(Fe,Cr)_2B$

Arup Dasgupta[1,2]*, Akhil G Nair[1,2], and Chanchal Ghosh[1,2]

[1] *Metallurgy and Materials Group, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, India*

[2]*Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India*

***Corresponding author e-mail:** arup@igcar.gov.in

ABSTRACT

The probe aberration-corrected Scanning Transmission Electron Microscopy (STEM) has established itself as an extremely powerful tool for conducting structural, chemical, and spectroscopic studies on crystalline domains in materials. However, the technique also brings unprecedented levels of information that have never been seen before. Therefore, understanding the images or spectra generated by such a tool requires a detailed analysis.

In this talk, a concentrated boron (5 wt.%) - added P91 steel will be discussed, with emphasis on the boride phase. The material is a boride (Fe2B) – ferrite (α-Fe) composite with the former being the major component. STEM-iDPC imaging and image simulations confirmed Cr substitution for Fe in the Fe2B lattice [1], resulting in the formation of $(Fe,Cr)_2B$ borides. However, there were delocalisation observed in the B atom positions which were studied using DFT simulations [2].

Extended Energy-Loss Fine Structure (EXELFS) analysis supported by Density Functional Theory (DFT) simulations was used to estimate Fe-B, Cr-B, and B-B bond lengths [3]. Cr doping of Fe2B was also found to exhibit magnetic skyrmions [4], not expected in the centrosymmetric bct crystal structure of Fe2B. The antiferromagnetic Cr was believed to assist the formation of skyrmions in $(Fe,Cr)_2B$ system at room temperature. Investigations on the effect of chromium concentration on skyrmion formation in the $(Fe,Cr)_2B$ system at room temperature were carried out using Lorentz Transmission Electron Microscopy (LTEM). This study is among the first to report direct observation of skyrmion formation at room temperature in the $(Fe,Cr)_2B$ system.

References:

1. Chanchal Ghosh, Akhil G. Nair, Arup Dasgupta, R. Mythili, R. Divakar, Atom column analysis of (Fe,Cr)2B phase in high B-containing ferritic steel, Materialia, Volume 33, 2024, 102007.
2. Akhil G. Nair, Namit Pai, Chanchal Ghosh, Arup Dasgupta, Indradev Samajdar, J. Ganesh Kumar, Alka Kumari, G. V. Prasad Reddy, Microstructural evolution and mechanical property correlation in boron-added modified 9Cr-1Mo steel, Materials Today Communications, Volume 40, 2024, 109489.
3. Akhil G. Nair, Chanchal Ghosh, Namit Pai, Indradev Samajdar, Arup Dasgupta, Effect of Cr addition on the bond characteristics of Fe2B: Insights from electron spectrometry and DFT simulations, Physica B: Condensed Matter, Volume 715, 2025, 417596,
4. Chanchal Ghosh, Akhil G. Nair, R. Mythili, Arup Dasgupta, R. Divakar, Correlation between Cr concentration and magnetic texture formation in (Fe,Cr)2B system at room temperature as revealed by Lorentz microscopy, Materials Characterization, Volume 230, Part A, 2025, 115668.

From Reactive-Species Composition to Function: A Design Framework for Non-Ablative, Reversible Biointerface Modulation

Kazuo Shimizu*[1,2], Alam Md Jahangir[1], Mahedi Hasan[2], Jaroslav Kristof[1]

[1] *Graduate School of Medical Photonics, Shizuoka University, Hamamatsu, Japan*

[2] *Graduate School of Science and Technology, Shizuoka University, Hamamatsu, Japan*

***Corresponding author e-mail:** shimizu.kazuo@shizuoka.ac.jp

ABSTRACT

A key bottleneck in soft-matter surface engineering for CNS drug delivery is designing a living barrier surface that permits nanometer-scale macromolecule transport while preserving integrity and recovery. Here we propose a composition-to-function (process–state–function) framework, defined as a quantitative mapping from controllable process inputs to biointerface state and transport output. Cold atmospheric microplasma generates tunable reactive oxygen/nitrogen species (RONS) in the surrounding medium; in this abstract, a "RONS composition vector (profile)" denotes the measurable set (vector) of redox-relevant chemical parameters produced under a given plasma condition (e.g., H_2O_2/NO_2^-/NO_3^-/pH/ORP measured at a defined post-treatment time). Using FITC–dextran FD-150 (150 kDa; ~10 nm-class probe) as a practical DDS (drug delivery system)-relevant metric, we quantify intracellular accessibility in the mouse brain endothelial cell line bEnd.3 and relate it to membrane physicochemical descriptors. Microplasma exposure enhances FD-150 uptake in bEnd.3 within a definable operating window, indicating controllable transport modulation rather than irreversible disruption. To translate this biointerface modulation into materials language, we connect uptake to surface-state descriptors: plasma conditions that increase FD-150 uptake coincide with reduced membrane lipid order (lower packing/greater lipid disorder) and membrane depolarization, consistent with a RONS-mediated reversible shift in membrane surface state. Complementary discharge studies further link operating conditions to cell integrity and intracellular absorption outcomes, supporting window-based operation (maximize delivery, constrain stress). As supporting evidence of generalizability, FD-150 uptake enhancement is also observed in suspension hematopoietic cells (HL-60), suggesting portability of the composition-to-function logic beyond BBB interfaces. Overall, we recast plasma–BBB modulation as a specification-driven materials problem: process parameters → RONS composition vector (profile) → membrane surface state (order/potential) → nanometer-scale transport function, providing a design route for reversible, non-genetic DDS interface engineering.

Keywords: microplasma; RONS composition vector (profile); surface-state modulation; transport window; reversible biointerface; BBB; nanometer-scale transport; FITC–dextran

References:

1. Alam, M.J., and Shimizu K., et al. Macromol, **4**, (2024), 597–609.
2. Alam, M.J., and Shimizu K., et al. Plasma, **8**, (2025), 19.
3. Rimi, S.A., and Shimizu K., et al. Plasma Med., **13**, (2023,) 15–32.
4. Rimi, S.A., and Shimizu K., et al. Applied Sciences, **14**, (2024), 3978.
5. Sadiq, A.H., and Shimizu K., et al. J. Electrostatics, **134**, (2025), 104040.
6. Hasan, M., and Shimizu K., et al. Membranes **15**, (2025), 156.
7. Shimizu, K. et al. Biointerphases, **10**(2), (2015), 029517.
8. Kristof, J. and Shimizu K., et al. Biointerphases, **12**(2), (2017), 02B402.
9. Shimizu, K. et al., IEEE Trans. Ind. Appl., **49**(5), (2013), 2308–2313.

IT-062

Quantum Spin Sensors for Open-Shell Molecules

Md. Ehesan Ali

Institute of Nano Science and Technology, Sector-81, Mohali, Punjab-140306, India

Corresponding author's email: ehesan.ali@inst.ac.in

ABSTRACT

Open-shell molecular systems, characterized by one or more unpaired electrons, provide a unique platform for spin-dependent quantum transport phenomena absent in closed-shell counterparts. In organic radicals, the presence of singly occupied molecular orbitals (SOMOs) leads to exchange splitting between spin channels, enabling spin-polarized currents and often enhanced conductance. While transport through monoradicals has been extensively explored, the role of multiple radical centers remains less clear. Here, we investigate quantum transport in di- and triradical molecular species based on stable Blatter's radicals, revealing that an increased number of SOMOs does not necessarily yield larger exchange splitting or improved conductance; instead, the spatial distribution of SOMOs and their coupling to electrodes critically determine transport characteristics. Extending this understanding to extended π-conjugated systems, we study the adsorption of closed- and open-shell molecules on zigzag graphene nanoribbons using NEGF-DFT methods. Closed-shell molecules physisorb weakly and act primarily as scattering centers, suppressing conductance, whereas open-shell paramagnetic molecules chemisorb strongly at ribbon edges, breaking spin symmetry and inducing pronounced spin-polarized transmission. This spin selectivity originates from quantum interference between localized molecular states and delocalized nanoribbon states, with the resulting spin current strongly dependent on the electronic structure of the adsorbed open-shell species. Taken together, our results demonstrate that spin-polarized quantum transport in open-shell systems is governed not merely by the number of unpaired electrons, but by the interplay of exchange splitting, orbital topology, molecule–electrode coupling, and quantum interference, offering design principles for molecular spintronics and quantum spin-sensing applications.

References

1. Bajaj, A., Ali, S., Khurana, R. & Ali, Md. E. Quantum Spin Transport Through Blatter's Diradicals and Triradicals J. Phys. Chem. A **129**, 4252–4264 (2025). Ali, S. & Ali, Md. E. Quantum spin sensors for open-shell molecules J. Mater. Chem. C **13**, 7760–7771 (2025).

Deriving Interface Physics from Correlations Between Electrical Properties and XPS in PECVD-SiO_2/Si

Sakura N. Takeda[1], Emilia E. Hashamova[2], Sai Hasegawa[1], Mutsunori Uenuma[3], Tomoyuki Miyao[1],
Naoaki Ono[1], Yukiharu Uraoka[1], and Kimito Funatsu[1]
[1]Nara Institute of Science and Technology, Ikoma, Nara, Japan, 630-0192
[2]Karlsruhe Institute of Technology, 76049 Karlsruhe, Germany
[3]National Institute of Advanced Industrial Science and Technology (AIST), 841-0052 Saga, Japan
***Corresponding author e-mail:** sakura@ms.naist.jp

ABSTRACT

Plasma-enhanced chemical vapor deposition (PECVD) SiO_2 films are widely used in semiconductor devices because of their compatibility with low-temperature processing1). A major challenge in PECVD SiO_2 is the need for extensive trial-and-error optimization of numerous process parameters to achieve high-quality electrical properties. Shortening this process requires a physical understanding of how process conditions determine electrical performance.

In this study2), we address this challenge by exploring correlations between electrical and spectroscopic properties in tetraethyl-orthosilicate (TEOS)-based PECVD-SiO_2/Si films. From systematic analysis of a large set of Si 2p x-ray photoelectron spectroscopy (XPS) data obtained from films fabricated under different process conditions (Fig. 1), a clear correlation between the Si 2p peak energy and electrical properties emerges (Fig. 2). Physical interpretation of this correlation reveals that the Si 2p peak energy provides direct information on charge accumulation within the oxide film. Furthermore, quantitative evaluation based on electrostatic considerations enables estimation of both the amount and spatial distribution of charges accumulated within the film (Fig. 3). Based on these findings, we discuss the mechanisms linking this charge distribution to process parameters and propose process conditions for achieving improved electrical properties.

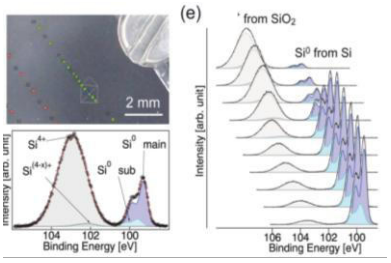


Fig. 1 XPS data collection at various SiO_2 thickness

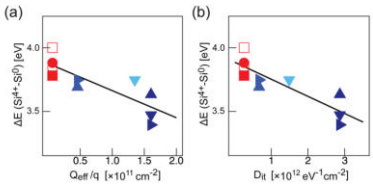


Fig. 2 Correlation between electrical properties and XPS

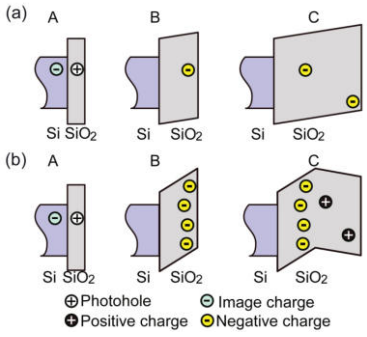


Fig. 3 Interface charge model derived from the XPS

References:

1. H. Li and K. Denpoh, J. Vac. Sci. Technol. A 42, 043002 (2024)
2. S. N. Takeda et al. J. Appl. Phys. 138, 175301 (2025).

IT-064

Representation of 3D X-ray CT Using Mixed Reality with Force Feedback for Density Information

Hiroki Kase[1,2]*, Katsuyuki Takagi[2], Toru Aoki[1,2]

[1]*Faculty of Informatics, Shizuoka University, Hamamatsu, Japan, 4328011*

[2]*Reseach Institute of Electronics, Shizuoka University, Hamamatsu, Japan*

***Corresponding author e-mail:** kase.hiroki@shizuoka.ac.jp

ABSTRACT

3D X-ray CT is an indispensable technology across diverse fields, including defect detection in materials and imaging of biological tissues. While visualization using Mixed Reality(MR) technologies has advanced in recent years, visual information alone has struggled to adequately represent the depth of complex, overlapping internal structures or the physical texture associated with density variations. Our laboratory has previously investigated methods for intuitively grasping internal structures by projecting X-ray CT data into an MR environment via spatial reconstruction displays. This research further develops this approach by proposing a new interface that integrates haptic information alongside visual input. By converting density information derived from CT values into force feedback, presented as reaction forces or resistance, we develop a highly integrated visual-tactile presentation method for internal structures. This system comprises a spatial reality display, motion capture, and a force-feedback device, as shown in Figure 1. First, the density gradient at each coordinate is calculated from the 3D X-ray CT voxel data. Next, a force-rendering algorithm is implemented that exhibits high rigidity in high-density regions and low resistance in low-density regions. When the user touches a virtual object in the MR space, the fingertip position and voxel coordinates are synchronized in real time, providing immediate force feedback. The proposed method enables tactile identification of subtle density variations that are difficult to discern visually. This facilitates faster and more accurate spatial understanding than conventional monitor observation, with applications including evaluating dissimilar material joints in materials science and monitoring crack progression. Beyond material diagnostics, this technique holds promise for applications across diverse fields that demand advanced spatial awareness, including surgical simulation and educational training.

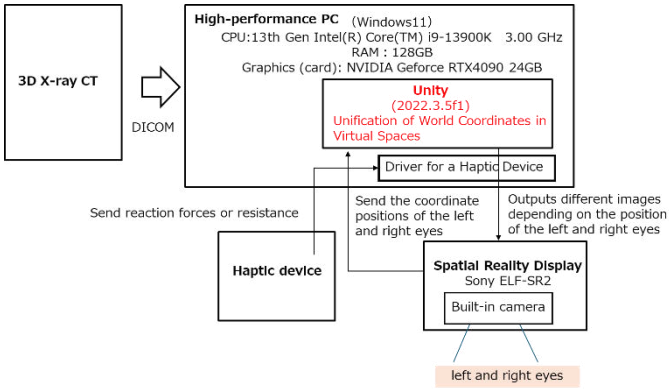


Fig. 1 System Configuration Diagram Using Haptic Devices

Keywords: 3D X-ray CT; Mixed Reality; Haptic Device;

Domain Engineering of Ferroelectric Nano-structures and Their piezoelectric properties

Tomoaki Yamada[1, 2]*

[1] *Department of Energy Engineering, Nagoya University, Nagoya 464-8603, Japan*

[2] *MDX Research Center for Element Strategy, International Research Frontiers Initiative, Institute of Science Tokyo, Yokohama 226–8503, Japan*

***Corresponding author e-mail:** yamada.tomoaki.h5@f.mail.nagoya-u.ac.jp

ABSTRACT

Domain structure control in nano-scale ferroelectric systems has been considered invaluable for improving dielectric and piezoelectric responses. Despite the significant need to control the domain structure, approaches for this are limited. For thin films, the most common approaches are to vary the orientation and strain of the films by selecting an appropriate substrate. However, the imperfect charge screening at the interface and/or surface, which generates a depolarizing field, can also affect the domain structure. This influence is larger for smaller structures.

In this presentation, we focus on such an influence in ferroelectric nanorods and artificial superlattice films. We fabricated epitaxial tetragonal $Pb(Zr, Ti)O_3$ (PZT) nanorods by using a focused ion beam (hereafter, FIB-rods)[1-3] and self-assembled nanorods by pulsed laser deposition (PLD) (hereafter, PLD-rods) [4,5]. We found that the *c*-domain fraction in the FIB-rods drastically increased with decreasing rod width (Fig.1(a)(b)). The preferred formation of the *c*-domain in narrow rods can be rationalized in terms of the large depolarizing field in the *a*-domain. Phase field simulations also supported the experimental observations. The narrow PLD-rods exhibited remarkably large piezoelectric response due to their complete *c*-domain structure and the reduced substrate clamping (Fig.1(c)). (111)-epitaxial tetragonal and rhombohedral PZT artificial superlattice films exhibited larger piezoelectric responses as compared with each single layer film [6,7] (Fig.2). This can be explained by the given mechanical and electrostatic boundary conditions, the details of which will be discussed in the presentation.

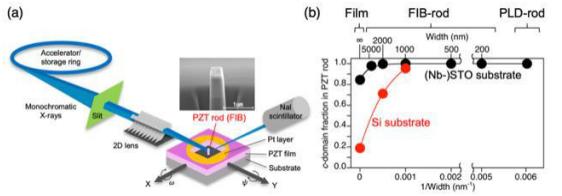


Fig. 1 Domain structure and piezoelectric property of PZT nanorods: (a) synchrotron XRD set-up, (b) c-domain fraction as a function of the inverse rod width, and (c) piezoelectric response.

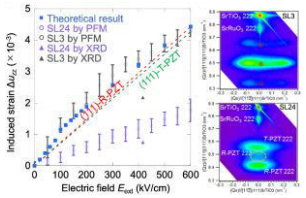


Fig. 1 Piezoelectric response of PZT artificial superlattice films.

Keywords: ferroelectric; domain; nanorod; superlattice; depolarizing field

References:

1. Jpn. J. Appl. Phys., **54**, 10NA07 (2015),
2. IEEE Trans. Ultrason., Ferroelect., Freq. Control, **63**, 1642 (2016),

IT-066

Sensing Experiments Based on Collaborative Research Activities in Tokyo University of Agriculture and Technology

Hiromasa SHIMIZU

Tokyo University of Agriculture and Technology, Japan

ABSTRACT

We have developed chemical sensors based on collaborative research activities in our university, for wide range of applications including health care, agriculture, food inspection, and environmental monitoring. I will give a seminar on 1) Sub-ppb detection of methyl jasmonate and methyl salicylate using SPR sensor with graphene oxide-Al films and violet light, 2) SPR Sensor Modified with Highly Cationic Polymers Toward Selective Detection of Acetic Acid and Ethanol [2], 3) Sensitivity Improvement of a silicon waveguide sensor decorated with olfactory receptors [3].

Exploring MBene: 2D Materials Pathways in Synthesis and Characterization for Optoelectronics devices

Madhurya Chandel [1]*

[1]*Faculty of Mechatronics, Warsaw University of Technology, Warsaw, Poland*

***Corresponding author e-mail:** madhurya.chandel@pw.edu.pl

ABSTRACT

Following the breakthroughs of graphene and MXenes, MBenes, early transition metal borides, have emerged as a compelling new class of two-dimensional (2D) materials. While they share nominal similarities with MXenes, the incorporation of boron introduces complex crystallographic arrangements and distinct transition metal–boron chemistry, resulting in alternative reaction pathways and structural transformations. These unique features position MBenes as a promising frontier in materials science, particularly for optoelectronic applications.

A major challenge in MBene synthesis lies in their pronounced susceptibility to oxidation, which limits the effectiveness of conventional wet-chemical etching and often leads to the formation of oxy-borides rather than pure MBenes. To overcome this, we employed microwave-assisted hydrothermal etching, combined with acid (HCl) and base (NaOH) pretreatments, to successfully remove aluminum from MoAlB and yield multilayered 2D MBene structures. This approach provides a controlled pathway for scalable synthesis, enhancing the structural integrity of the resulting materials.

Comprehensive characterization using X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), electron microscopy, and spectroscopic methods revealed fundamental insights into MBene chemistry and behavior. Optical absorption studies and time-resolved photoluminescence (TRPL) further demonstrated tunable optical properties, underscoring their potential in optoelectronic and energy-related technologies. Together, these findings establish a foundation for advancing MBene synthesis strategies and integrating these materials into next-generation device architectures.

Keywords: 2D materials, MBene; Characterization; Optical properties; optoelectronic devices

References

1. Madhurya Chandel, et al. "Multilayered MoAlB@ MBene structures using mild microwave-assisted etching and their optical properties." Materials Horizons 12.10 (2025): 3473-3484.

IT-068

Measurement of Hydrogen to Carbon Ratio in Amorphous Hydrogenated Carbon Products and the Effect Ion Irradiation

Ionut Topala[1]*, Cristina Gerber[2], Ilarion Mihaila[2], Valentin Pohoata[1], Decebal Iancu[3], Radu Florin Andrei[3], Ion Burducea[3], Mihai Straticiuc[3], Yvain Carpentier[4], Alessandro Faccinetto[5], Nicolas Nuns[6], Claire Pirim[4], Cristian Focsa[4]

[1]*Integrated Center of Environmental Science Studies in the North-Eastern Development Region (CERNESIM), Alexandru Ioan Cuza University of Iasi, Blvd. Carol I No. 11, Iasi 700506, Romania*

[2]*Iasi Plasma Advanced Research Center (IPARC), Faculty of Physics, Alexandru Ioan Cuza University of Iasi, Blvd. Carol I No. 11, Iasi 700506, Romania*

[3]*Applied Nuclear Physics Department (DFNA), Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN HH), Reactorului 30, Magurele 77125, Romania*

[4]*PhLAM –Physique des Lasers Atomes et Molecules, UMR 8523, Universite de Lille, CNRS, F-59000 Lille, France*

[5]*PC2A –Physicochimie des Processus de Combustion et de l'Atmosphere, UMR 8522, Universite de Lille, CNRS, F-59000 Lille, France*

[6]*UCCS –Unite de Catalyse et Chimie du Solide, UMR 8181, CNRS, Centrale Lille, Universite d'Artois, Universite de Lille, F-59000 Lille, France*

***Corresponding author e-mail:** ionut.topala@uaic.ro

ABSTRACT

Decades ago, laboratory experiments supported the idea that hydrogenated amorphous carbon (a-C:H) causes key infrared absorption bands in the interstellar medium, like the 3.4 μm aliphatic CH stretch and bands at 6.85 and 7.27 μm. However, a-C:H encompasses diverse carbonaceous solids with varying hydrogen to carbon (H/C) ratios and sp^1, sp^2, sp^3 contents, depending on production methods, making infrared signatures insufficient for clear differentiation. In space, the 3.4 μm feature appears in many environments, from the ISM in our galaxy and others to protoplanetary nebulae, dust particles, and meteorites. These factors significantly influence the resulting material's structure, including its hydrogen content, degree of graphitization, and aromatic-to-aliphatic ratio, which in turn affect its infrared spectral features. For instance, plasma-enhanced chemical vapor deposition often yields hydrogenated amorphous carbons with high porosity and tunable H/C ratios, mimicking diffuse ISM dust, while laser ablation produces more compact, graphitic nanoparticles are mimicking the materials in denser clouds. Overall, matching laboratory analogues to observed interstellar spectra requires optimizing many parameters to replicate the observed band profiles and carrier evolution across different astrophysical environments.

Recently, dielectric barrier discharge (DBD) plasma at atmospheric pressure has proven effective for synthesizing "fluffy" interstellar carbon dust analogues under low-temperature conditions. The H/C ratio serves as a key parameter for comparing interstellar carbon dust analogues to observations, with prior estimates for IRAS 08572 + 3915 ranging from 0.29 to 0.69, though these carry uncertainties from infrared band strength values. Most laboratory analogues exhibit H/C ratios in or near this range, showing trends toward values near 1 alongside decreasing densities approaching 1 g cm^{-3}. Complementary analytical techniques in the lab help refine these H/C measurements, reducing uncertainties in band strengths for complex hydrogenated carbonaceous materials.

In this paper, we thoroughly characterize the physico-chemical properties of interstellar dust analogues produced via low-temperature helium dielectric barrier discharge (DBD) plasma fed with 15% butane. We focus on their microscopic features, molecular structure, and carbon hybridization using complementary techniques—including electron and optical microscopy, mass spectrometry, Raman spectroscopy, and Fourier transform infrared (FTIR) spectroscopy—to probe surface and bulk composition. FTIR and electron microscopy further assess the analogues after 3 MeV H^+ irradiation to simulate energetic processing, with discussions emphasizing carbon structure evolution, aliphatic C-H bond destruction rates, and relevance to dust in diffuse and dense interstellar medium.

The average H/C ratio from multitechnique analysis guides the selection of absorption strength values for accurate FTIR spectral matching, addressing uncertainties in literature-based methods that can yield significant deviations for specific dust analogues. Upon 3 MeV H^+ irradiation, DBD-produced carbon dust exhibits morphological changes, including microscale modifications and ion etching across samples. The H/C ratio decreases due to proton-induced dehydrogenation, while the CH_2/CH_3 and sp^2/sp^3 ratios evolve with fluence, reflecting progressive graphitization.

Keywords: astrochemistry, plasmas, dust analogues, advanced characterizations, ISM

References:

1. B. Hodoroaba, I. C. Gerber, D. Ciubotaru, I. Mihaila, M. Dobromir, V. Pohoata, I. Topala, Mon. Not. R. Astron. Soc., 481 (2018) 2841.

IT-069

Studies on the Structure and Functional Properties of Some Nanocomposite Layers Based on Graphene and Graphene Oxide

Iacomi Felicia*[1], Maria Cazacu[2], Iulia Salaoru[3], Maria Ignat[4], Mirela Petruta Suchea[5], Luciana Punga[1], Alupului Teodor[1], Ovidiu Pana[7], Simona Cinta Pinzaru[6], Daniel Timpu[2], Elena-Laura Ursu[2], Lucel Sirghi[1], Ioan Valentin Tudose[8], Marius Dobromir[1]

[1] *faculty of Physics, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania*

[2]*Petru Poni Institute of Macromolecular Chemistry, 700487 Iasi, Romania*

[3]*Emerging Technologies Research Centre, De Montfort University, Leicester, LE1 9BH, UK*

[4]*Faculty of Chemistry, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania*

[5]*National Institute for Research and Development in Microtechnologies - IMT Bucharest, 077190, Voluntari-Bucharest, Romania;*

[6]*Faculty of Physics, Babeș-Bolyai University, 400084 Cluj-Napoca, Romania*

[7]*National Institute for R&D of Isotopic and Molecular Technology, 400295 Cluj-Napoca, Romania*

[8]*Center of Materials Technology and Photonics, School of Engineering, Hellenic Mediterranean University, 71410 Heraklion, Crete, Greece*

***Corresponding author e-mail:** iacomi@uaic.ro

ABSTRACT

Graphene and graphene oxide/polymer composite layers are critical for enhancing the mechanical, electrical, thermal, and barrier properties of polymers, transforming them into high-performance, lightweight materials for aerospace, electronics, and biomedical applications.

The present study regards the fabrication of four types of nanocomposite layers: graphene/PEDOT:PSS, graphene/PDMS, graphene/PDMS+SiO_2 and graphene oxide-/PVAc. Their structural and functional properties are investigated in comparison with the results presented in literature and discussed for possible applications. Semi-transparent Graphene-PEDOT:PSS layers with improved electrical conductivity were obtained for different graphene concentrations by air-carrier spray pyrolysis technique starting from commercially available graphene nanoplatelets. Thick layers of graphene-PDMS and thin films of graphene-PDMS+SiO_2 were obtained using the method of solution mixing and different concentrations of GNPs. Their optical and electrical properties and sensitivity to humidity were investigated and are discussed. Solutions of polyvinyl acetate in methanol with graphene oxides resulted from different oxidation processes were deposited by spin coating in a Al/PVAc+GO/Al structure on glass substrates. A comparative analysis of graphene oxidation processes is performed and the experimental results demonstrate that the oxidation level directly modulates the switching mechanism and stability, suggesting that an intermediate oxidation degree is essential for balancing low-power, forming-free operation with long-term device stability in graphene-based RRAM applications.

IT-070

Heusler Alloys as Spintronic and Spin-Caloritronic Applications

K. G. Suresh

Dept. of Physics, IIT Bombay

ABSTRACT

Heusler alloys have emerged as one of the most important materials in the field of applied magnetism in the recent past. These alloys are truly multifunctional and can be exploited for various applications. Apart from the magnetic shape memory related effects, Heusler alloys also play a vital role in spintronics. Spintronic materials can be classified into many groups, such as half metallic ferromagnets, spin gapless semiconductors, magnetic semiconductors etc. In addition to ferromagnets, antiferromagnets and ferrimagnets also attract a lot of interest in spintronics. All these categories have been found from the Heusler family. Several novel materials and novel phenomena have been discovered as a result of extensive experimental and theoretical investigations. Recently, the role of Heusler alloys as spin caloritronic materials is confirmed. In this talk, I will present some of the work that we have carried out in a variety of Heusler alloys in which the electronic band structure is systematically tuned to synthesize novel and better materials. The talk will also cover some of the very novel aspects that have come out of the extensive studies carried out on different classes of materials.

Generation and Detection of Orbital Currents

Dr. Arnab Bose

Assistant Professor, Department of Electrical Engineering, IIT Kanpur

ABSTRACT

Recent theoretical predictions, supported by emerging experimental evidence, confirm the existence of orbital currents under non-equilibrium conditions, even though orbital moments are strongly quenched at equilibrium [1]. A key advantage of orbital currents is that they can be significantly larger than spin currents and can be generated in a broad class of materials without the strict requirement of strong spin–orbit coupling. In our work, we demonstrate several mechanisms for generating orbital currents in nonmagnetic materials [2,3], noncollinear antiferromagnets [4], and ferromagnets [5]. First, we show how orbital currents generated via the orbital Hall effect can be experimentally disentangled from the conventional spin Hall effect in nonmagnetic metals such as Nb and Ru [2]. Using these systems, we also benchmark the efficiency of spin–orbit torque driven by orbital Hall currents [3]. Next, we reveal a new mechanism for orbital Hall current generation originating from spin fluctuations and magnetic chirality in noncollinear antiferromagnets [4]. Finally, we report a mechanism known as orbital pumping, in which a precessing magnet emits orbital currents analogous to spin pumping [5]. We further demonstrate experimental methodologies that enable the separation of orbital pumping signals from conventional spin pumping contributions. Together, these results establish both fundamental principles and practical benchmarks for the generation, detection, and potential technological application of orbital currents.

References:

1. D. Go, D. Jo, H. W. Lee, M. Kläui, and Y. Mokrousov, *Orbitronics: Orbital Currents in Solids*, EPL.
2. A. Bose, F. Kammerbauer, R. Gupta, D. Go, Y. Mokrousov, G. Jakob, and M. Kläui, Detection of long-range orbital-Hall torques, Phys. Rev. B **107**, 134423 (2023).
3. R. Gupta et al., Harnessing orbital Hall effect in spin-orbit torque MRAM, Nat. Commun. **16**, 130 (2025).
4. A. Bose et al., Fluctuation-Mediated Spin-Orbit Torque Enhancement in the Noncollinear Antiferromagnet Mn3Ni0.35Cu0.65N, Nano Lett. **25**, 8073 (2025).
5. N. Keller et al., Identification of Orbital Pumping from Spin Pumping and Rectification Effects, Nano Lett. **25**, 13462 (2025).

High Temperature Quantum Transport using Deep Dopant in Silicon

Arup Samanta[1,2], Pooja Yadav[1], Soumya Chakraborty[1] and Hemant Arora[1]

[1]*Quantum/Nano-Science and Technology Laboratory, Department of Physics, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

[2]*Centre for Nanotechnology, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

***Corresponding author e-mail**: arup.samanta@ph.iitr.ac.in

ABSTRACT

Over the past two decades, extensive research efforts have focused on developing silicon-based quantum devices using dopant atoms such as P, As, and B. These shallow dopants have enabled a variety of quantum electronic components, including single-electron transistors (SET), single-electron current metrology (SECM) devices, single-photon detectors (SPD), and spin- and charge-based quantum bits (qubits). Despite these advances, the practical deployment of such devices remains limited because shallow dopants possess small binding energies, which require device operation at extremely low temperatures. To overcome this limitation, we recently proposed a new approach based on deep dopants in silicon. Our theoretical studies indicate that nitrogen (N), acting as a deep dopant in silicon, can provide significantly stronger carrier confinement and improved thermal stability. This property opens a promising pathway toward roomtemperature single-electron transistor operation and high-temperature qubit architectures. In this talk, we will present the fundamental concept of deep-dopant quantum devices and discuss the potential advantages of nitrogen-doped silicon systems. A comparative analysis with conventional shallow dopant-based platforms will also be presented, highlighting the prospects of deep dopants for next-generation quantum electronics operating beyond cryogenic temperatures.

Topological Spin Textures in Van der Waals Magnets

Rana Saha

Indian Institute of Science Education and Research (IISER) Tirupati, India

***Corresponding author e-mail:** rana.saha@labs.iisertirupati.ac.in

ABSTRACT

Topological spin textures such as skyrmions have attracted significant interest for next-generation spintronic devices due to their nanoscale size, stability, and efficient manipulation by electric currents. While skyrmions typically arise in non-centrosymmetric magnets via Dzyaloshinskii–Moriya interactions, recent studies indicate that they can also emerge in nominally centrosymmetric materials through subtle structural modifications. In this talk, I will discuss our recent observations of skyrmions in the van der Waals magnets $CrTe_2$ and Fe_3GaTe_2 [1-3]. In $CrTe_2$, Cr self-intercalation between Te–Cr–Te trilayers forms a (2×2×2) superstructure that breaks inversion symmetry and stabilizes Néel-type skyrmions. In Fe_3GaTe_2 [2], Fe vacancies and intercalation induce symmetry breaking that promotes topological spin textures. Notably, Fe_3GaTe_2 [1] exhibits a high magnetic ordering temperature (~370 K), among the highest for vdW magnets. These results highlight defect and intercalation engineering as powerful strategies for realizing topological spin textures in two-dimensional magnets for high-temperature spintronic applications.

References:

1. R. Saha, H. L. Meyerheim, B. Göbel, B. K. Hazra, H. Deniz, K. Mohseni, V. Antonov, A. Ernst, D. Knyazev, A.B - Pinto, I. Mertig, S. S. P. Parkin, *Nat. Commun.* 13 (3965) 2022.
2. R. Saha, H. L. Meyerheim, B. Göbel, I. Mertig, S. S. P. Parkin, *npj Spintronics* 2 (21) 2024.
3. A. Chakraborty, A. K. Srivastava, A. K. Sharma, A. K. Gopi, K. Mohseni, A. Ernst, H. Deniz, B. K. Hazra, S. Das, P. Sessi, I. Kostanovskiy, T. Ma, H. L. Meyerheim, S. S. P. Parkin, *Adv. Mater.* 34 (2108637) 2022.

IT-075

Peptide-Based Nanomaterials for Organic Electronics: Tailoring Piezoelectric Properties through Nanostructural and Chiroptical Modulation

Aparna Ramesh, Goutam Ghosh*

Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru – 562162, India

***Corresponding author e-mail**: gghosh@cens.res.in

ABSTRACT

Peptide-based piezoelectric materials offer sustainable, biodegradable, and biocompatible alternatives to brittle and toxic inorganic systems; however, their structure–property relationships and potential integration into organic electronic devices—such as sensors, actuators, and energy harvesters—remain largely unexplored. In our first study,[1] we demonstrate that the dimension and morphology of nanostructures obtained via peptide self-assembly significantly influence their piezoresponse. The kinetic self-assembly led to nanorods or spherical nanoparticles, which were piezo-inactive (Scheme 1, left side). Remarkably, under thermodynamic conditions, these structures transformed into entangled nanofibers, which exhibited clear piezoelectric activity—highlighting the importance of supramolecular organization and dimensionality. In a second study,[2] we established a direct link between chiroptical activity and piezoresponse. Peptide self-assembly in water resulted in non-helical, chiroptically inactive nanofibers with no piezoelectric output. Upon introducing a small amount of cosolvent (DMSO), the same peptide system exhibited helical organization, became chiroptically active, and showed a pronounced piezoresponse (Scheme 1, right side). These results collectively underscore that precise control over supramolecular packing and chiroptical behavior governs the electromechanical properties of peptide-based nanomaterials. Our findings pave the way for the rational design of soft, tunable, and biocompatible piezoelectric systems for next-generation bioelectronic and energy applications.

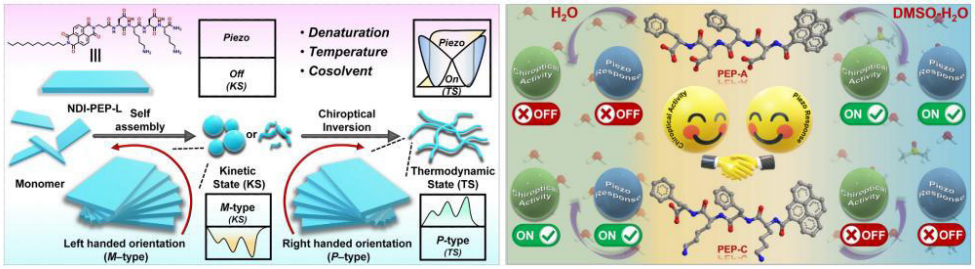


Fig 1. Influence of nanostructures on piezo-response (left) and effect of chiroptical activity on piezo-response.

References:

1. Ramesh, T. N. Das, T. K. Maji, G. Ghosh* Chemical Science, 2024, 15, 16355-16366.
2. Ramesh, S. Layek, T. N. Das, N. Sengupta, G. Ghosh* "Cosolvent-Modulated Supramolecular Chirality Unveils Pronounced Piezoelectric Response in Peptide-Based Nanomaterials" (Under Review).

IT-076

Efforts Toward Developing High-Performance Aqueous Rechargeable Zn-Ion Batteries

Ashutosh K. Singh

Centre for Nano and Soft Matter Sciences (CeNS),

Bangalore, Karnataka, 562162 India

***Corresponding author e-mail:** aksingh@cens.res.in

ABSTRACT

Zinc-ion batteries (ZIBs) are promising for safe and cost-effective energy storage for grid-scale applications, yet they face limitations due to unstable cathodes and problematic zinc anodes. This work addresses these dual challenges by presenting novel strategies for material engineering. For the cathode, we introduce a thermo-electrochemical activation strategy for V_2O_5, creating defect-rich ZnV_3O_8. This process induces a phase transition that enhances Zn^{2+} diffusion and structural robustness. The resulting cathode delivers a high specific capacity of 302 mAh g^{-1} at 0.1 A g^{-1} and demonstrates ultralong cycling stability over 4500 cycles [1]. Complementary studies on a homo-interphase vanadium oxide cathode further validate the performance gains from engineered mixed-valence states [2, 3]. For the anode, we address dendrite growth and side reactions by developing a free-standing composite film from waste generated during steel production at the TATA Steel plant, specifically as zinc dross powder. This optimized composite film has homogenized the electric field and Zn plating/stripping to mitigate the standard dendrite issues that occur in commercial Zn foils. It has commercial potential to replace the expensive Zn foil used for ZIBs fabrication [4]. Collectively, these straightforward and scalable approaches, targeting both cathode kinetics and anode stability, significantly advance the development of high-performance, practical ZIBs.

References:

1. R. Roy, P. Sharma, G. Mahendra, P. Dutta, V. Raghuraman, P. Singh, A. K. Singh, Thermo-Electrochemical Tuning of V2O5 to ZnV3O8 Enables Ultra-Stable Zinc-Ion Battery, Adv. Energy Mater., e02262 (2025).
2. R. Roy, A. Basith, P. Dutta, and A. K. Singh, " Homo-Interphase Engineering of Vanadium Oxide Cathode with Enhanced Diffusion Kinetics for High-Rate Aqueous Zinc-Ion Batteries." Small (2025): e08986.
3. R. Roy, T. Das, W. A. Goddard III and A. K. Singh, Ultra-robust Zinc-Ion Batteries with Co-solvent Water-in-Salt Electrolytes for Enhanced Stability and Capacity, J. Mater. Chem. A (2026), Accepted Manuscript.
4. K. Singh, R. Roy, A. Basith, C. Ghanty, M. Nidhi, An Anode Composite, Method of Preparation and Applications Thereof, Indian Patent Application No.: 202541078361, Date: 2025-December-04.

IT-077

Stimuli-Responsive Molecular Systems for Nanoscale Energy Harvesting Prospects

Pritam Sadhukhan[1], Osamu Sato[2]*, Shinji Kanegawa[2], Suhrit Ghosh[1]*, Anuja Datta[3]*

[1]Indian Association for the Cultivation of Science (IACS), Jadavpur, Kolkata, India 700032

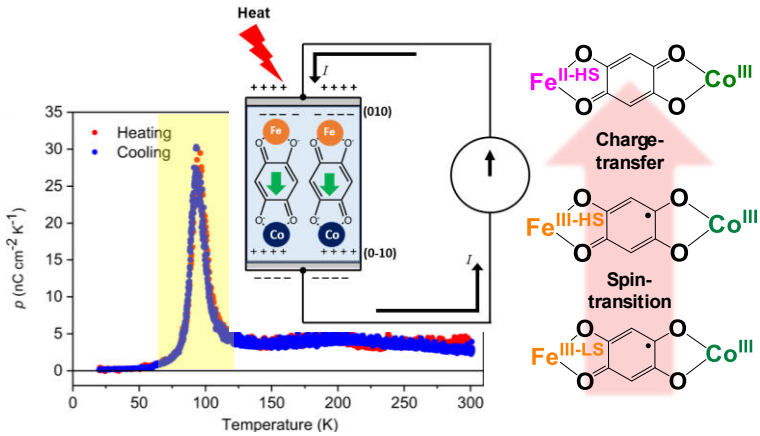
[2]Kyushu University, ITO Campus, Mootoka, Nishi-ku, Fukuoka, Japan 819-0395

[3]SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** sato@cm.kyushu-u.ac.jp, psusg2@iacs.res.in, psuad4@iacs.res.in

ABSTRACT

Polar molecular systems exhibiting switchable polarization hold promise for advanced applications in ferroelectric memory, pyroelectric sensing, and nanoscale energy harvesting. Yet, the intrinsic electronic correlations within conventional ferroelectrics pose significant challenges to material design and property modulation. Dynamic molecular crystals provide a compelling alternative, as phenomena like spin crossover and intramolecular charge transfer trigger pronounced electronic density redistributions that facilitate polarization switching. Building on this principle, we introduce a new class of materials, molecular electronic pyroelectrics, that exhibit polarization changes induced by electronic reorganization rather than lattice distortions. These materials demonstrate versatile light- and heat-responsive pyroelectric behaviour, paving the way for next-generation, molecule-based energy-harvesting systems.[1,2] More intriguingly, soft polymer systems also enable precise control of temperature-dependent spontaneous polarization in donor-acceptor π-architectures via reversible, thermally driven supramolecular assembly-disassembly transitions.[3] This approach provides a novel pathway for achieving and modulating electronic pyroelectricity in flexible, biocompatible organic materials.



References:

1. P. Sadhukhan et. al., Nature Communications, vol 12 (2021) 4836.
2. P. Sadhukhan et. al., Nature Communications, vol 14 (2023) 3394.
3. P. Sadhukhan et. al., Chemical Communications, vol 61 (2025) 5289.

IT-078

Development of Indigenous Electrode Materials for Li- and Na-Ion Batteries: From Lab-Scale Innovation to Technology Demonstration

Srinivasan Anandan

Centre for Advanced Materials & Batteries, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Balapur, Hyderabad, Telangana, India.

***Corresponding Author e mail :** anandan@arci.res.in

ABSTRACT

Translational research plays a crucial role in moving scientific innovations from the laboratory to real-world applications, particularly in strategic sectors such as energy storage. With India's rapidly expanding electric mobility and renewable energy landscape, the demand for indigenous, scalable, and commercially viable energy storage technologies has never been greater. This presentation highlights ARCI's efforts for the development, demonstration, and technology transfer of lithium-ion batteries (LIBs) and Na-ion batteries (NIB) materials. The first part of the presentation highlights ARCI's development of indigenous electrode material technologies for domestic LIB manufacturing. Lithium iron phosphate (LFP) is a preferred cathode chemistry owing to its intrinsic safety and strong thermal stability arising from robust P–O bonding, which prevents self-oxidation and thermal runaway. ARCI has developed a cost-effective high-energy milling process for synthesizing in-situ carbon-modified LFP (C-LFP), with 15–20 kg batch-scale production successfully demonstrated and validated at the cell level. Patents have been filed in India and internationally, and the technology has been transferred to M/s. Allox Minerals (India) and M/s. ALTMIN (Global & India). A 250 kg/day pilot plant has been established by M/s. ALTMIN at the ARCI incubator. Additionally, M/s. ALTMIN laid the foundation for its new plant recently, and the facility is expected to begin operations by Q4 2026, producing 20,000 MTPA of LFP CAM & meeting about 20% of India's projected LFP cell demand by 2028.

The second part of the presentation highlights ARCI's development of NVP and hard carbon materials for Na-ion batteries. $Na_3V_2(PO_4)_3$ (NVP) is a NASICON-type cathode for sodium-ion batteries, featuring a stable 3D framework with fast Na^+ diffusion. It operates at ~3.4 V (V^{3+}/V^{4+} redox) with a theoretical capacity of ~117 mAh g^{-1}, offering excellent cycling stability and safety. NVP synthesized by high energy milling using N,V, and P precursors at 1kg batch and subsequently calcined at 800oC under inert atm. The resulting pure NVP material delivers specific capacity of 110-115mAh/g with good rate capability and excellent cyclic stability retention (>80%) after 200 cycles. Currently, the up-scaling of the process for 20 kg batch is in progress and validation of material at pouch cell level is in progress. Hard carbon is considered a promising anode material for sodium-ion batteries due to its larger interlayer spacing (>0.35 nm), tunable microstructure, low specific surface area, and hierarchical porosity, which collectively facilitate efficient Na^+ storage and diffusion [1]. Further, ARCI also focus on synthesis of hard carbon (HC) using coconut husk biomass by . high-temperature carbonization at 1400 °C for 2 h under an inert atmosphere. The electrochemical performance is evaluated in a half-cell configuration vs. Na/Na^+ using 1 M $NaClO_4$ in EC:PC (1:1 vol%) electrolyte. Galvanostatic charge–discharge studies demonstrate specific capacities of 233, 142, 101, 48, and 33 mAh g^{-1} at current densities of 20, 50, 100, 500, and 1000 mA g^{-1}, respectively. Furthermore, the electrode exhibits good cycling stability with >80% capacity retention after 50 cycles at 50 mA g^{-1}. Further insights and technical details will be presented during the talk.

IT-079

Thermoelectric Properties of Nanocluster Composites consisting of Fullerene Molecules and Metal Oxide Nanoclusters

Masato Nakaya* and Jun Onoe

[3] *Department of Energy Science and Engineering, Nagoya University, Nagoya, Japan*

***Corresponding author e-mail:** m-nakaya@energy.nagoya-u.ac.jp

ABSTRACT

Thermoelectric (TE) conversion using flexible organic materials has been attractive to realize a power generator for various wearable devices in the future advanced information society. To realize a practical TE device, organic TE materials are desired to exhibit a dimensionless figureof-merit ($zT = \alpha^2 \sigma T/\kappa$) of more than unity for practical use, where T, α, σ, and κ denote absolute temperature, Seebeck coefficient, electrical conductivity, and thermal conductivity, respectively. Organic semiconductors such as pentacene, thiophene derivatives, and fullerene (C60) molecules have advantages for constructing high-performance organic TE devices owing to their low κ and exceptionally large α of 10−250 mV K^{-1}(giant Seebeck effect; GSE) 1 . Although the pristine C60 films exhibit a giant N-type α value (–121 mV K^{-1}), their ZT is 1.7×10^{-3} at RT, which is smaller by three orders of magnitude than that for practical use (ZT > 1) owing to a very low σ of 1.6 × 10−6 S cm^{-1} (see the blue circle in Fig. 1). In the present work, we have examined TE properties of C60 films doped with molybdenum trioxide (MoO3) nanoclusters, and succeeded in improving ZT value of 0.14 by increasing σ with maintaining the GSE (red circles of Fig. 1). In addition, the C60(MoO3)x films exhibited P-type TE properties within x of 0.01−11.8 by hole injection into C60 from MoO3 nanoclusters [2]. Furthermore, the temperature dependence of σ showed a strong positive correlation between |α| and the activation energy (Ea) of σ for the C60(MoO3)x films. For example, the GSE (|α| > 10 mV/K) emerged at Ea exceeding c.a. 0.27 eV [3].

Keywords: Thermoelectric conversion; Seebeck effect; nancomposite; fullerene; metal oxides.

References:

1. H. Kojima et al., Mater. Chem. Front. 2, 1276 (2018).
2. M. Nakaya et al., J. Chem. Phys. 158, 054701 (2023).
3. M. Nakaya et al., Carbon 241, 120374 (2025)

MOFs-derived and Chitosan-based Photocatalysts for Scalable VOCs Degradation in Photocatalytic Fluidized Beds

Ming-Wei Chen[1], Duo-Syuan Lin[1], Wei-Lun Huang[1], Yu-Che Hsiao[1], and Chao-Wei Huang[1*]

[1] *National Cheng Kung University, Department of Engineering Science, Tainan City, Taiwan*

***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

Photocatalytic fluidized beds (PFBs) synergistically couple photocatalysis with fluidized dynamics to enhance the degradation of volatile organic compounds (VOCs). By maintaining photocatalysts in suspension, PFBs improve light penetration and mass transfer, thereby overcoming the common limitations of fixed-bed systems such as light shielding and catalyst fouling. However, large-scale deployment remains constrained by catalyst attrition, loss, and insufficient mechanical stability. In this work, we introduce a MOFs-derived [1] and chitosan-based photocatalyst designed to address these challenges . Chitosan, a biodegradable and renewable biopolymer derived from natural biomass, provides low-cost, environmentally friendly, and mechanically robust support. Active photocatalytic particles were uniformly dispersed within a chitosan solution and solidified into spherical granules in an alkaline bath. These spheres exhibited superior abrasion resistance and maintained catalytic activity through progressive surface renewal as the outer layer eroded, continuously exposing fresh active sites. Our findings demonstrate that this chitosan-derived photocatalyst delivers long-term durability and scalability in fluidized bed operations, offering a sustainable pathway to practical VOC abatement. This approach provides both environmental and engineering benefits, establishing a promising strategy for advancing photocatalytic air pollution control technologies.

References:

1. Y.-C. Hsiao, D.-S. Lin, T.-Y. Wang, M.-W. Chen, C.-W. Huang, Enhanced photocatalytic degradation of VOCs using MOFs-derived nitrogen-doped TiO2 in a fluidized bed reactor, Journal of the Taiwan Institute of Chemical Engineers, (2025) 106358.

IT-081

Design of Sol–Gel Composite Materials for High-Temperature Ultrasonic/Piezoelectric Devices

Makiko Kobayashi[1]*, Mako Nakamura[1], Kei Nakatsuma[1]

[2]*Kumamoto University, Kumamoto, Japan*

***Corresponding author e-mail:** kobayashi@cs.kumamoto-u.ac.jp

ABSTRACT

In the realm of NDT 4.0 and industrial digital transformation (DX), continuous monitoring of operating industrial facilities is increasingly required; however, the exclusive use of high-Curie-point materials does not adequately address issues related to thermal vibration, the heat resistance limitations of backing materials, interfacial delamination, or the long-term durability of ultrasonic couplant. Sol–gel composite films offer an alternative design framework: the sol–gel process forms an oxide-based bonding layer directly on the substrate, enabling stable acoustic coupling without couplant, while intrinsic porosity suppresses excessive ringing and can eliminate the need for a separate backing layer, improving robustness under high-temperature vibration. Here, we investigate one of the sol–gel composites in which $LiNbO_3$ (LN) is the ferroelectric powder phase and a TiO_2 + $SrCO_3$ (TO+Sr) sol–gel phase; this material exhibits operational capability up to 1000 °C after heating to 400°C. A 200 µm-thick LN/TO+Sr film was fabricated on a 25mm thick steel substrate, and pulse–echo measurements were performed in an electric furnace at 750°C. Even after 10d, higher-order echoes with high signal-to-noise ratios were clearly observed, demonstrating sustained ultrasonic performance and thermal robustness at 750 C.

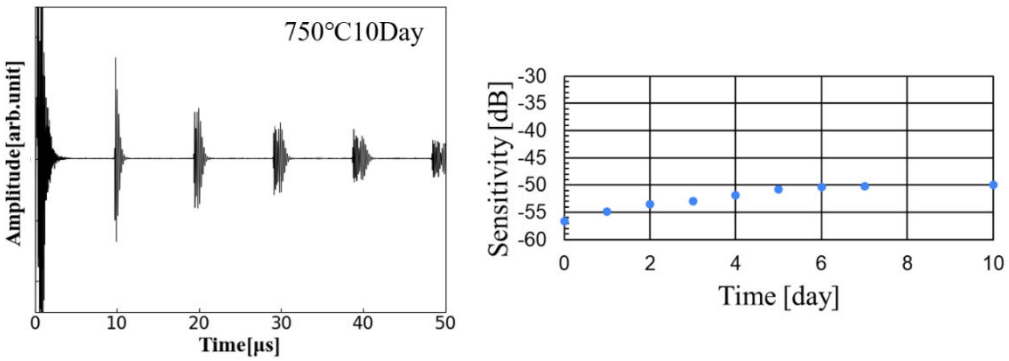


***Fig. 1 (a) Ultrasonic echoes at 750* °C after 10d *(b) Sensitivity transition at 750*°C**

Keywords: high-temperature; ultrasonic device; piezoelectric device; sol-gel composite

References:

1. N. Kambayashi, N. Zaito, H. Akatsuka, and M. Kobayashi, Jpn. J. Appl. Phys., **61**, SG1060 (2022).

IT-083

Seebeck-Coefficient Evaluation of Si Microribbon by Kelvin-Probe Force Microscopy

Hiroya Ikeda[1]*, Koteeswaran Kalaiarasan[1], Yuto Nakahara[1], Haruya Ozaki[1], Hiromu Hamasaki[1]

[1]*Shizuoka University, Hamamatsu, Japan*

***Corresponding author e-mail:** ikeda.hiroya@shizuoka.ac.jp

ABSTRACT

We have constructed a novel technique for evaluating the Seebeck coefficient in micro/ nanometer scale materials by Kelvin-probe force microscopy (KPFM) [1-3]. In this study, the Seebeck coefficient of a n-type Si microribbon formed on a silicon-on-insulator (SOI) substrate was determined by our technique. Because the evaluation of the Seebeck coefficient requires local measurement of the thermoelectromotive force (TEMF) and temperature difference, we first confirmed that the temperature difference measurement was possible using KPFM, and then measured the TEMF generated in the Si microribbon to evaluate the Seebeck coefficient. Figure 1 shows the KPFM (surface potential) image of the Si temperature-probe when a temperature gradient is applied to the sample [3]. The upper part of the image is the low temperature, and the lower part is the high temperature. From this result, it is found that the two Si probes have almost the same potential before the temperature gradient is applied (V_h=0V), as shown in Fig. 1(a). However, when the temperature gradient is applied (V_h=1V), the potential of the high temperature probe is lower than that of the low temperature probe, in Fig. 1(b). The temperature difference obtained from these potential images was 1.67K. Moreover, the Seebeck coefficient of the n-type Si microribbon could be evaluated to be -0.32 mV/K.

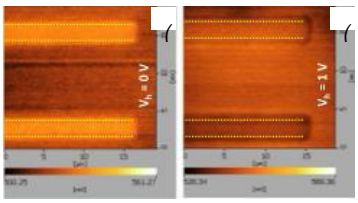


Fig. 1 Surface potential image of Si temperature-probes (a) at room temperature and (b) under a temperature gradient [3]

Keywords: Seebeck coefficient; Si microribbon; Kelvin-probe force microscopy

References:

1. H. Ikeda, K. Miwa, F. Salleh, *AIP Conf. Proc.*, **1449** (2012) 377-380.
2. H. Ikeda, Y. Suzuki, K. Miwa, F. Salleh, *2013 Int. Conf. on QiR* (2013) 35-38.
3. K. Kalaiarasan, Y. Nakahara, H. Hamasaki, H. Ikeda, et al., *Emergent Mater.*, **7** (2024) 3053-3060.

IT-084

A Traceable Digital Thread for UAV Propulsion: MBSE Architecture Linked with Performance Simulation

Chanakarn Phoopat, Bing-Han Huang, Yueh-Heng Li*

Department of Aeronautics and Astronautics, National Cheng Kung University, Tainan, Taiwan, 701

***Corresponding author e-mail:** yueheng@mail.ncku.edu.tw

ABSTRACT

Vacuum Arc Thrusters (VATs) is a micro-propulsion device for CubeSat attitude control due to their compact size, low power demand, and ability to perform without relying on the outside environment. The conventional Attitude Determination and Control Systems (ADCS) usually depends on the magnetic torque of a reaction wheel for the detumbling phase after launching the satellite. However, these devices have limitations in a deep space environment or when subjected to momentum saturation. Thruster-based detumbling using pulse plasma actuation, therefore, provides a viable alternative for post-deployment stabilization [1]. This research illustrates a simulation-based study on VAT-assisted detumbling control for a 3U CubeSat, with an emphasis on material-dependent thruster behavior and simple discrete control strategies. Copper (Cu) is adopted in experimental VAT systems [2], while tungsten (W) is considered as a comparative material due to its higher impulse bit and erosion resistance reported in prior studies [3]. Material effects are incorporated through impulse-bit modeling that captures variability and degradation characteristics associated with different electrode materials. The three-degree-of-freedom (3-DOF) rigid-body attitude dynamics model with realistic pulsed VAT actuation is developed. Two low-complexity detumbling control laws, which are Bang-Bang control and Logic-Based control, are used and evaluated under identical initial tumbling conditions. Logic-based control is widely used and offers flexibility in on-off thruster control principles, which require minimal tuning and computational effort [4]. The efficiency of two control laws is assessed in terms of angular-rate convergence, detumbling time, and firing activity. Simulation results demonstrate that angular rate of the satellite by using VAT is feasible under the limitation of the impulse bit constraints, and that material-dependent thruster characteristics significantly influence control performance. Bang-Bang control rapidly reduces the angular rate but results in higher firing frequency, while logic-based control exhibits improved robustness to impulse variability and material degradations.

References:

1. N. A. Gastonias, Y. Lu, J. Blandino, M. A. Demetriou, J. Spacecraft Rockets, 53 (2016) 57–75.
2. Y.-H. Li, J.-Y. Pan, G. Hendrich, Acta Astronautica, 172 (2020) 33–46.
3. I. Scheinin, N. Qi, R. Binder, M. Krishnan, I. K. Ziemer, I. E. Polk, A. Anders, Proc. Int. Electric Propulsion Conf., IEPC-01-228 (2001).

Bandgap Widening of Evaporated In-Se Films By Room Temperature Annealing

Tamihiro Gotoh*, Taiyo Hirai

Department of Physics, Graduate School of Science and Technology, Gunma University, Maebashi 371-8510, Japan

***Corresponding author e-mail:** tgotoh@gunma-u.ac.jp

ABSTRACT

Amorphous chalcogenide materials are highly desirable for phase-change memories and electrical switches. These two-terminal devices have emerged as promising candidates for highdensity memory applications due to their simple configuration1). However, drift in resistance and switching-threshold voltage2) poses significant challenges for their application. In this study, we investigated the fundamental physical properties of evaporated In-Se films, a type of chalcogenide semiconductors, and found significant changes in their properties at room temperature. Figure 1 shows the change in transmittance of In-Se evaporated films at room temperature. The transmittance at the absorption edge increased over a long period of more than one year after deposition. This result suggests that the bandgap widens upon room temperature annealing. Annealing at room temperature showed similar changes in film thickness, refractive index, and electrical conductivity, while the XRD patterns indicated the retention of an amorphous structure. This study clarified the structural relaxation process in amorphous In-Se and demonstrated that appropriate heat treatment can improve its structural stability.

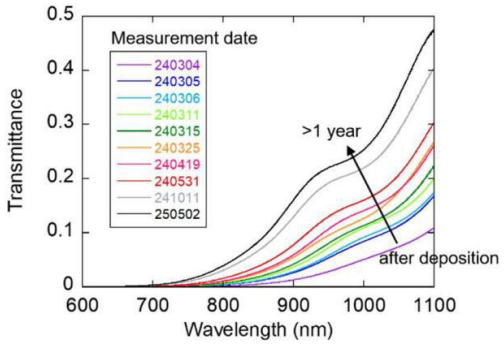


Fig. 1 Change in transmittance of In-Se evaporated films at room temperature

Keywords: amorphous chalcogenides; In-Se; transmittance; bandgap; structural relaxation

References:

1. S.-O. Park, S. Hong, S.-J. Sung, D. Kim, S. Seo, H. Jeong, T. Park, W. J. Cho, and J. Kim, S. Choi, Nature 628 (2024) 293.
2. V. Karpov, M. Mitra, D. Kau, G. Spadini, Y. A. Kryukov, and V. G. Karpov, J. Appl. Phys. 102 (2007) 124503.

IT-086

Transforming Electronics: The Future of Transparent and Paper Electronics

Rodrigo Martins, P. Barquinha, L. Pereira, R. Silva, D. Vieira, E. Carlos, A. Kiazadeh, J. Santanu, D. Gaspar, E. Fortunato

CENIMAT\i3N, Department of Materials Science, School of Science and Technology, NOVA University Lisbon and CEMOP/UNINOVA, Caparica, Portugal

ABSTRACT

In today's digital age, our rapid technological advancements confront us with critical sustainability challenges, including material scarcity, mounting waste, and environmental pollution, often exacerbated by high-temperature manufacturing processes. The socio-economic growth driven by the demand for smart electronics and non-recyclable materials contributes to climate change and resource depletion.

As we embrace the Internet of Things (IoT) and wearable technology, the need for sustainable materials becomes more urgent. Emerging nanoscale devices provide promising alternatives to silicon-based options, particularly in the field of so called transparent and paper electronics, which have the potential to revolutionize our approach to electronic devices, transforming it.

This presentation explores strategies to minimize electronic waste while advancing eco-friendly technology solutions. We are committed to developing green electronic products that meet consumer needs and promote environmental stewardship, going from micro to nanoscale approaches. Our efforts also focus on raising social awareness about sustainable technologies, engaging with communities and policymakers to advocate for practices that harmonize technology with environmental responsibility.

Join us in this exploration of innovative approaches to sustainability, as we aim to significantly impact our environment and foster a resilient future empowered by green technology.

Stimuli-Responsive Soft Molecular Materials

Manas K Panda

Department of Chemistry, Jadavpur University, Kolkata-700032

***Corresponding author e-mail:** mannup25@gmail.com, manaspanda.chemistry@jadavpuruniversity.com

ABSTRACT

Nature provides numerous examples of light-powered devices that can autonomously change their shape, size or display static/ dynamic motion in presence of natural light. Mimicking such function in the laboratory, i.e developing light powered autonomous micro/macro-machines using soft organic/metal organic molecular material represents one of the most difficult challenges in today's research and demands huge imagination, skills and tedious efforts from the involved researchers. Smart organic crystalline materials that are capable of displaying macroscopic responses such as shape deformation, size alteration or motion under light illumination have emerged as potential candidates for this purpose. The design of such molecules is accomplished by incorporating a photo-active unit that can absorb photons to initiate photoresponse and a suitable supramolecular synthon for non-covalent interactions for the propagation. On the simplest mechanistic view, the molecular motion triggered by light is cooperatively amplified to supramolecular to macroscopic scale with the help of intermolecular cooperative mechanism involving reconfigurable non-covalent interactions. While few such molecular crystals have been reported to exhibit fascinating macroscopic mechanical responses, the quest for developing new molecular systems having superior or novel mechanical responses is a never-ending process in material chemistry research. In this talk, we shall discuss about some of the novel light responsive materials that have recently been developed in our laboratory.

References

1. D. Bhattacharjee et al., *Cryst. Growth Des.*, 2025, **25**, 8157.
2. P. Mazumder et al., *Cryst. Growth Des.*, 2024, **24**, 7925.
3. P. Giri et al., *Chem. Eur. J.*, 2024, 202303836.
4. D. Dey et al., *J. Photochem. Photobiol. A*, 2023, **437**, 114480.
5. A. Shabashini et al., *Mater. Adv.*, 2024, D3MA00870C.

IT-088

Upconversion Luminescence of SrF_2-ErF_3 Solid Solutions

S.V. Gushchin*[1], S.V. Kuznetsov[2], V.A. Konyushkin[2], A.N. Nakladov[2], A.A. Lyapin[1], V.Yu. Proydakova[2], P.A. Ryabochkina[1], P.P. Fedorov[2]

[1]*National Research Ogarev Mordovia State University, Saransk, Russia, 430005*

[2]*Prokhorov General Physics Institute, RAS, Moscow, Russia, 119991*

***Corresponding author e-mail:**serg.guschin1703@gmail.com

ABSTRACT

Upconversion phosphors doped with rare-earth ions are the main object of study for many scientific groups. Because of their special optical properties, they have found various practical applications [1, 2].

In the present paper, we have investigated concentration series of fluoride single crystals and powders with a fluorite structure SrF_2-ErF_3. Single crystals were grown by vertical directional crystallization (Bridgman method). Powders were synthesized by using a co-precipitation from an aqueous nitrate solution technique.

The aim of work is comparison of upconversion luminescence characteristics of fluoride single crystals and powders SrF_2-ErF_3 upon excitation near-infrared laser radiation. Single crystals provide a more controlled and well-defined system for fundamental studies of mechanisms of upconversion energy transfer. Powders are a more complex object of investigate compared to crystals due to the presence of a number of factors. Firstly, powders have a significantly larger surface area compared to single crystals. This leads to a higher concentration of surface defects, acting as traps for excitation energy. These defects provide non-radiative relaxation pathways, resulting in energy loss as heat. Secondly, light scattering is more pronounced in powders due to the random arrangement and varying sizes of particles. This scattering reduces the effective path length of photons within the material, decreasing the probability of photon absorption and ultimately lowering luminescence output. Thirdly, powder particles tend to agglomerate, further increasing scattering effects. However, despite a number of restrictions, powders offer advantages in terms of ease of synthesis and cost-effectiveness.

In summary, the choice between crystals and powders depends on the specific research goals and practical application.

References:

1. X. Liu, H. Chen, et al, Nat. Commun., 12 (2021) 5662.
2. A. Ghazy, M. Safdar, ChemComm, Sol. Energy Mater. Sol. Cells. 230 (2021) 111234.

IT-089

A Proposal for Infrastructure Management Using Motorcycle Dynamics Data and Rider Vital Signals

Tomoya Kitani*[1]

[1]*Shizuoka University, Hamamatsu, Shizuoka 432-8011, Japan*

***Corresponding author e-mail :** t-kitani@inf.shizuoka.ac.jp

ABSTRACT

This study describes a method for quantifying road surface conditions by integrating motorcycle dynamics data with rider vital signals to provide data for infrastructure management. Current maintenance practices utilize indicators such as pavement cracking, rut depth, and the International Roughness Index (IRI). The measurement of these indicators traditionally requires specialized survey vehicles, a process that influences the frequency and spatial coverage of monitoring activities. Recent research has examined participatory sensing using smartphone sensors; however, these methods demonstrate lower measurement accuracy compared to dedicated instrumentation. Additionally, physical surface irregularities do not always correlate with the structural condition of the pavement or the physiological state of the road user. To address these factors, this study introduces a framework that synchronizes motorcycle dynamics data with rider vital signals. Vehicle motion is captured using inertial measurement units (IMUs) to record three-axis acceleration and angular velocity, combined with Global Navigation Satellite System (GNSS) positioning to provide centimeter-level coordinate data. Simultaneously, rider vital signals, specifically heart rate variability (HRV) and electrodermal activity (EDA), are collected via wearable sensors. The methodology involves correlating time-series data of vehicle attitude changes with physiological responses to identify road segments associated with specific rider reactions. This presentation details the sensing framework and the data acquisition methodology developed for integrating vehicle dynamics and human physiological data within the context of infrastructure management.

References:

1. M. Inagi, K. Tomiyama, R. Kohama, M. Eguchi, and M. Sato, “Human-centered Evaluation with Biosignals for Localized Surface Roughness on Expressway Pavements,” Proc. SURF2022, 9, ID-350 (2022).
2. Abdul Manan, Muhammad Marizwan and Abd Ghani, Muhammad Ruhaizat, “Road surface condition monitoring system utilizing motorcycle (ROCOM) – System development, validation and field test,” J. IOP Conference Series: Materials Science and Engineering, 512 (1), pp. 1-10, doi:10.1088/1757-899X/512/1/012017, (2019).

IT-090

Design of Electrodeposition-Driven Phosphide Catalysts for Green Hydrogen and Ammonia Synthesis

Bharati Debnath[1,2*]

[1]*Research Institute for Sustainable Energy (RISE), TCG-CREST, Salt Lake, 700091 Kolkata, India*

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002 India*

***Corresponding author's email address**: bharati.debnath@tcgcrest.org

ABSTRACT

Green hydrogen and ammonia are foundational to the emerging carbon-neutral energy landscape, functioning as clean fuels and carbon-free energy carriers, respectively. However, their industrial production remains dominated by fossil-fuel-intensive technologies, notably steam methane reforming for hydrogen and the Haber-Bosch process for ammonia. Developing sustainable electrochemical routes powered by renewable electricity therefore represents a critical scientific and technological challenge. Recent advances reveal that exceptional catalytic performance can be achieved through deliberate control of catalyst composition, electronic structure, and surface architecture, particularly in transition-metal phosphide systems.

Electrodeposition offers a versatile and scalable strategy to construct phosphide-based catalysts with tunable morphology, composition and controlled defect density. By modulating deposition parameters, charge distribution, and active-site environments, it becomes possible to optimize adsorption energetics of the reactant. Establishing systematic structure-function correlations provides mechanistic insight into how phosphide regulates intermediate stabilization, suppresses competing reactions, and enhances catalytic performance.

In this talk, I will present our recent progress on the design of phosphide-based catalysts using electrodeposition technique for hydrogen production and ammonia synthesis under ambient conditions. This presentation will highlight structure-activity correlations, mechanistic insights, and the role of surface engineering in achieving improved catalytic efficiency and durability.

References:

1. Bagaria, T.; Rahman, A.; U K, S.; Adalder, A.; Basak, H. K.; Ghorai, U. K.; Chakraborty, B.; Bano, A.;* Debnath, B.* Small 2025, 10.1002/smll.202513455.
2. Bagaria, T.; Borgohain, T.; Jadhav, S.; Das. T.;* Debnath, B.* Small 2025, 21, 2503368.
3. Bagaria, T.; Saha, S.; Pati, S. K.;* Sadhu, A.;* Debnath, B.* J. Mater. Chem. A 2025, 13, 15818-15831.

IT-091

Toward a Resilient Society: Dialogue between Engineering and the Social Sciences in Disaster Contexts

Miki Mochizuki*

Shizuoka University, Hamamatsu, Japan

***Corresponding author e-mail:** mochizuki.miki@shizuoka.ac.jp

ABSTRACT

Informatics is an interdisciplinary field encompassing engineering and the social sciences. From this perspective, this contribution explores dialogue between engineering and the social sciences, focusing on *resilience* as a common language bridging materials engineering and sociology. As natural disasters increase worldwide, resilience has become a key concept in disaster sociology. Originally used in materials engineering, resilience refers to the ability to store strain energy and deflect elastically under a load without breaking or being deformed [(1)]. In recent years, the concept has been applied to disaster research to describe the capacity of communities and societies exposed to hazards to recover from disruption [(2)]. In this expanded usage, resilience extends beyond the engineering notion of *bouncing back* to include adaptation and transformation—*bouncing forward*.

What does it mean to build a resilient society after disaster? We address this question through the case of the 2011 Great East Japan Earthquake, which had long-term impacts on Japanese society. During recovery, infrastructural measures such as collective relocation from tsunami-affected areas and the construction of seawalls were implemented to reduce future risks. However, in affected communities, disaster-related deaths and the deterioration of mental health became significant concerns. These realities suggest that building a resilient society cannot be reduced solely to structural or engineering considerations and underscore the importance of social resilience—the collective and communal dimensions of post-disaster life. Empirical research in sociology has focused on survivors and communities experiencing social disruption through evacuation and relocation, investigating the causes of disaster-related deaths and social responses. My research examines the frequently expressed experience of *having nothing to do* among survivors, revealing its close connection to the loss of community ties, livelihoods, and living environments following displacement.

Building a resilient society therefore requires not only safe infrastructure but also social environments in which people regain meaning, roles, and purpose in everyday life. Dialogue between engineering resilience and social resilience offers complementary perspectives for envisioning a more desirable society.

Keywords: Resilience; Sociology; Disaster Recovery; Great East Japan Earthquake

References:

1. Gordon, James Edward. 1978. Structures. Harmondsworth, UK: Penguin Books.
2. United Nations Office for Disaster Risk Reduction (UNDRR). 2017. The Sendai Framework Terminology on Disaster Risk Reduction. "Resilience". Accessed 14 February 2026.

IT-092

Theoretical Study of Phonon-Induced Negative Thermal Expansion Materials

Yasuhide Mochizuki[1]*

[1]*Institute of Science Tokyo, Tokyo, Japan*

***Corresponding author e-mail:** mochizuki.yasuhide@mct.isct.ac.jp

ABSTRACT

Negative thermal expansion (NTE) materials are attracting significant interest due to their potential applications as heat-resistant fillers, microdevices, power semiconductors, and micro-positioners in telescopes. Yet, despite a century of discoveries, the rational design of NTE materials has remained a challenging research topic. In this presentation, I introduce a comprehensive theoretical framework that clarifies the microscopic origins of NTE and establishes general guidelines for identifying new NTE candidates.

We present the systematic calculations of volumetric thermal expansion coefficients α_V, bulk moduli B_T, average atomic volumes V, and Grüneisen parameters γ for 46 unary solids and 45 binary oxides within the quasi-harmonic approximation (QHA). We have found that the magnitude of α_V is primarily governed by B_T, while its sign is determined by the Grüneisen parameter γ, which is determined by the crystal structure and local coordination environment. These correlations reveal that compounds with large structural void space and low-frequency transverse vibrational modes drive NTE behavior [1].

Building on this analysis, we have clarified that the NTE behavior of monoclinic $Cu_2P_2O_7$ is triggered by the transverse O–Cu–O vibrations [2]. Furthermore, we discovered biaxial NTE in $KNbSi_2O_7$ using molecular dynamics calculations within the on-the-fly machine-learning scheme and experiment [3].

Overall, our findings establish a phonon-based, symmetry-guided description of NTE, offering a foundation for the rational discovery and design of practical NTE materials.

Keywords: negative thermal expansion; lattice dynamics; quasi-harmonic approximation; Grüneisen parameter; machine-learning force fields

References:

1. Y. Mochizuki, H. Koiso, K. Nagamatsu, S. Bae, T. Isobe, and A. Nakajima, *J. Phys. Chem. C*, **128** (2024) 525.
2. Y. Mochizuki, K. Nagamatsu, H. Koiso, T. Isobe, and A. Nakajima, *J. Phys. Chem. Lett.*, **15** (2024) 156.
3. H. Koiso, S. Kawasoe, J. Zhang, T. Isobe, A. Nakajima, and Y. Mochizuki, *J. Phys. Chem. C*, **129** (2025) 9509.

IT-093

The Expanding Attack Surface of AI-Enabled Biometric Infrastructures

Tetsushi Ohki[1]*

[1]*Shizuoka University, Hamamatsu, Japan*

***Corresponding author e-mail:** ohki@inf.shizuoka.ac.jp

ABSTRACT

Biometric authentication is widely deployed across the world for identity verification in public services, finance, border control, and digital platforms. In particular, India operates Aadhaar, the world's largest biometric-based national identification system, which assigns a unique ID number to over a billion residents based on fingerprint, iris, and facial data. In recent years, rapid advances in artificial intelligence, especially deep learning, have significantly improved the accuracy and scalability of biometric recognition. However, these technological developments have also introduced new security, privacy, and fairness risks.

Emerging threats include sophisticated spoofing and impersonation attacks using AI-generated content, large-scale data breaches, model inversion[1] and template reconstruction attacks, adversarial examples, and risks of function creep and mass surveillance[2]. In addition, growing evidence suggests that biometric systems may exhibit demographic biases, leading to disparate error rates across gender, age, and ethnic groups, thereby raising concerns about fairness[3], discrimination, and unequal access to essential services. As biometric systems become increasingly interconnected and AI-driven, their technical and societal attack surface expands accordingly.

This talk introduces the evolving threat landscape of biometric authentication in the AI era and examines how these risks may manifest in large-scale national systems. By analyzing technical, security, privacy, and fairness perspectives, we discuss the implications for the robustness, trustworthiness, inclusiveness, and governance of next-generation biometric infrastructures.

Keywords: Biometric Authentication, Deep Learning, Adversarial Attacks, Privacy and Surveillance

References:

1. M. Akasaka, S. Maeda, Y. Sato, M. Nishigaki, and T. Ohki, "Model-free template reconstruction attack with feature converter," in Proc. BIOSIG 2022, pp. 14-22, 2022.
2. T. Ohki, N. Abe, H. Uchida, and S. Yamada, "A human-centered risk evaluation of biometric systems using conjoint analysis," in Proc. IEEE Int. Joint Conf. Biometrics (IJCB 2024), pp. 1-8, 2024.
3. T. Ohki, Y. Sato, M. Nishigaki, and K. Ito, "LabellessFace: Fair metric learning for face recognition without attribute labels," in Proc. IEEE Int. Joint Conf. Biometrics (IJCB 2024), pp. 1-8, 2024.

IT-094

Effect of Tandem-Type Stabilization of Two-Dimensional (2D) Nb_2CT_x Mxene on Their Colloidal and Cytotoxic Properties

M. Jakubczak and A. M. Jastrzębska

Faculty of Mechatronics, Warsaw University of Technology, św. Andrzeja Boboli 8, 02-525 Warsaw, Poland

ABSTRACT

Two-dimensional (2D) Nb2CTx MXene holds great promise for biomedical applications due to its tunable surface chemistry and biocompatibility. However, their practical use requires long-term colloidal and oxidative stability. Here, we propose a tandem-type stabilization strategy that combines antioxidant protection with macromolecular surface functionalization. Nb2CTx was first treated with L-ascorbic acid (LA) to suppress oxidation by binding to reactive edges, followed by modification with polyethylene glycol (PEG), poly-L-lysine (PLL), or polydopamine (PDA). This dual approach enhanced stability in biological media — phosphate-buffered saline (PBS) and Dulbecco's Modified Eagle's Medium (DMEM) — while maintaining non-cytotoxicity toward A375 and HaCaT skin cell lines across a concentration range of 0–100 mg·L−1. Among the tested systems, LA/PEG and LA/PDA-modified MXenes maintained stable zeta potentials (−15 to −12 mV) and particle sizes for 72 h, whereas LA/PLL samples showed aggregation and charge loss. This tandem stabilization effectively prevents oxidation and aggregation without compromising biocompatibility, offering a versatile route for developing oxidation-resistant MXenes for biomedical and nanomedicine applications.

AC-001

Structural, Morphological, and Magnetic Properties of Eu – Doped Nanocrystalline $La_{0.9}Ba_{0.1}MnO_3$

Dharm Singh[1], Rabindra Nath Mahato[1]*

[1]*School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India*

***Corresponding author e-mail:** rnmahato@jnu.ac.in

ABSTRACT

In this study, we have investigated the structural, morphological, and magnetic properties of $La_{0.85}Eu_{0.05}Ba_{0.1}MnO_3$ nanocrystalline compound synthesised by the Sol-gel method. Rietveld refinement of X-ray diffraction was done using Full Prof software, and it confirms the orthorhombic crystal structure with the Pnma space group. The Debye-Scherrer method was used to calculate the crystallite size, and the average crystallite size was found to be ~ 15 nm. Transmission electron microscopy (TEM) images show that the particles are spherical in shape and the average particle size is ~ 40 nm. The selected area electron diffraction pattern confirms the crystallinity, and high-resolution TEM gives a fringe width corresponding to planes. The temperature-dependent magnetic measurements were carried out in the temperature range of 2–300 K under an external magnetic field of 0.05 T, revealing a ferromagnetic to paramagnetic phase transition at a temperature of ~ 182 K. In this high temperature Curie-Weiss law, Debye's and paramagnetic Curie temperature were found to be 214 K. Using the Curie-Weiss fit data, the effective magnetic moment was calculated μ_{eff} = 7.9 μ_B/f.u. The magnetic field dependent magnetization M(H) data show a ferromagnetic loop at low temperature (2 K) and paramagnetic behaviour at room temperature. The M(H) data showed the Coercivity at 2 K is 0.0244 T and retentivity 19.6 emu/g. The hysteresis loop with a small Coercive field is important for magnetic refrigeration in the intermediate temperatures.

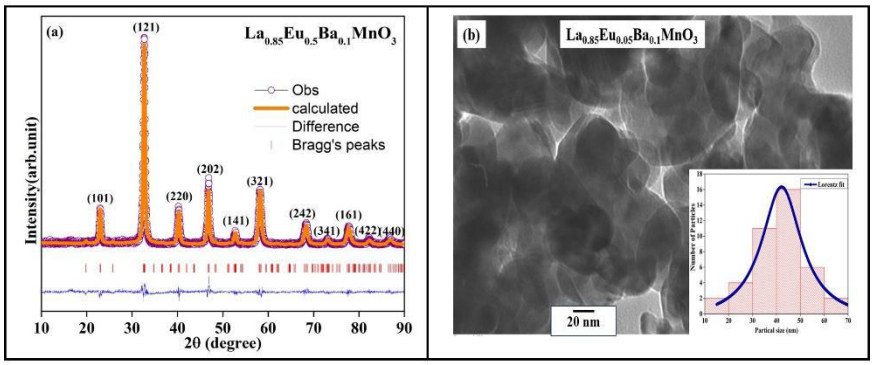


Fig. 1 (a) Rietveld-refined X-ray diffraction (XRD) pattern of the nanocrystalline LEBMO sample. (b) TEM images with the particle size distribution histogram and Lorentz fit of the nanocrystalline LEBMO sample

Keywords: Sol-gel method; X-ray diffraction; Magnetic materials; Magnetic refrigeration

References:

1. Li, L. Wei, Z. Ti, L. Ma, Y. Yan, G. Zhang, and P.-F. Liu, *Phys. Rev. B*, **108** (2023) 224302.

AC-002

Designer Colour-Tunable NIR-Reflective Cool Pigments in the Ternary Vanadate Phenacite-Inverse Spinel Phase Regime

Kshatri Durga Lalitha Bai[1], U.V. Varadaraju[1], SS. Halkarni[2], Ch. Subrahmanyam[3], M. Pardha Saradhi[1]*

[1]*Department of Chemistry, School of Engineering and Sciences, SRM University – AP, Andhra Pradesh 522240, India*

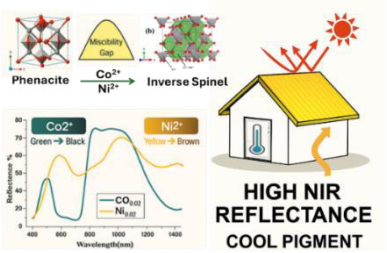
[2]*Department of Mechanical Engineering, School of Engineering and Sciences, SRM University – AP, Andhra Pradesh 522240, India*

[3]*Indian Institute of Technology Hyderabad, Sangareddy, Kandi-502284, Telangana, India*

***Corresponding author e-mail:** pardha.m@srmap.edu.in

ABSTRACT

Li-containing ternary vanadates are known for their remarkable structural diversity and tunable physical properties, making them attractive for advanced functional applications. In this study, we present a systematic investigation of Co^{2+} and Ni^{2+}-doped $LiZnVO_4$ to elucidate their structural transitions, optical behaviour, and potential for energy-efficient coating technologies. A clear miscibility gap is observed in intermediate compositions, indicating limited solid solubility between the two end members. The local lithium environments were probed using magic angle spinning 7Li solid-state nuclear magnetic resonance spectroscopy, providing direct evidence for the incorporation of two paramagnetic dopant ions into the crystal lattice. At low dopant concentrations, the 7Li isotropic peak intensity increases due to paramagnetic relaxation enhancement, whereas higher concentrations lead to characteristic peak broadening. CIELAB colour space shows systematic colour tuning with increasing dopant concentration: green → brown → black for Co-doping and light greenish yellow → yellow → brown for Ni-doping. Importantly, the doped LZVO-0.02Ni and LZVO-0.02Co compositions exhibited high NIR solar reflectance of 87% and 70% respectively, in the 750-2200 nm range, enabling effective solar heat management. The combination of phase-selective doping, tunable colour properties, and strong NIR solar reflectivity positions these materials as promising candidates for next-generation cool pigments in sustainable building and coating applications.



Keywords: Ternary vanadates; Structural transition; Paramagnetic relaxation enhancement (PRE); NIR reflectance; Cool coating pigments.

AC-003

Multifaceted Characterization of PVDF/ $Bi_{12}GeO_{20}$ Nanocomposite Films: Insights into Structural, Optical, Thermal, Mechanical and Dielectric Properties

Nimisha Babu Raj[1,2], Arun K.J[1]*

[1]*Sree Kerala Varma College, Trissur, Kerala, India, 680011*

[2]*Sree Narayana Guru College, Chelannur, Kerala, India, 673006*

***Corresponding author e-mail:** drarunkj@gmail.com

ABSTRACT

Bismuth Germanium Oxide ($Bi_{12}GeO_{20}$) reinforced polyvinylidene difluoride (PVDF) nanocomposite films were prepared by solution casting method and studied in detail for the enhanced physical properties. The prepared PVDF/$Bi_{12}GeO_{20}$ nanocomposite films were characterized using X- Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) spectroscopy and FT Raman spectroscopy for analysing structure, morphology and functional groups. SEM analysis confirmed the uniform distribution of $Bi_{12}GeO_{20}$ nanoparticles within the PVDF matrix. FTIR and FT Raman studies revealed a significant enhancement of the electroactive β-phase in PVDF upon the addition of $Bi_{12}GeO_{20}$ nanoparticles. Optical studies via photoluminescence and UV- Visible spectroscopy show an enhancement of emission intensity with the addition of $Bi_{12}GeO_{20}$ nanoparticles. Furthermore, the nanocomposite films exhibited improved thermal stability, mechanical strength, and a higher dielectric constant compared to pristine PVDF. These findings demonstrate the significant potential of PVDF/$Bi_{12}GeO_{20}$ nanocomposite films for developing a high performance, flexible sensor devices for advanced optoelectronic applications.

Keywords: Bismuth germanium oxide, polyvinylidene difluoride, solution casting method

References:

1. T. A. Taha, M. H. Mahmoud, and H. H. Hamdeh, J. Polym. Res., 28 (2021) 148.
2. L. Ruan, X. Yao, Y. Chang, L. Zhou, G. Qin, and X. Zhang, Polymers, 10 (2018) 228.
3. K. J. Arun, V. S. Hiran, A. K. Batra, and M. D. Aggarwal, Mater. Today Proc., 50 (2022) 81–84.
4. R. Gregorio Jr., J. Appl. Polym. Sci., 100 (2006) 3272–3279.

AC-004

Microstructural and Mechanical Performance of Laser Beam Welded Joint between Inconel 625 and SAE 304 Stainless Steel

Nivruth Narayan V M , Pradyun Shylesh, Santosh Sampath*

Programmable Responsive Intelligent Structures and Materials (PRISM) Group, Department of Mechanical Engineering, Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, INDIA.

***Corresponding author e-mail:** santoshs@ssn.edu.in

ABSTRACT

This study investigates the microstructural nature and tensile strength of the laser welded joint between two alloys – SAE 304 Stainless Steel and Inconel 625, with a constant laser power of 48 % and a pulse mode frequency of 12 Hz. Laser beam welding of these alloys provides significant advantages in the aerospace and chemical processing industries requiring high corrosion resistance and high surface temperature protection. However, challenges are posed due to different thermal properties such as thermal coefficients and different solidification behaviours in the weld joint. The base metals and the fusion zone were analysed using metallurgical microscope, FESEM and EDS techniques and the results showed that the base metals exhibited FCC lattice with austenitic grains and the fusion zone displayed dendritic pattern due to rapid solidification towards the centre line. Moreover, inclusions, striations and cracks were observed in the base metals and fusion zone respectively. Tensile testing specimen was cut out from the welded sample using Wire EDM machining process according to ASTM-E8 flat sample standards. This specimen was used in the tensile test. The UTS was recorded to be 235.07 N/mm2, typically lower than other welding processes. The load vs displacement curve was plotted and it showed an initial region of low stiffness with progressive increase in non-linear elongation.

References:

1. Vani Shankar, K Bhanu Shankar Rao, & S.L Mannan, Journal of Nuclear Materials, 288 (2001), 222-232
2. Manwatkar S. K., Kuhite K. S., Murty S. V. S., & Narayanan P. R, Metallography, Microstructure, and Analysis, 4(2015), 497–507.

Tailoring Laser Fluence to Enhance Piezoresistive Sensitivity in Laser-Induced Graphene-Based Flexible Sensors

Arun V[1]*, Krishnapriya U K[2], Adarsh V J[1], Shyam Kumar C N[1]

[1]*Department of Materials Science and Engineering, National Institute of Technology, Calicut, Kerala, India, 673601*

[2]*Department of Physics, P.T.M Government College, Perinthalmanna, Malappuram, Kerala, India, 679322.*

***Corresponding author e-mail:** arun_p230680mt@nitc.ac.in

ABSTRACT

The rapid advancement of flexible and wearable electronics demands materials that combine superior mechanical flexibility with high electrical sensitivity and stability. In this work, laser-induced graphene (LIG) derived from polyimide (PI) tape laminated on polyethylene terephthalate (PET) substrates was systematically investigated as a piezoresistive sensing material. The LIG was fabricated using a Snapmaker A350T laser system operated in dot-filled mode, with laser fluence precisely varied between 0.4 and 0.9 J/mm² to study its influence on microstructure, degree of graphitization, and piezoresistive response. Optical microscopy and FE-SEM analyses revealed a distinct morphological transition from isolated carbon dots at lower fluences to a continuous, interconnected spongy network at moderate fluence (0.7 J/mm²), beyond which thermal degradation and delamination occurred. Raman spectroscopy confirmed progressive graphitization with decreasing ID/IG ratios, from 0.819 to 0.218, as the fluence increased. Meanwhile, XRD analysis showed an enhancement in the (002) graphitic peak intensity and a reduction in interlayer spacing, indicating improved structural ordering. The electrical conductivity of LIG films increased significantly with fluence, from 1.70×10^{-4} S/m to 89.98 S/m, indicating efficient conversion of the PI matrix into conductive graphitic carbon. Piezoresistive characterization demonstrated a strong inverse correlation between conductivity and sensitivity, with the sample fabricated at 0.5 J/mm² exhibiting the highest gauge factor (GF = 89.04 ± 2.49), attributed to optimal defect density and inter-flake contact modulation. These findings establish laser fluence as a key parameter in tailoring the morphology, electrical, and piezoresistive properties of LIG, providing a reliable pathway for the rational design of high-performance, flexible strain sensors for wearable and biomedical applications.

Keywords: laser-induced graphene; laser fluence; piezoresistive behaviour; gauge factor; flexible strain sensor.

References:

1. Y. Wang et al., Appl. Phys. Lett., 126 (2025).
2. G. Chen et al., J. Mater. Chem. A, 13 (2025) 25400–25411.

AC-006

Investigation on the Linear and Non-Linear Optical Properties of Indole-Ringed Amino Acid Infused Thiourea-Metal Complexes

Kalaivani H, Chitra M*

Department of Physics, Anna University, Chennai, Tamil Nadu, India – 600025.

***Corresponding author e-mail:** chitrashadrach@annauniv.edu

ABSTRACT

Rapid technological development demands efficient nonlinear optical (NLO) materials, which play a crucial role in microelectronics, laser technology, optoelectronics, and optical communication, among other applications. Metal-organic NLO materials possess the required high nonlinearity with added metallic stability, especially metal-thiourea complexes, which exhibit superior performance in various NLO applications, such as frequency doublers. In this work, a novel attempt is made to analyze the optical properties of indole-ringed L-tryptophan doped zinc thiourea sulphate (ZTST) complexes. The parent and doped complexes were prepared using the solution growth technique. The effect of the dopant was studied in different concentrations. The structural analyses were carried out using P-XRD, SC-XRD, and SEM. The analysis revealed that the dopant induced minor strain without changing the parent structure. The optical absorption analysis was done to study parameters such as absorbance, refractive index, extinction coefficient, conductivity, etc. The dielectric analysis was carried out as the dielectric behaviour impacts the NLO property. The non-linear optical analyses were done using SHG and the Z-scan method. The figure of merit shows a significant improvement in NLO property due to the dopant.

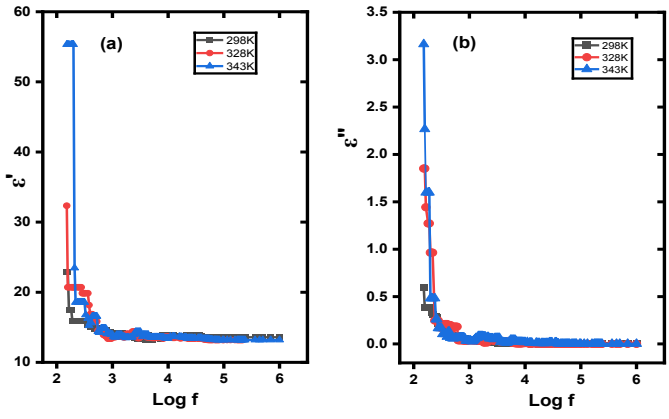


Fig 1: (a) Dielectric constant & (b) Dielectric loss profile of ZTST complex

Keywords: NLO material; Semi-organic complex; Z-scan analysis

References:

1. H. Merina Albert, T. Jemima, and C. Alosious Gonsago, J. Fluoresc., 34 (2024) 1057–1063.

An Experimental Analysis of Zinc MMCs Reinforced with SiC and Graphite

Selvabharathi V[1], Tamizhselvan G[1], Santosh Sampath[1]*

[1]*Programmable Responsive Intelligent Structures and Materials (PRISM) Group, Department of Mechanical Engineering, Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, INDIA.*

***Corresponding author e-mail:** santoshs@ssn.edu.in

ABSTRACT

This study looks at the creation and microstructural analysis of Zinc based Hybrid Metal Matrix Composite reinforced with Silicon Carbide and Graphite The composite is waws used to make stir casting of composition included Zinc 98% (433g) ,Graphite 1% (8.5g) and Silicon Carbide 1% (8.5g).The molten zinc was stirred mechanically by means of stir casting machine where dispersion of materials takes place in molecular view and the metal is finally made into dimensions of 30mm diameter and 200mm long The goal was to investigate how hybrid reinforcements affect the structural features of the Zinc matrix. Microstructural Analysis is done on Scanning Electron Microscopy (SEM),Energy Dispersive X-ray (EDX) is used to confirm the presence of Zinc, Silicon Carbide, Graphite and they are successfully incorporated into atomic particles and followed by wear test for to calculate how much the metal done by casting resists abrasion and surface damage .The experimental results show better structural uniformity and improved distribution of the reinforcement compared to pure Zinc. These findings suggest that Zn-SiC-Graphite composites are promising for lightweight and moderate-load engineering applications.

References:

1. M. Fan, F. Zhao, Y. Liu, S. Yin, S. Peng, and Z. Zhang, Crystals, 12 (2022) 1110.
2. Q. Dai, S. Peng, Z. Zhang, Y. Liu, M. Fan, F. Zhao, Front. Bioeng. Biotechnol., 9 (2021) 635338.
3. A. Owhal, A. D. Pingale, S. U. Belgamwar, and J. S. Rathore, Mater. Today Proc., 44 (2021) 222–228.

AC-008

Advancements in Soft/Hard Ferrite Nanocomposites: Magnetic, Dielectric, and Optical Perspectives

Bindu Sharma[1], Ankush Chauhan[2], Supreet Kaur[1], Suman[3], Rohit Jasrotia[4,5]*, Ritesh Verma[6]*

[1]*Department of Physics, Amity University Haryana, Gurugram, India-122413*

[2]*Centre for Herbal Pharmacology and Environmental Sustainability, Chettinad Hospital and Research Institute, Chettinad Academy of Research and Education, Kelambakkam, Tamil Nadu, 603103, India*

[3]*University Centre for Research and Development, Chandigarh University, Mohali, Punjab, India*

[4]*School of Physics and Materials Science, Shoolini University, Solan, Himachal Pradesh, India-173212*

[5]*Division of Research and Development, Lovely Professional University, Phagwara Punjab India-144411*

[6]*Department of Physics, Graphic Era (Deemed to be University), Dehradun, Uttarakhand, India-248002*

***Corresponding author e-mail:** vermaritesh.rv40@gmail.com, rohitsinghjasrotia4444@gmail.com

ABSTRACT

The outstanding thermal and chemical stability, high coercivity, and substantial magnetic anisotropy of barium hexaferrite make it an ideal candidate for use in permanent magnets, microwave devices, and EMI shielding. Cobalt zinc ferrite, on the other hand, is perfect for use in transformers, inductors, magnetic storage, and biological applications because of its low coercivity and high saturation magnetism. Enhancements to magnetic behavior, dielectric properties, and microwave absorption capacity are brought about by the incorporation of exchange coupling interactions into these ferrites through nanocomposites. Phase formation, crystallite size, microstructure, and cation distribution are all thoroughly examined in this study, along with the effects of doping elements, processing parameters (calcination and annealing temperatures), and various synthesis processes (sol-gel, co-precipitation, hydrothermal, etc.). The review emphasizes the importance of magnetic exchange coupling for tailoring the performance of soft/hard ferrite nanocomposites. Integrating these materials that enhance coercivity and saturation magnetization across interfaces is crucial for their use in high-frequency electronics, EMI shielding, and high-density data storage. The presence of both spinel and hexagonal phases in the composites is confirmed by structural as the primary cause. Optical characterization using UV-Vis spectroscopy shows that altering the doping concentration and crystallite size can modulate bandgap energies, leading to a greater potential for use in photocatalysis and optoelectronics. When it comes to microwave and RF technology, nanocomposites' consistent performance throughout frequency ranges and decreased dielectric losses are crucial. Optimal electrical, magnetic, and multifunctional materials are created when nanocomposites of barium hexaferrite and cobalt zinc ferrite are combined. The next generation of electrical, spintronic, and communication technologies.

Keywords: Nanoferrites; Barium Hexaferrite; Cobalt Zinc Ferrite; Nanocomposite; Dielectric; Vibrating Sample Magnetometer; UV-Visible

AC-009

Fatigue Behaviour of FeMnSi Shape Memory Alloy

S. Santosh[1]*, S. Vivithkumar[1], N. Yashvanth[1]

[1]*Programmable Responsive Intelligent Structures and Materials (PRISM) Group, Department of Mechanical Engineering, Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, India.*

***Corresponding author e-mail:** santoshs@ssn.edu.in

ABSTRACT

FeMnSi shape memory alloys are attractive for structural applications due to their reliable shape recovery, low alloying cost, and good workability, enabling use in large and complex components. Their functional behaviour is governed by the reversible γ (austenite) ↔ ε (martensite) transformation, which stabilises deformation and enhances energy dissipation during cyclic loading. Since many components experience fluctuating axial stresses, high cycle fatigue performance is a key factor for long term reliability. Previous studies mainly reported general transformation behaviour and overall fatigue trends, with limited focus on precise failure conditions. This study addresses that gap through controlled load based fatigue testing under accurate axial alignment. A $Fe_{30}Mn_6Si$ alloy was produced using vacuum induction melting followed by hot working to ensure microstructural uniformity. Dog bone specimens were carefully machined and polished to minimise surface induced crack initiation. High cycle fatigue tests were conducted in load control mode at a peak load of 27.5kN. Stable cyclic behaviour was observed initially due to stress assisted ε-martensite formation and gradual work hardening. With continued cycling, microstructural damage accumulated progressively. Final fracture occurred at approximately 11,000 cycles. This fatigue life is comparable to previously reported FeMnSi systems. The results show that fatigue performance is governed by transformation induced damage and crack growth. Despite stable behaviour at moderate stresses, fatigue limits remain finite. These findings support the selective use of FeMnSi alloys in structural connectors and vibration control applications.

References:

1. Otsuka, Hiroaki, et al. "Effects of alloying additions on Fe-Mn-Si shape memory alloys." ISIJ international 30.8 (1990): 674-679.
2. Koster, M., et al. "Cyclic deformation and structural fatigue behavior of an FE–Mn–Si shape memory alloy." Materials Science and Engineering: A 637 (2015): 29-39.

AC-010

Investigations on the Structural and Photoluminescence Properties of Alkali-Doped Cesium Copper Iodide Single Crystals

Jeevika S [1,2], Aryalakshmi S [1,2], Akshai Shyam [1,2], Krishnendu R [1,2], Janani Krishnamoorthy [3], Ramasubramanian Swaminathan [1,2] *

[1]*Department of Physics, Amrita School of Physical Sciences Coimbatore, Amrita Vishwa Vidyapeetham, India*

[2]*Functional Materials Lab, Amrita School of Engineering Coimbatore, Amrita Vishwa Vidyapeetham, India*

[3]*Department of Science and Humanities, Nehru Institute of Technology, Kaliapuram, Thirumalayampalayam, Coimbatore*

***Corresponding author e-mail:** s_ramasubramanian@cb.amrita.edu

ABSTRACT

Cesium copper iodide ($CsCu_2I_3$) is one of the promising lead-free metal halide perovskites exhibiting superior environmental stability, minimal toxicity, and cost-effective preparations. This study investigates the luminescence properties of pure and alkali-doped CsCu2I3 single crystals grown using anti-solvent vapor-assisted diffusion (AVD) method. The incorporation of potassium (K+) and sodium (Na+) ions as dopants has been explored to understand their impact on crystal growth, structural changes, and optoelectronic behaviour of the material. The CsCu2I3 single crystals have been synthesized in DMF-DMSO mixture using methanol as antisolvent in a 48-hour reaction. Structural and optical characterizations have been employed to characterize the single crystals. XRD analysis confirmed that undoped CsCu2I3 retained an orthorhombic crystal structure while the doped samples exhibited a random preferred growth. From SEM analysis, micrometer rod-shaped crystals have been observed with an average diameter of 138 µm for pure and above 100 µm for doped. According to photoluminescence studies, alkali doping has significantly impacted the stability and intensity of the emission. Pure $CsCu_2I_3$ showed a bright yellow emission at 570-580 nm at an excitation wavelength of 355 nm. At low dopant concentrations (1% K^+ or Na^+), photoluminescence intensity showed a higher value while, with increasing dopant concentrations, a quenching effect has been observed. Increase in luminescence efficiency at optimal dopant concentrations has indicated that the significance of precise regulation of doping for tuning optical performance. This work provides valuable insights into the role of alkali doping in perovskites in the fabrication of luminescence-based sensing devices.

Keywords: Perovskite; Photoluminescence; Single Crystals

References:

1. Z. Zhao et al., J. Lumin., 241 (2022) 118482.
2. F. Qiu, Y. Lei, and Z. Jin, Front. Optoelectron., 15 (2022) 47.

AC-011

Structural and Magnetic Properties of Tryphtophan-capped Iron Oxide Nanocomposites

Syed Mohamed. A[1], Jeba Sherin. R[1]*

[1]*Department of Chemistry, Sadakathullah Appa College,Tirunelveli, Tamilnadu, India, 627011*

***Corresponding author e-mail:** jebasherinjs2020@gmail.com

ABSTRACT

Iron Oxide Nanocomposites capped with L-tryptophan represnts a class of amino-acid-modified magnetic nanomaterial in which surface chemistry is governed by biologically relevant ligands. The incorporation of tryptophan onto iron oxide nanocomposites introduces an indole-containing, zwitterionic moeity capable of influencing nanocomposites stability. Such systems are commonly synthesized using co-prepitation method in alternative route, this paper focused on tryptophan capped iron oxide nanocomposites via microwave assisted solvothermal method. The resulting materials are characterised by techniques including X-ray diffraction, Fourier -transform infraref spectroscopy, electron microscopy, electron microscopy and magnetic measurements to confirm the phase purity, surface functionalisation and superparamagnetic behaviour. Investigation of tryptophan - capped iron oxide nanocomposites provides insights into amino acid-nanocomposites interactions and establishes a basis for examining their physiochemical and biological properties under controlled conditions.

Keywords: amino acid; microwave; iron oxide; nanocomposites

References:

1. A. S. Angela, L. M. Ludmila, C.-I. Cornelia, et al., Sci. Rep., 14 (2024) 26228.
2. R. Mathur, R. P. Chauhan, G. Singh, et al., J. Mater. Sci. Mater. Med., 31 (2020) 87.

AC-012

Disorder Induced Interband Dynamics of Spin–Orbit Coupled Tilted Nodal Line Semimetals

Vivek Pandey[1], Pankaj Bhalla[2]*

[1]*Department of Physics, School of Engineering and Sciences, SRM University AP, Amaravati, 522240, India*

[2]*Centre for Computational and Integrative Sciences, SRM University AP, Amaravati, 522240, India*

***Corresponding author e-mail:** pankaj.b@srmap.edu.in

ABSTRACT

We investigate the role of disorder on the interband conductivity of tilted nodal line semimetals (NLSMs) in the presence of spin-orbit coupling (SOC). The inclusion of SOC brakes spin degeneracy, hereby altering the band dispersion and transport properties. In the absence of the tilt term, the system anomalous response vanishes due to the underlying symmetry of the nodal ring. However, a finite tilt in the system breaks the inversion symmetry, giving rise to a non-zero anomalous response. Using a quantum kinetic framework, we analyze the total interband conductivity, which contains both disorder-driven (extrinsic) and field-driven (intrinsic) mechanisms. Using DFT-fitted parameters for a realistic system, we provide a numerical estimation for the response, highlighting the potential applications for photonic and spintronic devices.

References:

1. Chen Wang, Wen-Hui Xu, Phys. Rev. B 103 (2021), 165104.
2. Chen Fang, Hongming Weng, Chin. Phys. B. 25 (2016) 117106.
3. Chen Fang, Yige Chen, Phys. Rev. B 92 (2015),081201(R).
4. Vivek Pandey, Pankaj Bhalla, New J. Phys. 27 (2025) 073501.

AC-013

Application of X-Ray Radiography for Detection and Repair of Bulges Observed in Composite Rocket Motor Casing

Umashankar. D[1]*, Sanyaja Kumar Sahoo[1], Rajesh Addanki[1]

[1]*Advanced Systems laboratory (ASL), DRDO, Kanchanbagh, Hyderabad, India,500058.*

***Corresponding author e-mail:** sriuma2001@gmail.com

ABSTRACT

Composite rocket motor casings, fabricated from advanced materials through a filament winding process involving helical, hoop, and fabric layers, offer enhanced efficiency and simplified manufacturing. Non-destructive evaluation (NDE) plays a vital role in ensuring the structural integrity of these casings, with X-ray radiography being particularly effective in detecting defects such as porosity, inclusions, delamination, and non-uniform fiber or matrix distribution. Delamination, a common and severe defect often introduced during manufacturing, can significantly impact the service life of the component.

In this context, this paper examines the delamination defects (bulges) identified in a large composite rocket motor casing and the subsequent steps taken to address them. Radiographic Testing (RT) was utilized to accurately characterize the delamination, providing critical insights that informed the development of an effective repair strategy. The repair scheme developed was validated through post-repair non-destructive testing (NDT), which allowed the casing to undergo further processing and a subsequent static test. The success of this static test not only confirmed the efficacy of the repair but also corroborated the RT findings. Additional post-static test radiography was conducted to evaluate the condition of the repaired area, ensuring the casing's readiness for continued use.

Throughout the manufacturing process of the composite rocket motor casing, RT played a pivotal role. From the initial detection and investigation of defects to the rectification of those issues, RT provided valuable data that was essential for ensuring the integrity of the rocket motor casing.

References:

1. R. A. Smith, Mater. Sci. Eng., 3 (2009) 103.
2. S. T. Peters, in Composite Filament Winding, ASM Int., (2011) 1.
3. M. Munro, Polym. Compos., 9 (1988) 352.

AC-014

Additive manufacturing of Anisotropic Honeycomb Lattice Materials Embedded with Shape Memory Alloys: Mechanical and microstructural characterization

Sandhya[1], Samyuktha[1], Santosh Sampath[1]*

Programmable Responsive Intelligent Structures and Materials (PRISM) Group, Department of Mechanical Engineering, Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, INDIA.

***Corresponding author e-mail:** santoshs@ssn.edu.in

ABSTRACT

This study deals with layer-by-layer deposition of PLA based materials with certain special reinforcements. Anisotropic honeycomb lattice-based materials composed of unique microstructures were built by incorporating shape memory alloys into the PLA matrix. Shape Memory Alloys (SMAs) are smart materials, which can change their shape, size and properties according to the external triggers such as temperature, stress or magnetic field. Initially, using CAD software (Fusion 360), the anisotropic honeycomb structure was designed, and the 3D printing process was carried out using Fused Filament Deposition (FDM) technique. The prepared samples were further subjected to mechanical and microstructural characterisation. This property tailored materials are of great importance in the current world, because of their unique characteristics such as light weight, high impact strength, stiffness, Shape Memory Effect and superelasticity. All these properties make them ideal for their applications in aerospace, biomedical and various other fields.

Keywords: additive manufacturing; metamaterials design; shape memory alloy

AC-015

Phase Evolution and Dielectric Response of Lead-Free $BiTiO_3$, NBT, and KBT-Based Perovskites

Nilesh Kumar Prasad[1], Satya Prakash pati[1]

[1] *North-Eastern Hill University, Shillong, Meghalaya*

***Corresponding author e-mail:** nileshprasad700@gmail.com

ABSTRACT

A comparative investigation was conducted on lead-free perovskite ceramics $BiTiO_3$ (BiT), $Na_{0.5}Bi_{0.5}TiO_3$ (NBT), and K0.5Bi0.5TiO3 (KBT) to establish structure-property correlations. Rietveld refinement of X-ray diffraction data confirmed a single-phase tetragonal structure (P4mm) for BiTiO3 and KBT, with refined lattice parameters of a = 3.9366 Å and c = 3.9623 Å for KBT. NBT exhibited its characteristic perovskite structure with refined lattice parameters of a = 5.5036(14) Å and c = 3.8793(19) Å. Raman spectroscopy further verified phase purity and structural consistency across all compositions. AC conductivity studies as a function of frequency and temperature indicated a thermally activated conduction mechanism. Charge density distribution analysis revealed the influence of the KBT phase on the NBT lattice. A negative real dielectric permittivity (εr′) was detected over a broad frequency range (1 kHz-2 MHz), reflecting anomalous polarization effects intrinsic to the lead-free compositions.

References:

1. Mesrar, Mohammed, et al. ACS omega 7.42 (2022): 37142-37163.
2. Elkechai, O., M. Manier, and J. P. Mercurio. 157.2 (1996): 499-506.

AC-016

A Comparative Analysis of Alternate Refrigerant-Lubricant Pairs for Enhanced and Sustainable VCR System Performance.

Subramani N[1], Shrilakshmi B[1], Rahul AK[1]

[1]*Easwari Engineering College, Department of Mechanical Engineering, Chennai,India,600089*

***Corresponding author e-mail:** subramani.n@eec.srmrmp.edu.in

ABSTRACT

The refrigeration industry has significantly advanced food preservation by extending the shelf life of perishables and limiting microbial growth. With widespread household adoption, refrigerator production has increased rapidly, making energy efficiency a critical concern due to continuous operation. Improving system efficiency can reduce power consumption and support long-term sustainability. Refrigerants and lubricants play a major role in the performance of vapor compression refrigeration (VCR) systems. Lubricants reduce mechanical friction and enhance efficiency; however, conventional lubricants often raise environmental concerns due to limited biodegradability. Refrigerant selection is equally important, as commonly used refrigerants contribute significantly to global warming. This study evaluates a sustainable refrigerant–lubricant combination by varying capillary tube diameters and lengths. A hydrocarbon blend of R290 and R600a is used with a blended lubricant consisting of polyol ester and sesame oil. System performance is assessed in terms of coefficient of performance (COP), suction pressure, refrigeration effect, and power consumption. Compared to the conventional POE + R134a system, the synthesized blend demonstrates a 9.26% improvement in COP and up to a 4% increase in suction pressure for optimized capillary dimensions. Pull-down temperature analysis indicates an enhancement in refrigeration effect of nearly 44% for the optimal capillary diameter, while power consumption shows only a 2.7% increase, confirming improved energy efficiency and sustainability

Keywords: COP; Refrigeration effect; Capillary tube; R290/R600a; POE/sesame oil

References:

1. A. Ruggiero, R. D'Amato, M. Merola, P. Valasek and M. Müller, Tribol. Int., 2017, 109, 529–540.
2. S. N. Sabarinath, K. Prabhakaran Nair and P. K. Rajendrakumar, Lubr. Sci., 2019, 31, 179–193.
3. Irnawati, S. Riyanto, S. Martono and A. Rohman, Food Res., 2019, 4, 135–142.
4. S. Narayanasarma and B. T. Kuzhiveli, Powder Technol., 2019, 356, 1029–1044.
5. A. Sajeeb and P. K. Rajendrakumar, J. Clean. Prod., 2019, 240, 118255.

AC-017

Disorder Induced Interband Dynamics of Spin–Orbit Coupled Tilted Nodal Line Semimetals

Vivek Pandey[1], Pankaj Bhalla[2]*

[1]*Department of Physics, School of Engineering and Sciences, SRM University AP, Amaravati, 522240, India*

[2]*Centre for Computational and Integrative Sciences, SRM University AP, Amaravati, 522240, India*

***Corresponding author e-mail:** pankaj.b@srmap.edu.in

ABSTRACT

We investigate the role of disorder on the interband conductivity of tilted nodal line semimetals (NLSMs) in the presence of spin-orbit coupling (SOC). The inclusion of SOC brakes spin degeneracy, hereby altering the band dispersion and transport properties. In the absence of the tilt term, the system anomalous response vanishes due to the underlying symmetry of the nodal ring. However, a finite tilt in the system breaks the inversion symmetry, giving rise to a non-zero anomalous response. Using a quantum kinetic framework, we analyze the total interband conductivity, which contains both disorder-driven (extrinsic) and field-driven (intrinsic) mechanisms. Using DFT-fitted parameters for a realistic system, we provide a numerical estimation for the response, highlighting the potential applications for photonic and spintronic devices.

References:

1. Chen Wang, Wen-Hui Xu, Phys. Rev. B 103 (2021), 165104.
2. Chen Fang, Hongming Weng, Chin. Phys. B. 25 (2016) 117106.
3. Chen Fang, Yige Chen, Phys. Rev. B 92 (2015),081201(R).
4. Vivek Pandey, Pankaj Bhalla, New J. Phys. 27 (2025) 073501.
5. Vivek Pandey, Dayana Joy, Phys. Rev. B 110 (2024), 155108.

AC-018

Effect of Pre-Milling (Ni And Al) on the Oxidation Behaviour of Nialfecocr High Entropy Alloy

Uma Maheswara Rao, U. Devi Sushma, Sheela Singh*

Department of Mechanical Engineering, School of Engineering and Applied Sciences, SRM University AP, Amaravati, Andhra Pradesh, 522502, India.

* **Corresponding author e-mail:** sheela2k5@gmail.com, Sheela.s@srmap.edu.in

ABSTRACT

This study explores the impact of pre-milling Ni and Al powders on the synthesis and high-temperature oxidation behavior of NiAlFeCoCr high-entropy alloy (HEA). Two alloy types were synthesized via mechanical alloying: (1) as-milled (all elements milled together for 10 h), and (2) pre-milled (Ni and Al pre-milled for 5 h, then mixed with Fe, Co, and Cr and milled for another 10 h). Both powders were consolidated using vacuum hot pressing (VHP). X-ray diffraction analysis confirmed the formation of BCC and FCC phases in both alloys. The coefficient of thermal expansion (CTE) was also lower in the pre-milled alloy (13.37×10^{-6}/K) than in the as-milled alloy (16.11×10^{-6}/K). Isothermal oxidation studies at 1050 °C over 5, 50, and 100 hours revealed the formation of stable Al_2O_3. SEM-EDS confirmed equiatomic composition and the development of an oxide layer. The pre-milled alloy exhibits better oxidation resistance, mechanical, and thermal properties compared to the as-milled alloy. The obtained results demonstrate the benefit of pre-alloying in tailoring material properties.

References:

1. W. Ji et al., J. Alloys Compd., 589 (2014) 61–66.
2. E. J. Pickering and N. G. Jones, Int. Mater. Rev., 61 (2016) 183–202.
3. M. Jadhav, S. Singh, M. Srivastava, and G. S. Vinod Kumar, J. Alloys Compd., 783 (2019) 662–673.
4. H. Chen and W. Luo, J. Mater. Res. Technol., 37 (2025) 1737–1747.

AC-019

Fe–Co–Gd Alloy Synthesized by Mechanical Alloying: Structural and Magnetic Properties

Sanjeev Kumar Gupt, Rajeev Singh, and Biswanath Bhoi*

Nano-Magnetism and Quantum Technology Lab, Department of Physics, Indian Institute of Technology (Banaras Hindu University) Varanasi, Uttar Pradesh - 221005, India

***Corresponding author e-mail:** biswanath.phy@itbhu.ac.in

ABSTRACT

Rare-earth–transition-metal alloys such as FeCoGd are emerging as highly promising synthetic antiferromagnets due to their strong spin–orbit coupling, ultrafast spin dynamics, and low magnetic damping [1], making them attractive for next-generation spintronic technologies [2]. While most prior studies have focused on thin-film systems, the role of structural phase, crystallite size, and lattice disorder in governing their magnetic behavior remains largely unexplored.

In this work, we report the first successful synthesis of nanocrystalline FeCoGd alloys in powder form using a simple and scalable mechanical alloying route. X-ray diffraction confirms the formation of a well-defined body-centered cubic phase, while SEM–EDX mapping reveals a homogeneous elemental distribution across the alloyed particles. The mechanically alloyed FeCoGd exhibits nanoscale crystallite sizes accompanied by lattice strain and defect-driven disorder, characteristic of non-equilibrium solid-state processing [3].

Magnetic measurements demonstrate that antiferromagnetic exchange coupling between the Fe/Co and Gd sublattices dominates the magnetic response, leading to compensated or reduced net magnetization depending on composition and microstructure. The results further show that crystallite size, strain, and defect density significantly modulate the strength of magnetic interactions, offering additional degrees of freedom for tuning material performance.

These findings establish mechanical alloying as a versatile platform for producing FeCoGd alloys over a wide compositional range and for systematically exploring structure–magnetism correlations. The insights gained from this nanocrystalline system provide a valuable foundation for optimizing FeCoGd-based thin films and synthetic antiferromagnets for ultrafast and energy-efficient spintronic applications.

References:

1. D. Huang, D. Zhang, et. al. Phys. Rev. B 107 (2023) 214438.
2. R.A. Duine, K.J. Lee, et. al. Nat. Phys. 14 (2018) 217–219.
3. B. Bhoi, V. Singh, et.al. J. Alloys Compd. 496 (2010) 423–428.

Effect of Graphene Filler in ARB Fibers in Araldite LY 556 Epoxy Resin and Aradur HY 951 Hardener Polymer Composites: Experimental Study of Fractography and Moisture Absorption

Ananda G K[1]*,Raviprakash M[2], Prashanth B[3], Venkatesh N[4],Raghu P[3],Manju Venu[1]*

[1]*Center for Polymer Testing Lab, Faculty of Engineering, AMC Engineering, Bengaluru-560083 India*

[2]*Center for Design Systems Lab, Faculty of Engineering, The Oxford College of Engineering, Bengaluru-560068 India*

[3]*Center for Nano-Materials Lab, Faculty of Engineering, Cambridge Institute of Technology, North Campus, Bengaluru-562110 India*

[4]*Center for Materials Testing Lab, Faculty of Engineering, University Visvesvaraya College of Engineering, Bengaluru-560001 India*

***Corresponding author e-mail:** ananda.ullegowda@amceducation.in, manju.venu@amceducation.in

ABSTRACT

The study investigates the moisture absorption capabilities and fractography performance of created reinforced barrier fibres inserted in epoxy resin polymer composites, with a focus on the influence of graphene fillers integration by augmentation ultrasonic machining. The Araldite LY 556 epoxy resin and Aradur HY 951 hardener are mixed with a proportion of 10:1 ratio for creating the matrix polymer. To achieve a homogeneous mixture, the graphene fillers based powders is sonicated using acetone liquid for 1 hr. The chopped alkalized ARB fibres are placed into the mould, which follows a mixture of required epoxy resins, hardener, and graphene powder for 30 minutes at a temperature of 140°C via compression moulding process. FESEM and AFM results revealed that the surface roughness of various types of alkalized ARB fibers has significantly improved, resulting in better bonding between the alkalized ARB fibers and the polymerized resin during composite processing. Additionally, the composite's flexure strengths dropped drastically from 163.25 MPa (60E36A4G) to 146.95 MPa (60E34A6G) after adding 10 wt. % graphene fillers, which was even lower than the flexural strength of 60E40A. This abrupt decrease in flexural strength shows that greater volumes of filler cannot be effectively integrated into the matrix.

Keywords: Acetone liquid, composite processing, dropped drastically, ultrasonic machining, compression moulding process.

AC-021

Lightweight and Absorption-Dominant PVA/PANI/$CeNiO_3$@GNP Polymer Nanocomposites for EMI Shielding

Supreetha M[1, 2], Veena M G[2], Bindya S[4], Shubhada H C[4], Pawandeep Kaur.[5], Maalti Puri[6], Gnana Prakash A P [3*]

[1]*Department of Studies in Electronics, PG Center, Hemagangotri, University of Mysore, Hassan 573220, India*

[2]*Department of Electronics and Communication Engg, JSS Science and Technology University, SJCE, Mysuru 570006, India*

[3]*Department of Studies in Physics, Manasagangotri, University of Mysore, Mysuru 570006, India*

[4]*Department of Chemistry, JSS Science and Technology University, SJCE, Mysuru 570006, India*

[5]*Department of Electronics Technology, Guru Nanak Dev University, Amritsar 143005, India*

[6]*Department of Electronics and Communication Engg, Khalsa College of Engineering and Technology, Amritsar 143005, India*

***Corresponding author e-mail:** gnanaprakash@physics.uni-mysore.ac.in

ABSTRACT

The increasing electromagnetic pollution from high-frequency electronic devices requires the development of lightweight, flexible, and absorption-dominant electromagnetic interference (EMI) shielding materials. Polymer-based electromagnetic interference shielding nanocomposites through absorption-dominant characteristics are significantly desirable for next-generation electronic applications. In this work, polymer nanocomposites were fabricated and systematically examined for EMI shielding applications in the X-band frequency range (8.2–12.4 GHz). Cerium Nickelate **(**$CeNiO_3$) nanoparticles were synthesized via the solution combustion method, while Polyaniline (PANI) was prepared through in-situ oxidative polymerization. Polymer nanocomposites were fabricated by incorporating conductive PANI, magnetic perovskite $CeNiO_3$, and graphene nanoplatelets (GNP) into a polyvinyl alcohol (PVA) matrix resulting in a PVA/PANI/$CeNiO_3$@GNP films. Structural characterization using X-ray diffraction (XRD) confirmed the crystalline nature of $CeNiO_3$, while Fourier transform infrared spectroscopy (FTIR) revealed strong interfacial interactions among PVA, PANI, $CeNiO_3$, and GNP. Morphological studies were carried out using scanning electron microscopy (SEM), the micrographs demonstrated homogeneous dispersion of fillers and the formation of interconnected conductive networks at higher filler loadings. The nanocomposites exhibited frequency-dependent AC conductivity, reduced skin depth, enhanced dielectric and magnetic loss tangents in the X-band (8.2–12.4 GHz). With the synergistic effects of conductive, dielectric, and magnetic loss mechanisms, the composites demonstrated absorption-dominated EMI shielding behavior. The EMI shielding performance showed a strong dependence on filler concentration, with the shielding effectiveness due to absorption (SE_A) increasing from ~5 dB to ~18 dB as the filler content increased. In contrast, the shielding effectiveness due to reflection (SE_R) remained relatively low (2–11 dB), minimizing secondary electromagnetic interference.The sample fabricated with greater perovskite loading achieved total shielding effectiveness of ~25–27 dB. These results emphasize the ability of PVA/PANI/$CeNiO_3$@GNP nanocomposites as a flexible, lightweight, absorption dominant EMI shielding materials for high-frequency applications.

Keywords: Absorption dominant, EMI shielding, oxidative polymerization, solution combustion method

AC-022

Extraordinary Magnetoresistance and Temperature-Dependent Electronic Transport in WTe_2

Sharvari Kulkarni[1], R S Patel[1]*

[1]*Department of Physics, Birla Institute of Technology & Science Pilani – K K Birla Goa Campus, Zurainagar, Goa, India, 403 726*

***Corresponding author e-mail:** rsp@goa.bits-pilani.ac.in*

ABSTRACT

Tungsten ditelluride (WTe_2), a layered transition-metal dichalcogenide, exhibits extraordinarily large, positive, and non-saturating magnetoresistance (MR) over a wide range of magnetic fields and temperatures. In this work, we analyse the magnetotransport properties of 1T′ -WTe_2, emphasizing the role of carrier compensation and electronic structure. Special attention is given to the temperature dependence of electrical resistance in zero magnetic field and under applied magnetic fields, where a pronounced magnetic-field-induced resistive upturn is observed. These findings highlight the interplay between carrier mobility, compensation, and external magnetic fields in determining the unique transport characteristics of WTe_2. We report MR at 4 K approximately 2200 % with the application of field of 8 T (black curve in Fig. 1(b)). The MR curves remain symmetric and non-saturating up to the highest applied field, reinforcing that we observe near-perfect electron-hole compensation in our samples. Overall, the observed low-temperature magnetoresistance in 1T′-WTe_2 is predominantly governed by classical electron–hole compensation mechanisms. In the absence of an external magnetic field (red curve in Fig. 1(b)), the resistance drops monotonically from 300 to 3 K, indicating enhanced carrier mobility at low temperatures due to reduced phonon scattering. This metallic trend aligns well with conventional transport mechanisms in high-mobility semimetals where delocalized electrons dominate conduction.

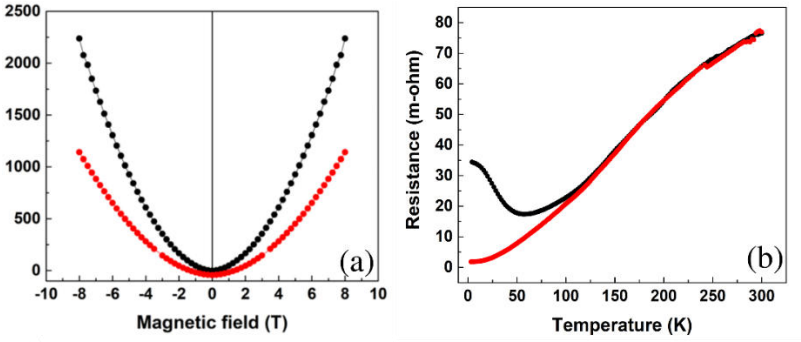


Fig. 1 (a) MR of 1T'-WTe_2 flake at 10K (red circles) and 4K (black circles). (b) Resistance vs Temperature of 1T'-WTe_2 flake without magnetic field (red) and with magnetic field of 8T (black).

References:

1. M. N. Ali, J. Xiong, S. Flynn, J. Tao, Q. D. Gibson, L. M. Schoop, T. Liang, N. Haldolaarachchige, M. Hirschberger, N. P. Ong, and R. J. Cava, Nature, 514 (2014) 205.
2. L. R. E. A. Thoutam, Phys. Rev. Lett., 115 (2015) 046602.
3. Y. E. A. Zhao, Phys. Rev. B, 92 (2015) 041104.

AC-023

Microstructural Evolution and Mechanical Tailoring of Fe-Al-Ni Alloys via Controlled Annealing and Normalizing Heat Treatments

A. Siddartha*, K. Sai Maneesh, Md. Owais Ahmed Sajjad, Radhika Chada

Mechanical Engineering, KUCE&T, Kakatiya University, Warangal, 506009

***Corresponding author e-mail:** siddartha.arukonda@gmail.com

ABSTRACT

Fe-Al-Ni (Iron-Aluminum-Nickel) alloys represent a critical class of advanced engineering materials, valued for their synergistic combination of high-temperature mechanical strength, superior corrosion resistance, and lightweight characteristics. These alloys are increasingly utilized in high-performance sectors, including aerospace propulsion and automotive components, where stability under extreme thermal stress is paramount. Their performance is fundamentally governed by complex phase evolutions; specifically, studies by Massalski et al. [1] have mapped the ternary Fe-Al-Ni phase diagram, demonstrating that nickel additions serve to stabilize the gamma (fcc) and B2 (FeAl/NiAl) structures while effectively suppressing DO_3 formation in aluminum-rich compositions. This study investigates the correlation between specific thermal processing regimes—annealing and normalizing—and the resulting structural and mechanical behavior of these alloys. The research methodology involved a comprehensive characterization of the alloy in its as-casted, annealed, and normalized conditions. X-Ray Diffraction (XRD) was employed to monitor phase stability, while Scanning Electron Microscopy (SEM) coupled with Energy Dispersive Spectroscopy (EDS) was utilized to analyze grain morphology and elemental partitioning. Literature suggests that B2 ordering increases significantly with Ni content [2], and our experimental results confirm that annealing at intermediate temperatures facilitates the transformation from metastable to equilibrium phases. Specifically, annealing was observed to promote the nucleation and growth of ordered intermetallic precipitates, such as Ni_3Al, within the solid solution matrix. Conversely, normalizing treatments induced significant crystallographic texture modifications, altering preferred planar orientations without necessitating major phase transformations. These divergent mechanisms—precipitation hardening in annealed samples versus texture-induced strengthening in normalized samples—both provide effective pathways for enhancing mechanical hardness. By integrating findings from thermomechanical processing studies, this work elucidates the critical structure-property relationships required to tailor Fe-Al-Ni alloys for targeted industrial applications. The results suggest that by strategically manipulating heat treatment parameters, engineers can optimize the trade-offs between ductility, hardness, and long-term microstructural stability in advanced functional environments

References:

1. T. B. Massalski, H. Okamoto, P. R. Subramanian, L. Kacprzak, *Binary Alloy Phase Diagrams*, vol (1990) 120-145.
2. S. Yuan, S. O. Samuel, G. J. Shiflet, *J. Alloys Compd.*, 614 (2014) 115-122.

AC-024

Multi-Scale Microstructural and Indentation Evaluation of Glass Fibre Reinforced Expired ABS for Sustainable Additive Manufacturing

G. A. Munshi*[,1], Venkatesh M. Kulkarni[1]

[1]*Department of Mechanical Engineering, Visvesvaraya Technological University, Belagavi, Karnataka, India, 590014*

***Corresponding author e-mail:** iamnihalmunshi05@gmail.com

ABSTRACT

The progressive ageing of acrylonitrile-butadiene-styrene (ABS) significantly compromises its structural integrity, reducing its reuse in additive manufacturing, thus increasing wastage. To recycle this wastage and add to the circular economy, this study investigates the structural restoration of expired ABS through glass fibre reinforcements in 5, 10, 15 and 20 wt% and establishes a microstructure-property correlation using multi-scale characterization. Virgin ABS (vABS), expired ABS (eABS) and their corresponding glass fibre (GF) reinforced composites (i.e., vABS/GF and eABS/GF) were systematically analyzed using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and macro and micro indentation testing. FTIR spectra of eABS revealed oxidative modifications and subtle alterations in characteristic functional group intensities, indicating molecular-level degradation. On adding GFs, the C≡N stretch at 2234 cm^{-1} indicates better fibre-matrix interactions, signifying fibre dispersion and interfacial bonding. XRD patterns confirmed the predominantly amorphous structure of ABS, with reinforcements including minor changes in structural ordering. SEM observations showed microcrack formation and surface embrittlement in eABS, whereas GF incorporation improves morphological uniformity and demonstrates effective fibre-matrix interaction with crack-bridging features. Indentation measurements indicated progressive recovery in hardness in eABS/GF compared to vABS/GF at both macro and micro scales. The enhancement in localized deformation resistance is attributed to load transfer mechanisms and microstructural constraint imparted by the dispersed fibres. This multi-scale evaluation demonstrates a viable pathway for valorising the mechanical integrity of eABS in sustainable additive manufacturing, thus advancing circular material utilization without complex reprocessing routes.

References:

1. E. Lobov, I. Vindokurov, and M. Tashkinov, Polymers (Basel), 16 (2024) 1106.

AC-025

Raman Spectroscopic Characterization of Fly Ash and Bottom Ash from a Coal Power Plant of Eastern India

Jajneswar Biswal[1*], Tushar Gupta[2], Himanshu Bhushan Sahu[3]

Department of Mining Engineering, National Institute of Technology Rourkela, Rourkela, Odisha, India-769008

***Corresponding author e-mail:** 521mn1006@nitrkl.ac.in ; biswaljajneswar@gmail.com

ABSTRACT

Fly ash (FA) and bottom ash (BA), the principal solid residues generated from coal combustion in thermal power plants, pose significant environmental challenges due to their large volumes and compositional heterogeneity. Although the bulk chemical characteristics of FA are well documented, comparative phase-level investigations addressing variability among different ash fractions and bottom ash remain limited, particularly for Indian coal ashes. In this study, coarse, medium, and fine fractions of FA, along with BA, collected from a coal-fired thermal power plant in eastern India were systematically characterized using Raman spectroscopy, supported by complementary compositional analysis. Raman spectra revealed the dominance of quartz (457–460 cm^{-1}) across all FA fractions, accompanied by hematite (196, 200, 417–430 cm^{-1}), magnetite (259 cm^{-1}), and anatase (107–140, 394 cm^{-1}), reflecting high-temperature silicate transformations during combustion. In contrast, BA exhibited more pronounced crystalline signatures of quartz (125, 196, 463 cm^{-1}), magnetite (320–380 cm^{-1}), and minor rutile (240–265 cm^{-1}), indicating differences in cooling history and oxidation conditions relative to FA. The concurrent presence of quartz and mullite phases supports the potential reuse of FA in cementitious and ceramic applications, whereas the detection of unburned carbon and metal oxide phases highlights the need for appropriate stabilization and leaching control prior to utilization. Overall, this study demonstrates that fraction-wise Raman spectroscopic analysis provides critical insight into the mineralogical heterogeneity of coal ash materials, offering a reliable basis for evaluating their utilization potential and informing strategies for safe and sustainable ash management.

Keywords: Fly ash; Bottom ash; Raman Spectroscopy; Phase Characterisation; Coal Combustion Residues

AC-026

Synthesis of high purity Zeolite from Water Treatment Sludge for Fluoride Removal from Coal Mine Water

Satish Chandra Bhuyan[1*], Pallavi Behera[2], Himanshu Bhushan Sahu[3]

Department of Mining Engineering, National Institute of Technology Rourkela, Rourkela, Odisha, India-769008

***Corresponding author e-mail:** 520mn6002@nitrkl.ac.in

ABSTRACT

Water treatment sludge (WTS), generated in large quantities from drinking water treatment plants, presents significant disposal and environmental challenges due to its high alumina-silicate and metal hydroxide content. This study investigates the sustainable conversion of WTS into zeolitic material and its application for fluoride removal from coal mine water. The sludge was subjected to alkali activation followed by hydrothermal method for synthesis of zeolite. Structural and morphological characterization using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), and Brunauer–Emmett–Teller (BET) analysis confirmed the formation of crystalline zeolite phases with enhanced porosity and surface functionality. Batch adsorption experiments were conducted to evaluate fluoride removal efficiency under varying pH, contact time, adsorbent dosage, and initial fluoride concentration. The synthesized zeolite demonstrated significant fluoride uptake, particularly within near-neutral pH ranges relevant to mine discharge waters. Adsorption equilibrium data were best described by the Langmuir isotherm model, indicating monolayer adsorption, while kinetic studies followed pseudo-second-order behaviour, suggesting chemisorption mechanisms. The primary removal pathways include ion exchange, electrostatic interactions, and surface complexation with aluminum-rich active sites. The findings highlight a circular economy approach by transforming water treatment sludge into a value added adsorbent for remediation of fluoride contaminated coal mine water. This approach addresses dual environmental concerns waste sludge disposal and mine water contamination offering a cost effective and sustainable solution for mining affected regions.

Keywords: Water treatment sludge, Zeolite, Fluoride, Coal mine water, Sustainable remediation.

AC-027

Alginate – Silica Functionalized Magnetic Nanoparticle for Targeted Cancer Cell Isolation

Kaavya Purushothaman [1], Ashwin Kumar Narasimhan[2], S. Gnanavel*[3]

[1]*Biomaterials Laboratory, Department of Biomedical Engineering, SRM Institute of Science and Technology, Kattankulathur campus, Chengalpattu, Tamil Nadu, 603203, India*

[2]*Department of Biomedical Engineering, College of Engineering and Applied Science, University of Wisconsin Milwaukee, Milwaukee, WI, 53211, USA*

***Corresponding author e-mail:** gnanaves@srmist.edu.in

ABSTRACT

Circulating tumour cells (CTCs), are the transitional metastatic agent that enables tumour dissemination is crucial in metastatic progression. CTC isolation remains challenging due to the mechanical instability, low ligand density and non-specific binding of the conventional immunomagnetic beads. Existing silica – based magnetic nanoparticle often limits biocompatibility and its robust structure that reduces the capturing efficiency in complex biological fluids. Here, we developed alginate-silica functionalized nanoparticle that integrates bio functional versatility of alginate. The controlled multilayer structure will lead to controlled surface modification through silane-mediated conjugation of folic acid. High ligand accessibility is maintained while polymer swelling is suppressed by the strengthened inorganic shell, improving magnetic responsiveness and colloidal stability. In comparison to their traditional silica-coated counterparts, the modified nanoparticles exhibit greater shear stability and selective cancer cell capture under dynamic flow circumstances. A strong and flexible framework for next-generation immunomagnetic cancer diagnostics is offered by this organic–inorganic approach.

References:

1. Deng, Z., Wu, S., Wang, Y., & Shi, D. (2022). Circulating tumor cell isolation for cancer diagnosis and prognosis. *EBioMedicine*, *83*.
2. Kim, G., Yong, Y., Kang, H. J., Park, K., Kim, S. I., Lee, M., & Huh, N. (2014). Zwitterionic polymer-coated immunobeads for blood-based cancer diagnostics. *Biomaterials*, *35*(1), 294-303.
3. Yu, Y., Zhang, Y., Chen, Y., Wang, X., Kang, K., Zhu, N., ... & Yi, Q. (2023). Floating immunomagnetic microspheres for highly efficient circulating tumor cell isolation under facile magnetic manipulation. *ACS sensors*, *8*(4), 1858-1866.
4. Pollema, C. H., Ruzicka, J., Christian, G. D., & Lernmark, A. (1992). Sequential injection immunoassay utilizing immunomagnetic beads. *Analytical chemistry*, *64*(13), 1356-1361.

AC-028

A Comprehensive Review on PVDF Nanocomposites Reinforced with Maleic Anhydride and Silane-Treated Short Carbon Fiber

Shalini M S[1]*, M G Veena[1], Lakshmi Swaminathan[2] G Gayathri [1]

[1]*Dept. of ECE, JSS Science and Technology University, SJCE, Mysuru*

[2] *Dept. of ECE, MS Ramaiah Institute of Technology, Bengaluru*

***Corresponding author e-mail:** shalinims@jssstuniv.in

ABSTRACT

Polyvinylidene fluoride (PVDF) based polymers with polar covalent bonds are next-generation dielectric materials for electric energy storage applications. PVDF and its copolymers have attracted considerable attention as promising polymer matrices for dielectric applications owing to their excellent flexibility particularly the β-phase, thermal stability, and high breakdown strength. However, the relatively low dielectric constant, challenges in fabricating complex geometries limits its performance in advanced electronic and energy storage devices. To overcome this limitation, nanocomposite approaches have been developed by incorporating metal oxides, high-permittivity ceramic or conductive nanofillers. This paper reviews the PVDF based nanocomposite materials like multi-walled carbon nanotubes (MWCNTs), Graphene oxide, Short carbon fibres etc. The optimized PVDF nanocomposite exhibits a significant enhancement in dielectric constant while maintaining low dielectric loss and good mechanical flexibility. The interfacial polarization of PVDF contributes to improved dielectric behaviour, making these composites suitable for electromagnetic shielding, embedded capacitors, flexible electronics, and energy storage systems. The work comprehensively presents the PVDF based nano composites materials for the futuristic comprehensive understanding, there by facilitating the design and development of next-generation multifunctional materials.

Keywords: Nanocomposites, dielectric constant, energy storage, interfacial polarization, Polar Covalent bond

AC-029

Titanium Dioxide Nanoparticles: An Eco-Friendly Material for Versatile Applications with Self-Cleaning Abilities

M. Sneka[1], J. Balaji[1], R. Lakshmipathy*[1,2]

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamilnadu,India*

[2] *Directorate of Learning and Development SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India*

***Corresponding author e-mail:** lakshmir11@srmist.edu.in

ABSTRACT

In the present work, Titanium dioxide (TiO_2) nanoparticles were synthesized by a green synthesis approach using seed extract of the *Manilkara zapota* plant as a caping and stabilizing agent. The aqueous extract solution contains alkaloids, coumarins, and flavonoids which favours the formation of TiO_2 nanoparticles. The synthesised nanoparticles were surface characterized using UV-Visible, FTIR, XRD, TEM and EDX techniques. The anatase phase of TiO_2 NPs with an average crystalline size of 20-22 nm was revealed from the XRD pattern. TEM analysis showed nearly spherical TiO_2 nanoparticles in the less 2 nm in size with visible lattice fringes, confirming their crystalline nature. We synthesis the TiO_2 nanoparticles were coated onto cotton cloth and clay pot substrates using a dip coating method. The coated materials showed good antibacterial activity against both Gram-positive and Gram-negative bacteria under light irradiation due to reactive oxygen species (ROS) generation. TiO_2 coated fibric exhibit good Photocatalytic activity against synthetic dye strain in presence sunlight. TiO_2 coated clay exhibited good resistance toward abrasion. These results demonstrate that green-synthesized TiO_2 integrated onto low-cost substrates can serve as a dual-functional material for antimicrobial and photocatalytic applications, offering a practical and environmentally sustainable approach for self-cleaning textiles and clay pot.

Keywords: TiO_2 Nanoparticles; Self-cleaning; antibacterial; green synthesis; photocatalysis

References:

1. Q. Li et al., Nanotechnol. Rev., 2025, 14, 20250237.
2. A. K. Shimi et al., J. Nanomater., 2022, 7060388.

AC-030

High Hardness Lanthanum Borate Glasses Containing Eu^{3+}, Dy^{3+} and Er^{3+}

Kajal Dadwal[1], Atul Khanna[1]*

[1]*Department of Physics, Guru Nanak Dev University, Amritsar, India*

***Corresponding author e-mail:** atul.phy@gndu.ac.in

ABSTRACT

Eu^{3+}, Dy^{3+} and Er^{3+} incorporated lanthanum borate glasses of composition: (25-x)La_2O_3-75B_2O_3-xRE_2O_3 (where RE= Eu, Dy and Er, x = 0, 1 and 5 mol%) were synthesized by the melt quenching in the temperature range: 1200–1400 °C. The structural, thermal and optical properties of glasses were studied by X-ray diffraction, Differential Scanning Calorimetry, Vickers' hardness tests and UV–visible absorption studies. The density and glass transition temperature of lanthanum borate glass samples increases, with an increase in Eu_2O_3, Dy_2O_3 and Er_2O_3 concentration from 1 to 5 mol%. The hardness of lanthanum borate glass is 8.82±0.06 GPa while the hardness of glass sample containing 5 mol% of Eu_2O_3 is maximum and is 9.49±0.04 GPa. UV–visible spectra of glasses exhibit absorption bands due to transitions of Eu^{3+}, Dy^{3+} and Er^{3+} from the $^7F_{0,1}$, $^6H_{15/2}$ and $^4I_{15/2}$ ground states different to the excited states of Eu^{3+}, Dy^{3+} and Er^{3+} respectively.

Keywords: Borate glasses, differential scanning calorimetry, hardness, UV-visible.

AC-031

Electrical and Electrochemical Properties of Barium Vanadate Glass Cathode

Uday Bhatia[1], Kriti[1], Atul Khanna[1]*

[1]*Glass and Sensors Lab, Department of Physics, Guru Nanak Dev University, Amritsar-143005, India*

***Corresponding author e-mail:** atul.phy@gndu.ac.in

ABSTRACT

Barium vanadate glass of composition: 25BaO-75V_2O_5 was synthesized by splat quenching and used as cathode in aqueous zinc ion rechargeable cells that generated open circuit voltage of 1.4±0.1 V when used with Zn anode in 1 M solution of $ZnSO_4$. The glass sample was characterized by X-ray Diffraction data (XRD), Raman spectroscopy, Differential scanning calorimetry, temperature dependent dc electrical conductivity, Cyclic Voltammetry and Galvanostatic charge-discharge studies. The XRD studies confirm the glassy phase of the sample. The temperature dependent dc electrical conductivity studies shows that conductivity of sample is 2.15×10^{-7} S cm^{-1} at 296 K and 1.39×10^{-5} S cm^{-1} at 416 K. The Raman spectra of vanadate glass show broadband at 664 cm^{-1} due to the stretching vibrations of V_2-O bonds and another band at 876 cm^{-1} due to the symmetric stretching vibrations of O-V-O linkages in the VO_4 units. The sample exhibits a maximum specific capacitance of 1107 F kg^{-1} and highest specific energy of 0.098 Wh kg^{-1} at the current density of 0.008 A g^{-1}.

Keywords: Barium vanadate glass; cathodes; Raman spectra; electrochemical properties

AC-032

Analysis of Steel Structure infilled with ACC Blocks Subjected to Seismic Loads

Pradeep A R[1], Punith N R[2], Siddesha H[3], Vijayanand M[4],

[1] *Department of Civil Engineering, Sri Siddhartha Institute of Technology, Tumkur-572107, Karnataka, India*

[2]*Research scholar, Department of Civil Engineering, Sri Siddhartha Institute of Technology, Tumakuru-572103, Karnataka, India*

[3]*Department of Civil Engineering, Siddaganga Institute of Technology, Tumakuru-572103, Karnataka, India*

[4]*School of Architecture MSRIT Bengaluru, Karnataka, India*

***Corresponding author e-mail**: arpradeepmtech@gmail.com)

ABSTRACT

A structure consisting of both frame elements and infill masonry elements forms a complex composite system in which the dynamic responses of both components are altered under seismic conditions. This study evaluates the behavior of infilled frames, focusing on the transition from primary frame action mechanisms to diagonal strut action. The integration of masonry infill increases both lateral stiffness and strength, resulting in reduced interstory drifts. However, this enhancement in stiffness comes at the cost of reduced global ductility and altered failure modes. Using a G+6 story model analyzed with ANSYS software, this research investigates the trade-off between increased stiffness and heightened seismic demand hallow concrete (HC) blocks are used as infill masonry material. The introduction of hallow concrete(HC) blocks demonstrated improved seismic performance by reducing inertial mass and promoting a more sacrificial, ductile failure pattern.This study advances knowledge in the field of structural engineering by emphasizing that maintaining structural integrity and mitigating localized stress concentrations during high-intensity ground shaking require integrated modeling of the infill-frame interaction using ANSYS software.

Keywords: ACC Blocks, Steel frame, Seismic, MS frames.Infill.

AC-033

A Review on Polyaniline Based Hybrid Nanocomposites: The Role of Maleic Anhydride Compatibilizer and Silane-Treated Short Carbon Fibers

Usha Rani C M[1*], M G Veena[2], Dinesh Rangappa[3] Shankaraiah N[4]

[1,2,4]*Dept. of Electronics and Communication Engineering, JSS Science and Technology University, SJCE, Mysuru, Karnataka, India.*

[3]*Dept. of Applied Science, Visvesvaraya Technological University, Muddenahalli Campus, Chikkaballapura, Karnataka, India.*

***Corresponding author e-mail:** usharani@jssstuniv.in

ABSTRACT

Polyaniline (PANI) has developed as a multifaceted conducting polymer with adjustable electrical, mechanical, and thermal properties, rendering it an appealing matrix for sophisticated multifunctional composites. This paper thoroughly analyzes current progress in the design and development of PANI-based hybrid nanocomposites, which are enhanced with maleic anhydride as a compatibilizer, silane-treated short carbon fibers (SCFs), and diverse nanofillers. Additionally, the synergistic effects of hybrid nanofillers on electrical conductivity, thermal stability and mechanical strength performance are critically analyzed. The review focuses on hybrid nanocomposites, which combine PANI with carbon nanotubes (CNTs), graphene, and short carbon fibers to enhance electrical, mechanical, and thermal properties through synergistic effects. The inclusion of compatibilizers such as maleic anhydride and surface treatments such as silane coupling improves interfacial adhesion between PANI and fillers, resulting in better dispersion, higher conductivity, and increased efficiency. Composites are created by combining two or more distinct materials, resulting in a new material with unique features. Polyaniline composites retain constituent identities while enhancing overall qualities like electrical conductivity and mechanical strength. Finally, potential applications in sensors, energy storage, and structural electronics are explored, alongside future challenges in scalability, environmental stability, and sustainable processing. This work aims to provide a comprehensive understanding of PANI-based hybrid nanocomposites systems to guide the development for next-generation multifunctional materials.

Keywords: Conducting Polymers, Polyaniline, Maleic anhydride compatibilizer, Silane-treated short carbon fibers, Nanocomposites.

QD-001

Strategies for Light Management in Thin and Flexible C-Si Solar Cells Utilizing Cadmium Selenide (CdSe) Nanoparticles

Sandeep Kumar Reddy Anumareddy[1], Arjit Bardhan Roy[2]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** as2985@srmist.edu.in*

ABSTRACT

As the next-generation photovoltaic devices, thin and flexible crystalline silicon(c-Si) solar cells have generated a lot of attention because of their lightweight, bendable design and potential for incorporation into wearable and portable applications. Never the less, their smaller thickness restricts optical absorption, which results in a reduction in efficiency. In order to overcome this difficulty sophisticated light management techniques are necessary. This study explores the use of Cadmium selenide (CdSe) nanoparticles as a practical means of improving light absorption and trapping in thin c-Si solar cells. While CdSe nanoparticles scattering and plasmonic- like behavior help to increase optical path lengths within the active layer, their significant absorption coefficient and tunable bandgap enable better photon harvesting over a wide spectrum range. Almost 6% reduction of reflectance is shown in the proposed structure. The work describes design strategies, material integration methods, and optical simulations that show how CdSe nanoparticles can maximize photocurrent generation, reduce reflection losses, and enhance light coupling. The suggested tactics show a possible technique to achieve sophisticated nanostructured light management schemes in c-Si solar cells that are mechanically flexible, lightweight, and efficient.

References:

1. M. A. Green et al., Prog. Photovolt. Res. Appl., 27 (2019) 3–12.
2. H. A. Atwater and A. Polman, Nat. Mater., 9 (2010) 205–213.
3. A. B. Roy, IEEE Trans. Electr. Electron. Mater., 1 (2025).
4. B. Roy, A. Dhar, M. Chowdhury, S. Das, N. Mukherjee, and A. Kundu, Mater. Today Chem., 29 (2023) 101446.
5. P. K. Basu and N. K. Das, Sol. Energy Mater. Sol. Cells, 180 (2018) 301–310.
6. S. Pak, I. Pak, U. Kim, and B. Ryu, J. Comput. Electron., 24 (2025) 93.

QD-002

Effect of B-Site Doping on the Structural, Morphological, AC Susceptibility, and Magnetic Properties of Nanocrystalline $Pr_{0.7}Ba_{0.3}Mn_{1-x}Ni_xO_3$ (x=0.1,0.2)

Sondinglen Haokip and Rabindra Nath Mahato*

School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067

***Corresponding author e-mail:** rnmahato@jnu.ac.in

ABSTRACT

This study presents the structural, morphological, AC susceptibility, and magnetic properties of $Pr_{0.7}Ba_{0.3}Mn_{1-x}Ni_xO_3$(x = 0.1, 0.2). Rietveld refinement analysis was done using FullProf software. The crystallite size, micro-strain, and particle size were calculated using the Scherrer equation, Williamson-Hall Plot, and Transmission Electron Microscopy (TEM) analysis. The morphological image was studied using Scanning Electron Microscopy (SEM), and the crystallinity of the sample was also analysed using Selected Area Electron Diffraction (SAED). Temperature-dependent magnetisation data show a paramagnetic to ferromagnetic transition at 166K with an external applied magnetic field of 0.05T. Alternating Current (AC) susceptibility data suggest cluster-like behaviour. The maximum magnetic entropy changes for x = 0.1 is ~ 2.9 J/Kg K near its transition temperature, and the activation energy is about 0.543 eV.

Keywords: Rietveld refinement, crystallinity, susceptibility

References:

1. Balli, M., et.al, Phys. Rev. B 96, 146401
2. Heilman, A. K., et.al, Phys. Rev. B 65, 214423
3. Shames, A. I., et.al, Phys. Rev. B 70, 134433
4. G. Singh and R. N. Mahato, Emerg. Mater., (2024) 00810.

QD-003

Disorder-Induced Orbital Hall Conductivity in Three-Dimensional Weyl Semimetals

Dayana Joy[1], Vivek Pandey[1], Pankaj Bhalla[1,2]*

[1]*Department of Physics, School of Engineering and Sciences, SRM University – AP, Amaravati, Andhra Pradesh, India, 522 502*

[2]*Centre for Computational and Integrative Sciences SRM University – AP, Amaravati, Andhra Pradesh, India, 522 502*

***Corresponding author e-mail:** pankaj.b@srmap.edu.in

ABSTRACT

Our study presents the disorder-induced contribution to the orbital Hall conductivity in three-dimensional Weyl semimetals with broken time-reversal symmetry. Using the quantum kinetic approach, we analyze the impact of side-jump and skew-scattering contributions in the system. The dependence of the orbital Hall conductivity on both disorder potential and Fermi energy is explicitly demonstrated. Furthermore, we provide the orbital Hall response to an AC electric field that includes the skew-scattering and side-jump contributions, thereby enhancing the understanding of extrinsic orbital Hall conductivity. Finally, our results are supported by numerical estimations and highlight potential experimental relevance for advancing orbitronic device technologies.

References:

1. Dayana Joy, Vivek Pandey, Pankaj Bhalla, Phy. Rev. B, 111 (2025) 075149
2. Hong Liu, Dimitrie Culcer, Phys. Rev. Lett, 132, (2024) 186302

Quantum-Aided Deepfake Detection: A Critical Review of Classical Techniques, Existing Challenges, and the Emerging Role of Quantum Approaches

I. Pavani[1], S. Aruna Mastani[2]

[1]*Audisankara College of Engineering and Technology,*

[2]*Jawaharlal Nehru Technological University Anantapur College of Engineering (JNTUA).*

ABSTRACT

The rapid growth of generative models has enabled the creation of highly realistic synthetic images and videos, commonly known as deepfakes. While such content can support creative and educational applications, its misuse has raised significant concerns about misinformation, privacy breaches, and digital security. Research on deepfake detection has matured steadily from early Convolutional neural networks (CNNs) and temporal architectures to more advanced transformer- and graph-based systems. These developments have improved the ability to identify spatial and temporal irregularities; however, most existing methods still struggle to generalize across datasets, manipulation styles, and real-world distortions. Recent interest in quantum machine learning (QML) has added a new dimension to this field. Quantum feature embeddings, hybrid classical–quantum models, and tensor-based representations have been explored as potential solutions for more efficiently handling high-dimensional patterns. Although these efforts are still in early stages, they introduce promising ideas for compact modeling and richer feature interaction. This review critically examines the trajectory of deepfake detection research from the recent studies, highlighting strengths, limitations, and persistent challenges across major classical and transformer-based systems. It also mirrors the role that quantum-inspired methods might play in addressing longstanding challenges related to generalization, scalability, explainability, and computational efficiency. The discussion concludes with future research directions to build more robust and reliable deepfake detection frameworks.

Keywords: Deepfake Detection; Quantum Machine Learning; Hybrid Quantum–Classical Models; Transformer Networks; Graph Neural Networks; Media Forensics; Tensor Networks

QD-005

Collective Enhancement and Suppression of Coupling Strength Due to Photon-Mediated Magnon-Magnon Interaction

Sachin Verma, Abhishek Maurya, Rajeev Singh, and Biswanath Bhoi*

Nano-Magnetism and Quantum Technology Lab, Department of Physics, I.I.T. (BHU) Varanasi, Varanasi - 221005, India.

***Corresponding author e-mail:** biswanath.phy@iitbhu.ac.in

ABSTRACT

Photon–magnon coupling (PMC) is an emerging interdisciplinary research area that bridges microwave photonics, optics, and magnetism, offering a promising platform for hybrid quantum systems [1]. By combining the complementary advantages of these distinct physical systems, PMC enables the exploration of novel phenomena relevant to quantum information processing [2] and coherent signal manipulation. A deep understanding of the coupling mechanism and its controllability is crucial for advancing both fundamental studies and potential applications [3].

In this work, we experimentally demonstrate photon-mediated magnon–magnon coupling in a hybrid system based on a hexagonal ring resonator (HRR) coupled to spatially separated yttrium iron garnet (YIG) films. Through both experiments and numerical simulations, we observe the emergence of bright and dark magnon modes arising from the collective interaction between a single photon mode and two magnon modes positioned at different locations along the resonator track.

For a single YIG placed at angular positions of 0° and 180°, we observe a consistent coupling strength of approximately 126 MHz. Interestingly, when two YIG samples are simultaneously positioned at 0° and 180°, the coupling strength increases to 166 MHz, indicating the presence of photon-mediated magnon–magnon interaction. This enhanced coupling confirms the cooperative nature of the hybrid system.

Furthermore, we develop a theoretical model to validate our simulation results and to elucidate the physical origin of the photon-mediated magnon-magnon coupling. Our findings provide valuable insights into controllable multi-magnon interactions mediated by cavity photons and open new avenues for engineering hybrid quantum systems.

References:

1. Y. Tabuchi, et al, Science 349(6246), 405–408 (2015).
2. Y. Li et al, J. Appl. Phys. 128 (2020) 130902.
3. Z.-L. Xiang et al, Rev. Mod. Phys. 85 (2013) 623–653.

Planar Hybrid System for Photon-Magnon Coupling

Abhishek Maurya[1], Sachin Verma[1], Biswanath Bhoi[1] and Rajeev Singh[1]*

[1]*Department of Physics, Indian Institute of Technology (Banaras Hindu University) Varanasi, Varanasi - 221005, India*

***Corresponding author e-mail:** rajeevs.phy@iitbhu.ac.in

ABSTRACT

Photon–magnon coupling (PMC) is an emerging interdisciplinary research area that bridges the microwave, optical, and magnetism communities, with the goal of integrating the unique advantages of these systems into a single hybrid quantum platform. Such hybrid photon–magnon systems offer promising opportunities for exploring novel physical phenomena and developing functionalities relevant to quantum information science. In this work, we numerically investigate photon–magnon interaction in a planar hybrid architecture consisting of a ferrimagnetic thin film and an electrical resonator. Full-wave electromagnetic simulations were carried out using CST Microwave Studio, and the transmission response was analysed as a function of microwave frequency under varying bias magnetic field strengths. In the absence of an external magnetic field (H = 0 Oe), only a single resonant mode corresponding to the electrical resonator was observed. Upon application of the magnetic field, two distinct resonance peaks emerged, where one mode exhibited strong magnetic-field tunability across the studied frequency range, consistent with magnon excitation in the ferrimagnetic film. The evolution of resonance frequencies with increasing H reveals a pronounced avoided crossing (anti-crossing) behavior, confirming the formation of hybridized magnon–photon modes and demonstrating strong coupling between the microwave photon mode and the magnon resonance. These results highlight the potential of planar PMC systems for magnetically tunable microwave devices, reconfigurable metamaterials, and hybrid quantum technologies exploiting coherent magnon–photon interactions.

References:

1. M. Harder, P. Hyde, L. Bai, C. Match, C.-M. Hu, Phys. Rev. B 94 (2016) 054403.
2. B. Bhoi, T. Cliff, I. S. Maksymov, M. Kostylev, R. Aiyar, N. Venkataramani, S. Prasad, R. L. Stamps, J. Appl. Phys. 116 (2014) 243906.
3. X. Zhang, C. Zou, L. Jiang, H. X. Tang, J. Appl. Phys. 119 (2016) 023905.

Structural, Morphological and Optical Properties of Surfactant-Mediated ZnS QDs

Priya Chandra[1]*, K. S. Ojha[1]

[1]*Department of Physics, National Institute of Technology Raipur, Chhattisgarh, India, 492010*

***Corresponding author e-mail:** pchandra.phd2022.phy@nitrr.ac.in

ABSTRACT

ZnS is a well-known semiconductor material for optical, electronic, sensing and biomedical applications. The incorporation of surfactants during synthesis effectively controls particle growth and surface chemistry, leading to reduced agglomeration and affecting optical performance. In this article, ZnS nanoparticles were prepared using hydrothermal and solvothermal methods in the absence of any surfactant, and their preliminary analysis indicates that the solvothermal method gives a higher yield and smaller ZnS nanoparticles. Therefore, by employing the solvothermal approach, the influence of cetyltrimethylammonium bromide (CTAB), dodecyl trimethylammonium bromide (DTAB), dodecyl trimethylammonium chloride (DTAC) and sodium lauryl sulfate (SLS) surfactants have been investigated on the structural, morphological and optical properties of ZnS nanoparticles. The solvothermally synthesised ZnS nanoparticles exhibited a crystallite size of 1-2 nm, as calculated by XRD spectra. FTIR analysis confirmed the capping of different surfactants on ZnS nanocrystals. SEM images demonstrate that the solvothermally synthesised ZnS has a popcorn-like morphology, whereas the hydrothermally synthesised ZnS has a spherical, ball-like shape. EDX spectra confirmed the presence of all expected elements in appropriate stoichiometric ratios. The presence of surfactants results in decreased photoluminescence emission intensity, showing effectively suppressed surface defect states. The optical bandgap values were found to be 3.58 - 3.77 eV for all ZnS samples. The increased bandgap value is consistent with quantum confinement effects in ZnS quantum dots.

Keywords: ZnS, Surfactant, CTAB, DTAB, DTAC, SLS.

References:

1. A. K. Shahi, B. K. Pandey, B. P. Singh, B. K. Gupta, S. Singh, R. Gopal, Electron. Mater. Lett., 13, 2 (2017) 160–167.
2. Kumar, S. Verma, J. Park, V. Chandra Srivastava, M. Naushad, Chemosphere, 298, (2022).

QD-008

A New Semiconductor Quantum Dot for Optoelectronic Applications

Gopi N, Parthiban T, Raja R*

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** rajar@srmist.edu.in

ABSTRACT

Semiconductors are the backbone of modern electronics and future technologies, where continuous reduction in material dimensions has been employed to achieve superior performance. Among low-dimensional systems, quantum dots have attracted significant attention due to their size-dependent electronic and optical properties. However, most traditionally studied semiconductor quantum dots suffer from limitations such as toxicity, poor stability, complex synthesis routes, and limited property tunability.

To address these challenges, the present work focuses on the exploration of new quantum dot materials as alternatives to conventional systems. By developing novel quantum dots with controlled size and composition, this study aims to overcome the demerits of traditional semiconductor materials while enhancing their optoelectronic performance. The findings of this research are expected to provide new insights into material design and contribute to the development of next-generation electronic and optoelectronic devices.

References:

1. A. J. Houtepen, E. H. Sargent, I. Infante, Nat. Rev. Methods Primers, 5 (2025) 42.
2. Y. Zhang, G. Wu, Nanomaterials, 15 (2025) 1812.
3. J. W. Kim, J. Kim, J. Y. Woo, Y. Kim, J. Mater. Chem. A, 13 (2025) 29706–29735.
4. X. Deng, F. Zhang, Y. Zhang, H. Shen, J. Mater. Chem. C, 11 (2023) 14495–14514.
5. S. Aftab, G. Koyyada, M. Mukhtar, H. H. Hegazy, J. H. Kim, J. Mater. Chem. C, 12 (2024) 17789–17801.

Morphology-Driven Magnetization Reversal in Functional Ni Nanostar Chains

Sandhya Ravichandran, Jaivardhan Sinha, Arnab Ganguly

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** arnabg@srmist.edu.in

ABSTRACT

Magnetic nanoparticles and nanochains are of significant interest for data storage and biomedical applications due to their nanoscale dimensions, high aspect ratios, and unique magnetization reversal properties. Among these, nickel (Ni) nano stars assembled into chain-like structures exhibit distinctive magnetic behaviors, which are strongly influenced by their surface morphology and geometric configuration. This study systematically investigates the magnetization reversal and hysteretic properties of chemically synthesized Ni nano star chains and their individual constituent particles, with a particular focus on surface features and structural arrangements. Our analysis reveals that surface roughness, manifested as spikes on the nano stars, plays a critical role in shaping the magnetic reversal landscape. These protrusions act as localized nucleation sites, modifying the coercivity and remanence of the particles. Furthermore, we explore the effect of chain geometry and the arrangement of self-assembled clusters on the collective magnetic response. The spatial configuration and inter-particle interactions within these chains lead to complex reversal behavior, highlighting the interplay between individual particle morphology and overall chain architecture. By correlating the fine surface characteristics with the observed hysteretic responses, this work provides fundamental insights into the mechanisms governing magnetization reversal in nanostructured magnetic systems. The results underscore the importance of precise morphological and configurational control in chemically synthesized nanostructures to tailor their magnetic performance. These findings have direct implications for the design of high-density magnetic memory devices and advanced biomedical tools, where controlled magnetization behavior at the nanoscale is crucial. Overall, this study establishes a clear link between nanoscale structural features and functional magnetic properties, paving the way for rational engineering of nanomaterials with targeted magnetic functionalities.

Keywords: Nickel nano stars; Magnetic nanochains; Magnetization reversal; Hysteresis behavior; Surface roughness effects; Dipolar interactions

References:

1. Ravichandran, S., et al., Nanotechnol. Rev., (2025) 14(1), 20250223.
2. Ravichandran, S., et al., Mater. Lett., (2025) 383, 137922.

QD-010

Impact of Intermediate Diradical Character on Optical and Magnetic Properties in Croconaine Dyes

Takeshi Maeda*

Graduate School of Engineering, Osaka Metropolitan University, Sakai, Osaka 599-8531, Japan

***Corresponding author e-mail:** maeda@omu.ac.jp

ABSTRACT

Molecules with intermediate diradical character exhibit a unique electronic structure in which two electrons with antiparallel spins are not completely paired but are instead partially bonded in the ground state. This electronic state is associated with properties such as nonlinear optical responses and semiconducting behaviour, making these molecules attractive candidates for functional materials. In this study, we focus on short-wavelength infrared (SWIR)-absorbing croconaine dyes incorporating five-membered oxocarbon and chalcogenopyrylium skeletons.[1,2] These dyes exhibit intermediate diradical character, which contributes to their optical and magnetic properties. They show pronounced two-photon absorption in the SWIR region. This behaviour is related to the intermediate diradical character, which makes the electron distribution along the π-conjugated system more susceptible to distortion by the optical field generated by intense laser.[3] Furthermore, we examine the electron spin resonance (ESR) behaviour originating from unpaired electrons in the diradical structures and investigate how phase transitions in the solid state and molecular assembly structures influence the magnetic response.[4] This presentation discusses the relationship between molecular structure, intermediate diradical character, and optical and magnetic properties, and provides insights relevant to the design of optoelectronic and magnetic materials.

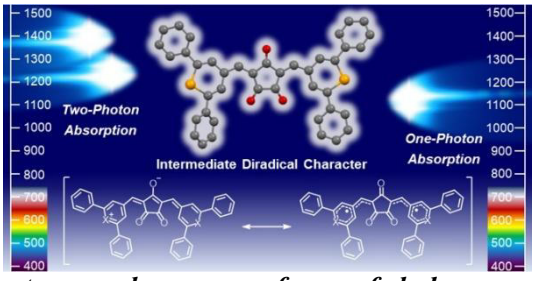


Fig. 1. Molecular structures and resonance forms of chalcogenopyrylium-based croconaine dyes with intermediate diradical character, and schematic illustrations of their one- and two-photon absorption in the SWIR region.

References:

1. T. Maeda, T. Oka, D. Sakamaki, H. Fujiwara, N. Suzuki, S. Yagi, T. Konishi, K. Kamada, Chem. Sci., 2023, 14, 1978.
2. T. Oka, T. Maeda, D. Sakamaki, N. Suzuki, S. Yagi, S. Kodama, H. Fujiwara, Org. Chem. Front., 2025, Advance Article (doi: 10.1039/D4QO01722F).
3. Oka, T.; Maeda, T.; Sakamaki, D.; Fujiwara, H.; Suzuki, N.; Yagi, S.; Mauric, L.; Kamada, K. 2025, 13, 11970.
4. T. Maeda, K. Ono, T. Ohno, D. Sakamaki, H. Fujiwara, N. Suzuki, S, Kodama, S. Yagi, *in preparation.*

QD-011

pH-Tunable Dual-Target Fluorescent Sensor for Selective Detection of Tartrazine and Ascorbic Acid Using N/O-Doped Carbon Quantum Dots

R. Mahalakshmi[1,2], K. Radhakrishnan[1,2*]

[1]*Department of Chemistry, Karpagam Academy of Higher Education, Coimbatore, Tamil Nadu, India,*

[2]*Centre for Material Chemistry, Karpagam Academy of Higher Education, Coimbatore, Tamil Nadu, India.*

[*]**Corresponding author e-mail:** raddhakrishnan21@gmail.

ABSTRACT

Fluorescent detection of multiple analytes requires dual-target fluorescent sensors in complex environments for precise monitoring. The synthesize nitrogen/oxygen-doped carbon quantum dots (N/O-CQDs) under hydrothermal conditions by incorporating cranberry extract with urea and citric acid as a sustainable precursor effective surface passivation. N/O-CQDs produced by optimized conditions reached an 18.6% quantum yield and maintained strong chemical stability while showing excellent photostability. The successful passivation of functional groups (-NH_2, -OH, -COOH) were confirmed on the surface through analysis by UV-Vis spectroscopy, fluorescence spectroscopy, X-ray photoelectron spectroscopy (XPS), N/O-CQDs functioned as a dual-target fluorescent sensor at different pH levels to selectively detect TZ and AA while displaying reversible fluorescence quenching. Fluorescence quenching triggered by tartrazine occurred via electrostatic interactions, while ascorbic acid facilitated fluorescence restoration through reduction processes. N/O-CQDs exhibited high sensitivity in quantifying tartrazine at 32 nM and ascorbic acid at 86 nM, with detection capabilities ranging from 0.5 to 10 µM and 0.5 to 15 µM respectively. The study introduces a cost-effective, environmentally sustainable approach for the large-scale production of dual-sensing functionalized carbon quantum dots. N/O-CQDs exhibit exceptional selectivity and sensitivity, indicating significant promise for the development of enhanced monitoring systems in food quality control, environmental protection, and biomedical applications.

Keywords: Carbon quantum dots, dual-target sensing, fluorescent probe, tartrazine, ascorbic acid, food safety, environmental monitoring.

References:

1. S. Jiang, F. Wang, Q. Li, H. Sun, H. Wang, Z. Yao, Environ Sci Pollut Res 28 (2021) 54511–54530.
2. B. Haridevamuthu, R. Murugan, B. Seenivasan, R. Meenatchi, R. Pachaiappan, B.O. Almutairi, S. Arokiyaraj, K. M. K, J. Arockiaraj, Journal of Hazardous Materials 461 (2024) 132524.

QD-012

Tailoring Topological Deflection and Mobility of Skyrmions in Synthetic Ferrimagnets

Vijay R[1], Sudharsun G[1], Nicolas Reyren[2],Vincent Cros[2], Sougata Mallick[1]*

[1]*SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

[2]*Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, Palaiseau, France*

***Corresponding author e-mail:** sougatam@srmist.edu.in

ABSTRACT

Magnetic skyrmions, nanoscale spin textures with topologically protected stability, are promising candidates for next-generation spintronic devices. Recent studies have demonstrated the linear motion of skyrmions in the domain-wall flow regime for compact skyrmions in synthetic ferrimagnetic and antiferromagnetic multilayers [1, 2]. In this context, we engineer skyrmion mobility (μ), dissipated power, and effective mass (Meff) to reach an optimal regime that combines minimal skyrmion size, high velocity (vSk), and a suppressed skyrmion Hall angle (θSkHA). To interpret these observations, we performed theoretical calculations based on the Thiele formalism, using experimentally measured parameters [3] for each sample (±10% uncertainty). Fig. 1(a), (b) illustrate the experimentally and simulation-observed skyrmion motion along the nanotrack. The dotted lines in Fig. 1(c), (d) represent these theoretical results, which map closely to experimental (large skyrmions: solid symbols) and micromagnetic simulation (small skyrmions: open symbols) data. We further show how geometric confinement enhances skyrmion propulsion along device edges, enabled by the non-inertial dynamics of the antiferromagnetic system. Our results exhibit excellent agreement between theory, micromagnetic simulations, and experiments, establishing a robust route toward efficient skyrmion-based spintronic devices.

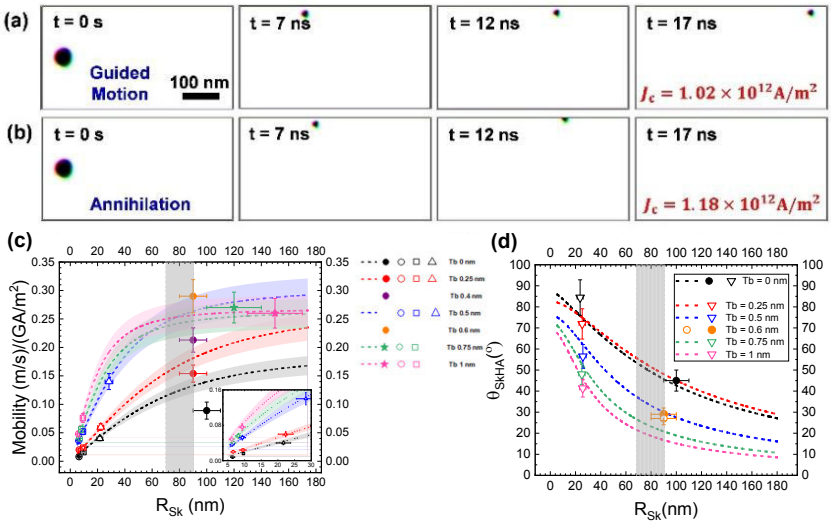


Fig. 1: (a) Skyrmion guided along the edge of the track below J_Th, and (b) annihilating beyond J_Th. (c), (d) Mobility (μ) and Skyrmion Hall angle (θ_SkHA) as a function of the skyrmion radius for theoretical calculations (dotted lines), experimental (solid symbols), and simulation data (open symbols).

References:

1. S. Mallick et al, Nature Communications 15, 8472 (2024)

QD-013

Exploring Static and Dynamic stability conditions of Skyrmions in Synthetic Ferrimagnets

S Sudharsun G, Vijay R, *Sougata Mallick

Department of Physics and Nanotechnology, SRM Institute of Science and Technology,Kattankulathur 603203, Tamil Nadu, India

***Corresponding author e-mail:** sougatam@srmist.edu.in

ABSTRACT

Magnetic skyrmions, topologically protected spin textures with fixed chirality, are promising candidates for next-generation spintronic devices. Recent studies report linear skyrmion motion in the domain-wall flow regime for compact skyrmions in synthetic antiferromagnetic and ferrimagnetic multilayers [1, 2]. In this work, using micromagnetic simulations (Mumax3), we explore a range of material parameters such as saturation magnetization (MS), uniaxial anisotropy (KU), and Dzyaloshinskii-Moriya interaction (D) to tune the skyrmion size and identify optimal conditions for efficient and stable skyrmion dynamics in Pt|Co|Tb|Al heterostructures. Maintaining a fixed skyrmion size during dynamics is essential for realistic device applications, where stability and controllable motion under current-induced spin-orbit torque (SOT) are required for reliable device operation. The phase diagrams (Fig. 1: a-c) reveal the parameter window for stable skyrmion formation and their evolution with Tb thickness (0.25–1 nm) [3]. The heterostructures with Tb = 0.25, 0.5, 0.75, and 1 nm, shown as solid black, red, blue, green and pink symbols, correspond to the experimentally studied samples.

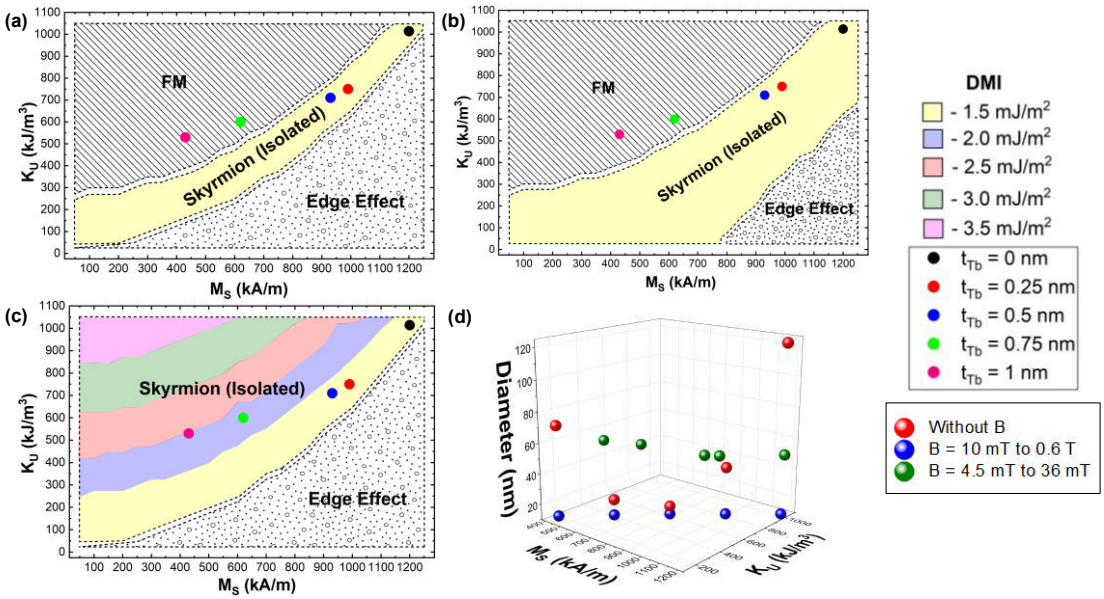


Fig. 1. Phase diagrams showing the regions of skyrmion stability under static conditions. (a), (b): Stability map for a fixed DMI without and with an external magnetic field respectively. (c): Stability map for varying DMI. (d): 3D plot illustrating the variation of skyrmion diameter as a function of MS and KU. The value of DMI energy -1.5 mJ/m2 is an experimentally measured parameter.

References:

1. V. T. Pham et al, Science 384, 6693 (2024).

EN-001

Thermoelectric and Phase Change Materials for Waste Heat Recovery

Benial V[1], Kondusamy V[1]*, Aadhithyaa C[1], Vinish R[1]*

[1]*Karpagam College of Engineering, Coimbatore, Tamil Nadu, India, 641032*

***Corresponding author e-mail:** kondusamy.v@kce.ac.in, vinishravi04@gmail.com

ABSTRACT

The need for renewable energy systems has promoted the advancement of effective solar water heating technology. In this study, a dual loop heat exchanger combined with PCM is presented to improve thermal storage and heat transfer capability in solar water heating systems. The controller is based on ESP32 for real time monitoring-automation and two DS18B20 waterproof temperature sensors that record the in/outlet water temperatures. Water circulation is performed using a 12 V DC pump, which is regulated by a relay to allow automatic water circulation and avoid overheating of the PCM unit/water loop. Power storage and supply are with a 12 V, 7Ah lead acid battery for independent operation. The temperature reading is being sent to Blynk all the time so you can monitor and take control of your system through a smartphone interface. The addition of PCM noticeably enhances heat storage ability, stabilizing the outlet water temperature and prolonging the duration of hot-water availability after sunset. Experimental results demonstrate that the new two-loop structure can enhance thermal performance with respect to the common single-loop case. This method proves to be an economical, feasible and automatic route for solar water heating systems both in domestic sector as well as industrial application and also has promising potential for smart hybrid RE system integration.

Keywords: Solar water heater, dual-loop heat exchanger, phase change material (PCM), ESP32, IoT monitoring, thermal energy storage, renewable energy.

References:

1. H. Hussein and H. M. T. Al-Najjar, Results in Engineering 27 (2025) 106805.
2. J. Li, L. Wei, Z. Ti, L. Ma, Y. Yan, G. Zhang, and P.-F. Liu, Phys. Rev. B 108 (2023) 224302.
3. M. A. Eleiwi, Energy Sources, Part A: Recovery, Utilization and Environmental Effects 45 (2023) 2013–2026.
4. M. H. S. Abd, Renewable and Sustainable Energy Reviews 189 (2024) 113904.
5. P. Lad, International Journal of Ambient Energy 43 (2022) 1–36.

EN-002

Catalyst-Enhanced ChCl-Ethylene Glycol Deep Eutectic Electrolytes for High-Performance Zinc-Ion Batteries

Nishanth Sudarsanan[1], and Vijayakumar.T[1]*

[1]*Futuristic Materials Research Centre for Planetary Exploration, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur campus, Chengalpattu-603203, Chennai, Tamil Nadu, India*

***Corresponding author e-mail:** ns5849@srmist.edu.in

ABSTRACT

A series of deep eutectic solvent (DES) electrolytes based on choline chloride (ChCl) and ethylene glycol (EG) were developed for zinc-ion batteries (ZIBs), incorporating various catalysts such as titanium chloride (TiCl), thioglycolic acid, and ethylene oxide to enhance electrochemical performance. These ChCl-EG DES electrolytes exhibit suppressed parasitic reactions and expanded electrochemical stability windows due to strong hydrogen bonding and chelation effects that stabilize Zn2+ ions and reduce dendrite formation. The inclusion of catalytic additives further improves ionic conductivity, zinc plating/stripping efficiency, and cycle life by facilitating uniform Zn deposition and mitigating corrosion. Electrochemical tests demonstrated enhanced rate capability and prolonged cycling stability in ZIB cells using the catalyst-modified DES electrolytes compared to conventional aqueous solutions. This work highlights the promise of functionalized DES electrolytes with tailored catalysts as efficient, stable, and eco-friendly media for high-performance zinc-ion battery applications

References:

1. R. Puttaswamy, H. Lee, H. W. Bae, D. Youb Kim, and D. Kim, Small 20 (2024) 2400692.
2. V. Verma, R. M. Chan, L. J. Yang, S. Kumar, S. Sattayaporn, R. Chua, Y. Cai, P. Kidkhunthod, W. Manalastas, and M. Srinivasan, Chem. Mater. 33 (2021) 1330–1340.

EN-003

Development and Characterization of Sustainable Metal Matrix Composites Reinforced with Industrial Waste and Minor Graphite Additives

Venugopal S[1]*, Edwin Paul N E[2], Balaji Venkatesan[3], Uma Devi A[4], Palani R[5]

[1]*Vels Institute of Science, Technology & Advanced Studies (VISTAS), Chennai, Tamilnadu, India, 600117.*

[2] *GRT Institute of Engineering and Technology, Tiruttani, Tamilnadu, India, 631209.*

[3] *Sri Sai Institute of Technology and Science, Rayachoty, Andhra Pradesh, India, 516270.*

[4]*St. Joseph's College of Engineering, Chennai, Tamilnadu, India, 600119.*

[5]*J.N.N Institute of Engineering (Autonomous), Kannigaipair, Tamil Nadu, India, 601102.*

***Corresponding author e-mail:** Venugopal.se@vistas.ac.in

ABSTRACT

In recent times, the environmental burden and low engineering/functional performance of synthetic alloys have driven the search for sustainable and low-cost engineering materials, leading to an increased interest in sustainable MMCs containing industrial waste as reinforcement in the matrix. In this present work, aluminium 6063 hybrid MMCs with fly ash (FA), red mud (RM), and graphite as reinforcement were developed. The tensile strength of the composites was tested according to the ASTM E8/E8M-21 standard, and it was found that the 5% FA + 5% RM + graphite hybrid composite exhibited the best tensile strength, which can be attributed to the improved load transfer and synergistic strengthening effect. Results also showed a gradual increase in hardness values with increasing reinforcement content, confirming the effective solution treatment of the matrix [21]. Tribological characterization (ASTM G99-17) revealed a pronounced reduction in wear rate and coefficient of friction, attributed to the higher surface hardness and the formation of a protective tribofilm throughout the sliding process. XRD analysis revealed the presence of SiO_2, Al_2O_3, and Fe_2O_3 phases; SEM micrographs showed a fine grain size, uniform inter-particle distribution, and good interfacial bonding. The density and porosity measurements showed a slightly lower density and low porosity (<3%) in all the composites. This study demonstrated the capability of a machine learning feature-importance analysis in identifying reinforcement type and porosity as the primary contributors to mechanical and tribological behaviours. FA–RM–graphite hybrid composites were more effective and eco-friendlier than lightweight structural application solutions.

Keywords: 0D halides; hybrid architecture; lone pair electrons; antibonding states

References:

1. S. Kumar and P. Senthil, “Advances in Aluminum Metal Matrix Composites: A Review,” J. Mater. Eng. Perform., vol. 30, no. 5, pp. 3124–3138, 2021.
2. T. Prasad and R. Rajesh, “Development of Lightweight MMCs for Automotive Applications,” Mater. Today Proc., vol. 52, pp. 1876–1882, 2023.

EN-004

Lewis Acid Site Engineering for Sustainable Ethanol-to-Ethylene Conversion

Ching-Chun Chang[1], Duo-Syuan Lin[1], Chao-Wei Huang[1]*

[1]*Department of Engineering Science, National Cheng Kung University, Tainan, Taiwan, 701401*

***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

In response to the European Union's increasingly stringent carbon-neutral policies, the global petrochemical industry is actively seeking carbon-neutral solutions. Ethylene is an indispensable raw material in modern industry, and its current production relies primarily on steam cracking of fossil fuels, which results in substantial carbon emissions. The high reaction temperatures also lead to significant energy consumption, and fossil fuels themselves are non-renewable resources. In recent years, the production of bioethanol has reached an industrial scale, making ethanol dehydration a feasible alternative route for ethylene synthesis.

The ethanol dehydration reaction requires the participation of high concentrations of acidic sites, and the introduction of metals can promote the generation of such sites. Therefore, this study attempts to introduce metals into dealuminated zeolites. The reaction products are analyzed using gas chromatography (GC). Because the role of Lewis acid sites in ethanol dehydration remains inconclusive in the literature, this study adjusts the ratio of dealuminated zeolite to metal in order to modify the Lewis acid content in the catalyst, and investigates its correlation with ethanol dehydration activity.

References:

1. Ouayloul, L., et al, ACS Catalysis, 14.23 (2024) 17360-17397.
2. Potter, Matthew E., et al, ACS Catalysis, 13.9 (2023) 5955-5968.
3. Ouayloul, L., et al, Green Chemistry, 25.9 (2023), 3644-3659.
4. PEARSON, RALPH G, Journal of the American Chemical Society, 85.22 (1963), 3533-3539.

EN-005

Hydrothermal synthesis of $CuMn_2O_4$/rGO composite and investigation of electrochemical properties for high performance supercapacitor electrode materials

Takhelchangbam Dayananda Sharma[1], Reema Gupta[2], V.K. Sachdeva[3], Arijit chowdhuri[4], Anjali Sharma[5], Monika Tomar[6], H. Basantakumar Sharma[1]*

[1]*Department of Physics, Manipur University, Imphal-795003, Manipur, India*

[2]*Department of Physics, Hindu College, University of Delhi, Delhi-110007, India*

[3]*Advisor, SMDL, Miranda House, University of Delhi, Delhi-110007, India*

[4]*Department of Physics, Acharya Narendra Dev College, University of Delhi, Delhi-110019, India*

[5]*Department of Physics and Astrophysics, University of Delhi, Delhi-110007, India*

[6]*Department of Physics, Miranda House, University of Delhi, Delhi-110007, India*

***Corresponding author e-mail**: hbslab.18@gmail.com

ABSTRACT

The rapid growth of the global population and continuous technological advancements has led to a significant increase in energy demand across various sectors. Meeting this demand require the development of efficient, reliable, cost effective and sustainable energy storage systems. In this context, supercapacitors have emerged as promising energy storage devices that effectively bridge the gap between conventional capacitors and batteries. Supercapacitors offer unique advantages like high power density, comparatively high energy density, fast charge–discharge capability and long cycle life.

In this study, spinel-structured $CuMn_2O_4$ nanomaterials have been synthesized with the help of hydrothermal process. The novelty of the present work lies in the strategic integration of $CuMn_4O_4$ with rGO to form hybrid composites aiming to enhance conductivity, surface area and electrochemical stability. Electrode materials, including pure $CuMn_2O_4$ and $CuMn_2O_4$/rGO were directly fabricated on to nickel foam to ensure robust electron transport pathways and practical applicability.

Structural and crystal phases of the synthesized materials are analysed using XRD and confirmed the formation of desired structures. SEM revealed the morphology of the synthesized composite materials. FTIR spectroscopy verified the presence of functional groups and lattice vibrations. The Brunauer-Emmett-Teller (BET) method demonstrated a significant surface area enhancement in the composites having a high value of 14.20m2/g, favouring ion accessibility. Electrochemical studies including Cyclic Voltammetry (CV), Galvanostatic Charge Discharge (GCD) and Electrochemical Impedance Spectroscopy (EIS) were performed in 1M of KOH electrolyte solution. Cyclic Voltammetry (CV) confirmed these electrode materials have pseudocapacitive behaviour due to the presence of distinct oxidation and reduction peaks. $CuMn_2O_4$/rGO delivered high specific capacitance of 671.7F/g at current density of 1A/g and excellent cycle stability even at higher current density. These results highlight that the hydrothermally synthesized $CuMn_2O_4$/rGO composite as a potential candidate for next-generation high-performance supercapacitors.

Keywords: Supercapacitor, Hydrothermal, composite materials, Specific Capacitance.

Thermoelectric Properties of Γ-Phase In_2Se_3 Thin Films Prepared by RF Magnetron Sputtering

Satyam Garg[1,2], Arijit Chowdhuri[3], Monika Tomar[2], Anjali Sharma[1]*

[1]*Department of Physics and Astrophysics, University of Delhi, Delhi – 110 007, INDIA*

[2]*Department of Physics, Miranda House (University of Delhi), Delhi – 110 007, INDIA*

[3]*Acharya Narendra Dev College (University of Delhi), Kalkaji, New Delhi – 110 019, INDIA*

***Corresponding author e-mail:** anjalisharma31@gmail.com

ABSTRACT

Global energy demands continue to rise with burgeoning anthropogenic requirements, while primary energy sources still remain heavily reliant on fossil fuels. This condition underscores an urgent need to explore alternative energy sources and technologies capable of efficiently harnessing waste energy from myriad sources. Amongst various approaches envisaged to address this challenge, thermoelectric energy conversion has emerged as a promising strategy, owing to its ability to directly convert thermal energy into electrical energy. In the present study, RF sputtered Indium Selenide (In_2Se_3) thin films were deposited onto Corning glass substrates and their structural characterization using X-ray diffraction (XRD) indicated formation of γ-phase In_2Se_3 at a substrate temperature of 400 °C. Further, UV-Visible spectroscopy confirmed a direct band gap energy of 1.8 eV for a 100 nm thick In_2Se_3 thin film. To investigate the thermoelectric property of the material, thermoelectric legs of In_2Se_3 were prepared having length = 2.5 cm, width = 3 mm and thickness = 100 nm. Three thermoelectric legs of In_2Se_3 were prepared and connected in series for measurements of the output voltage with temperature difference maintained at 200 °C for hot and cold sides of the In_2Se_3 thin film. The Seebeck coefficient were clearly discernible at 867 µV/K (heating cycle) and 848 µV/K (cooling cycle) respectively. The high Seebeck coefficient values exhibited by optimized In_2Se_3 thin films indicate their strong potential as thermoelectric materials for efficient conversion of waste heat into electrical power in future energy applications.

Keywords: In_2Se_3 thin films, X-ray diffraction, UV-Visible spectroscopy, Seebeck coefficient.

EN-007

Microwave-Synthesised Vanadium Oxide Incorporated $Mose_2$/Polypyrrole Nanocomposites for Improved Hydrogen Evolution Reaction

Aparna Unnikrishnan [1], J.Balavijayalakshmi [1]*

[1] *Department of Physics, PSGR Krishnammal College for Women,Coimbatore, Tamilnadu, India.*

***Corresponding author e-mail:** balavijayalakshmiroopa@gmail.com

ABSTRACT

Developing low-cost, efficient, and stable electrocatalysts is essential for accelerating the hydrogen evolution reaction (HER) toward sustainable hydrogen production. Transition-metal chalcogenides incorporated with conductive polymers and metal oxides provide a promising pathway to enhance catalytic activity through synergistic interface engineering.Co3O4 modified 2H-$MoSe_2$/polypyrrole (MSPVO) ternary nanocomposites were synthesised by a microwave-assisted method using Co3O4 ratios of 3:1, 3:2, and 3:3. Structural and morphological studies (XRD, FTIR, Raman, FESEM, EDAX, TGA/DTA) confirmed the successful integration of Co3O4 within the $MoSe_2$/polypyrrole composite. HER performance in alkaline medium showed composition-dependent behaviour, with sample MSPVO2 (3:2) exhibiting the lowest overpotential, smallest Tafel slope, and highest catalytic current density. Electrochemical impedance spectroscopy further revealed minimal charge-transfer resistance for MSPVO2, confirms the rapid electron transport and efficient proton reduction kinetics. The optimised ternary nanocomposite demonstrates strong potential as a scalable and cost-effective HER electrocatalyst for green hydrogen technologies.

Keywords: Microwave-assisted method, Hydrogen evolution reaction, Alkaline water splitting reaction.

References:

1. M. Y. Olangi, et al., Int. J. Hydrogen Energy 47 (2022) 3834–3845.
2. S. S. Kahandal, et al., Int. J. Hydrogen Energy 61 (2024) 710–720.

EN-008

Upcycled Paper Cup-Based Porous Activated Carbon for High-Performance Supercapacitors

Prathiksha P[2]*, Priyadharshini T[1], Govindaraj Rajamanickam[1]

[1]*Department of Electrical and Electronics Engineering, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam - 603 110, Tamil Nadu, India.*

[2]*Department of Physics, Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam - 603 110, Tamil Nadu, India.*

***Corresponding author e-mail:** prathiksha2310879@ssn.edu.in

ABSTRACT

The growing use of single-use disposable paper cups has raised significant environmental concerns due to their limited recyclability and tendency to accumulate as solid waste. In this study, a sustainable and environmentally friendly method is introduced for upcycling spent disposable paper cups into porous activated carbon (PAC) for high-performance supercapacitor applications. The waste paper cups were subjected to controlled carbonization followed by chemical activation to produce highly porous carbon materials with increased surface area and well-developed pore structures. The structural and morphological properties of the synthesized activated carbon were systematically investigated using XRD, FTIR, FESEM, EDS, and BET, confirming the formation of amorphous carbon with abundant surface functional groups and interconnected porous networks. Electrochemical performance was evaluated using CV, GCD, and EIS in an aqueous electrolyte system. The activated carbon electrode exhibited excellent capacitive behaviour, high specific capacitance, good rate capability, and superior cycling stability over prolonged charge–discharge cycles. The enhanced electrochemical performance is attributed to the synergistic effects of high surface area, hierarchical porosity, and favorable surface chemistry derived from the waste precursor. This study demonstrates that spent disposable paper cups can be effectively transformed into value-added functional carbon materials, offering a low-cost and sustainable alternative to conventional carbon sources for energy storage devices. The proposed waste-to-wealth strategy not only addresses environmental challenges associated with disposable paper cup waste but also contributes to the development of sustainable electrode materials for next-generation supercapacitors.

References:

1. V. Sankar Devi and P. Elumalai, Energy Storage 5 (2023) e440.
2. X. Zhu, Y. Liu, C. Zhou, and Y. Li, J. Energy Chem. 49 (2020) 289–298.

EN-009

Structural and Electrochemical Study of Template-Free Self-Standing MOF Electrocatalyst for OER in Alkaline Medium

Sreelekshmi.S[1], Karuvath Yoosaf [1,2]*

[1]*Department of Applied Chemistry, Cochin University of Science and Technology (CUSAT), Kochi, Kerala, India, 682022*

[2]*Inter University Centre for Nanomaterials and Devices, Cochin University of Science and Technology (CUSAT), Kochi, Kerala, India, 682022*

***Corresponding author e-mail:** yoosafk@cusat.ac.in

ABSTRACT

The escalating global energy crisis, caused by fossil fuel depletion, pollution, and growing demand, has spurred the urgent need for sustainable energy solutions. Electrochemical water splitting has become a promising method to produce clean hydrogen fuel. Hydrogen fuels generated in this way emit no carbon, offering a renewable alternative to fossil fuels. However, the oxygen evolution reaction (OER), the other half-cell reaction of water splitting involving the oxidation of water or hydroxide ions, is kinetically sluggish, which limits overall efficiency. So, it is necessary to overcome high overpotentials for OER. Therefore, developing efficient and stable OER electrocatalysts is vital to reducing energy loss and boosting sustainable hydrogen generation. Metal–organic frameworks (MOFs) are emerging as versatile catalysts due to their large surface area, tunable porosity, and abundant active sites. In alkaline media, bimetallic MOFs using nickel and cobalt show synergistic effects that improve electronic structure, lower energy barriers for oxygen evolution, and foster in-situ formation of active oxyhydroxide species, enhancing stability and durability. Here, we synthesized a bimetallic Ni–Co MOF via a solvothermal, template-free method, producing uniformly porous crystals. Electrochemical evaluation in a three-electrode setup with linear sweep voltammetry (LSV) demonstrated enhanced catalytic activity and electron transfer efficiency. The synergistic interaction of Ni and Co contributed to improved conductivity, abundant active sites, and superior redox kinetics, indicating strong potential for energy conversion technologies. This approach highlights MOFs' promise as next-generation electrocatalysts in clean energy systems.

References:

1. A. Dey, J. Pradhan, S. Biswas, F. A. Rahimi, K. Biswas, T. K. Maji, Angew. Chem. Int. Ed. 2024, 63, e202315596
2. S. Karmakar, S. Barman, F. A. Rahimi, S. Biswas, S. Nath, T. K. Maji, Energy Environ. Sci. 2023, 16, 2187-2198

CoS/Water Hyacinth-Based -Natural Metals and Activated Carbon Nanocomposite for Supercapacitor Application

Kalawati chute, Sushama Giripunje*

Visvesvaraya National Institute of Technology, Nagpur, Maharashtra, India 440011

***Corresponding author e-mail**: sushamagipunje9@gmail.com

ABSTRACT

Improving the energy density of supercapacitors, while considering environmental sustainability and cost-effectiveness, is a major focus in developing electrode materials. This study utilizes the inherent reducing properties of Tridax Procumbens L leaf extract to synthesize NiS nanoparticles. The water hyacinth activated carbon (WHAC) materials, naturally doped with various heteroatoms, can serve as green electrode materials for energy storage devices, offering a sustainable and eco-friendly alternative for advancing energy technologies. WHAC contains the presence of calcium carbonate, cellulose compound, and different unspecified elements observed in the elemental analysis. The CoS nanoparticles were combined with water hyacinth-activated carbon (WHAC) to create a CoS/WHAC nanocomposite electrode material. From cyclic voltammetry (CV) analysis, the CoS/WHAC nanocomposite exhibits a specific capacitance of 1913 F/g at a 5 mV/s scan rate. From Galvanostatic charge-discharge analysis (GCD) the specific capacitance was calculated of 1096 F/g at 6 A/g current density. Thus, the green synthesized composite CoS/WHAC will enhance the energy-storing capacity of the supercapacitor electrode.

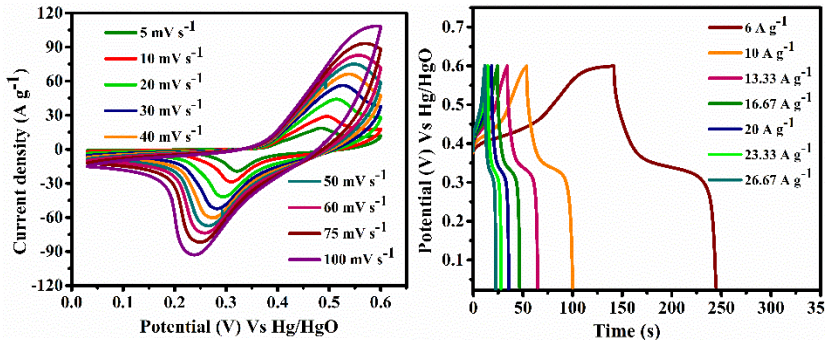


Fig. 1 (a) Cyclic voltammetry (CV) curves at different scan rates (b) Galvanostatic charge-discharge plot at different current densities of CoS/WHAC nanocomposite electrode.

Keywords: supercapacitor; activated carbon; green synthesis; water hyacinth

References:

1. Barik, R.; Ingole, P. P. Challenges and Prospects of Metal Sulfide Materials for Supercapacitors. Curr. Opin. Electrochem. 2020, 21, 327–334.
2. Xu, T.; Wang, Z.; Wang, G.; Lu, L.; Liu, S.; Gao, S.; Yu, Z. One-Pot Synthesis of a CoS–AC Electrode in a Redox Electrolyte for High-Performance Supercapacitors. J. Appl. Electrochem. 2019, 49, 1069–1077.

EN-011

Recycling of Spent Battery Electrode Materials for Textile Wastewater Remediation

Unmesha Ray[1]*, Sneha Das[1], Puspargha Roy[1], Sourav Sarkar[2]

[1]*Department of Electrical Engineering, Institute of Engineering & Management, University of Engineering and Management, Salt Lake, Kolkata-700091, West Bengal, India*

[2]*School of Material Science and Nanotechnology, Jadavpur University, Kolkata- 700032, West Bengal*

***Corresponding author e-mail:** unmesha.ray@iem.edu.in

ABSTRACT

Batteries have become an essential part of daily life as we have become a generation reliant on technology. Everything from self-heating coffee cups to robotic cleaners to morning alarms, charging our electronics, and smart watches that track our progress, we have become battery dependent. As a result, there is a generation of large quantity of the spent batteries which pose serious risk to environment and health. Also, wastewater discharge from the textile industry is increasing in tandem with their significant expansion. These contains hazardous substances such chemicals, pigments, dyes, and suspended particles, which are threat to the aquatic flora and fauna. To tackle this problem, photocatalytic degradation process is utilized to breakdown dyes in the wastewater from the textile industries. In this work, we propose to recover the spent battery electrode materials and use it as a photocatalysts for the degradation of textile wastewater. The battery electrode materials contain different transition elements, and carbonaceous materials which are often used to degrade the textile dyes like Rhodamine B, methylene blue, methyl orange, Congo Red, etc. The commercially used materials like graphite, LPF, NMC, LMNO are recovered from the spent battery packs. The recovery is carried-out via different techniques like acid leaching, hydrometallurgy, pyrometallurgy. After successful recovery of the spent battery electrodes, they are used as a photocatalyst. This solution's main advantage is that it simultaneously solves both problems, encouraging sustainability and lowering total costs.

Keywords: Wastewater, Spent battery electrode material, Photocatalysis, Recycling

References:

1. Gupta, N. K.; Epsztein, R. Upcycling Battery Waste into Photocatalysts for Sustainable Energy and Environmental Applications. ACS Sustainable Resour. Manag. 2025.
2. Panda, N. R.; Pati, S. P.; Sahu, D. Nickel Ion Doping–Induced Enhancement in Photocatalytic Degradation Efficiency of Tin Oxide Nanoparticles toward Mineralization of Reactive Blue 19 Textile Dye. Next Mater. 2026, 10, 101362.

EN-012

Exploring the Potential of Ag/NiO Cathode for the Fabrication of a Screen-Printed Silver-Zinc Rechargeable Microbattery

S. Vibavakumar[1,2], Gopika Mohandas[1,2], M. Pavithra[1,2], Satheesh Babu T.G [1,2,3], Suneesh P [1,2]*

[1]*Department of Chemistry, Amrita School of Physical Sciences Coimbatore, Amrita Vishwa Vidyapeetham, Coimbatore 641112, India*

[2]*Amrita Biosensor Research Laboratory, Amrita School of Engineering Coimbatore, Amrita Vishwa Vidyapeetham, India*

[3]*Amrita Biomedical Engineering Research Centre, Amrita School of Engineering Coimbatore, Amrita Vishwa Vidyapeetham, India*

***Corresponding author e-mail:** pv_suneesh@cb.amrita.edu

ABSTRACT

Rechargeable aqueous silver-zinc oxide (Ag – Zn) batteries are attractive for large-scale energy storage owing to their low cost, high safety, and environmental friendliness. However, the commercialization of Ag-based cathodes is limited by corrosion, dissolution, and structural instability during cycling. Herein, we report a stable and high-performance Ag–NiO composite cathode with optimized NiO content to address these challenges. The incorporation of NiO improves electrical conductivity and structural integrity, enabling higher utilization of Ag(II)/Ag(I) redox-active sites. Meanwhile, NiO provides additional pseudocapacitive contribution through the reversible NiO/NiOOH redox couple and buffers the volume changes associated with the AgO-to-Ag_2O/Ag phase transformation. This synergistic effect suppresses particle cracking, reduces polarization, and enhances cycling stability. Furthermore, NiO modifies the surface chemistry of silver oxide, promoting greater participation of Ag in electrochemical reactions. X-ray diffraction confirms the successful formation of the Ag–NiO composite. The assembled Ag– Zn battery delivers an operating voltage of ~1.5 V with two characteristic discharge plateaus of silver oxide, demonstrating that NiO does not disrupt Ag redox behavior. Overall, this work presents an effective strategy to improve the durability and performance of aqueous Ag– Zn secondary battery systems.

Reference:

1. Yin, Qisheng, Libao Chen, Yuejiao Chen, and Feng Zhan. Composites Communications 26 (2021): 100728.
2. Yang, Lufa, Shuai He, Zongyi Shang, Jie Zou, Yaoyue Yang, Zhigang Zhao, Dan Xiao, and Caixia Zhou. Applied Surface Science 608 (2023): 155236.

EN-013

Carbon-Integrated Co_3O_4 Cathodes with Enhanced Electrochemical Kinetics for Aqueous Zinc-Ion Batteries

Subashree M[1], Nithya C[1]*

[1]*PSGR Krishnammal college for women, Coimbatore, Tamil Nadu, India, 641004*

***Corresponding author e-mail:** nithyajcs@gmail.com

ABSTRACT

The development of Zinc-ion batteries (ZIBs) with high capacity, fast charge–discharge capability, and durable cathode materials has remained a major challenge. Cobalt oxide (Co3O4) has attracted considerable attention as a cathode material for ZIBs due to its abundance, safety, and environmental compatibility. In this work, a Co_3O_4/C composite has been synthesized and investigated as a cathode material for aqueous zinc-ion batteries. The composite has been prepared and systematically characterized using various structural and morphological techniques. Its electrochemical performance has been evaluated through cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). Compared with pristine Co_3O_4, the Co_3O_4/C composite cathode has exhibited enhanced specific capacity, improved cycling stability, and stable electrochemical behavior. These performance improvements have been attributed to the presence of the carbon matrix, which enhances electrical conductivity and facilitates faster charge-transfer kinetics. Overall, this study has demonstrated an effective strategy for improving the electrochemical performance of ZIB cathodes and has provided valuable insights for the rational design of high-performance zinc-ion battery systems.

References:

1. Ma, L., Chen, S., Li, H., Ruan, Z., Tang, Z., Liu, Z., Zhi, C. Energy & Environmental Science, 11(9), (2018), 2521-2530.
2. Wang, X., Wang, F., Wang, L., Li, M., Wang, Y., Chen, B., Huang, W. Advanced Materials, 28(24),(2016), 4904-4911.

Interfacial Engineering of Nickel Sulfide with Graphitic Carbon Nitride for Advanced Zinc-Ion Storage

Greeshma Jayan[1], C. Nithya[1]*

[1]PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India, 641004

***Corresponding author e-mail:** nithyajcs@gmail.com

ABSTRACT

Among multivalent metal-ion battery systems, aqueous zinc-ion batteries (AZIBs) have gained significant interest because of their high safety, environmental friendliness, natural abundance, low cost, and favorable energy and power densities. Despite these advantages, the widespread application of AZIBs is hindered by the limited capacity, poor cycling stability, and low operating voltage of existing cathode materials. In this context, transition metal chalcogenides (TMCs) have emerged as attractive cathode candidates due to their distinctive two-dimensional structures, which facilitate reversible Zn^{2+} insertion and extraction, tunable interlayer spacing, plentiful active edge sites and sulfur vacancies, and the high polarization of S2- ions that promotes rapid ion transport. Among various TMCs, nickel sulfide (NiS) stands out as a promising cathode material for aqueous zinc-ion batteries owing to its high theoretical capacity and cost-effectiveness. In this work, highly crystalline and phase-pure nickel sulfide has been synthesized using a two-step hydrothermal approach and evaluated as a cathode material for ZIBs. Its electrochemical performance was systematically investigated through cyclic voltammetry (CV), galvanostatic charge–discharge (GCD) measurements, and electrochemical impedance spectroscopy (EIS). Since inadequate capacity and unsatisfactory cycling stability remain major challenges for AZIB cathodes, rational engineering of electrode structure and composition is crucial. Accordingly, this study explores the synergistic contribution of multiple energy storage mechanisms and composite design to improve electrochemical performance. Specifically, the incorporation of graphitic carbon nitride (g-C_3N_4) with NiS is examined, demonstrating notable enhancements in capacity, rate capability, and long-term cycling stability in aqueous ZIBs.

References:

1. Huang, Z., He, L., Zhang, W., Huang, W., Mo, Q., Yang, L., ... & Gao, Q., J. colloid and interface science, 622 (2022) 728-737.
2. Yuan, C., Wei, H., Meng, X., & Shen, H. ACS Applied Materials & Interfaces, 17(43) (2025) 59266-59278.
3. Fan, Y., Wang, Q., Xie, Y., Zhou, N., Yang, Y., Ding, Y., ... & Qu, G, Progress in Materials Science, 149 (2025) 101393.

EN-015

Ag doped Activated Carbon as a Potential Energy Storage Material of Supercapacitor and Experimental Investigations

Mareeswaran P, T. Vijayakumar*

Futuristic Materials Research Centre for Planetary Exploration, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur, Chengalpattu, Chennai, Tamil Nadu 603203, India.

***Corresponding author e-mail address:** vijayakt1@srmist.edu.in

ABSTRACT

The need for high-performance energy storage devices is increasing due to the global transition towards sustainable and portable energy systems. This study involves the synthesis of silver (Ag)-doped activated carbon by a straightforward chemical activation method utilizing urea as a nitrogen dopant and stabilizing agent. The primary aim is to examine the influence of Ag doping on the structural, surface, and electrochemical characteristics of activated carbon for use as a supercapacitor electrode material. The synthesised Ag doped activated carbon demonstrates the enhanced porosity and electrical conductivity, High surface area due to the cooperative interactions of metallic silver and nitrogen functionalities transmitted by urea. Thorough characterisations through X-ray diffraction (XRD), Scanning electron microscopy (SEM), Brunauer-Emmett- Teller (BET) surface analysis, X-ray photoelectron spectroscopy (XPS), confirmed the integration of Ag nanoparticles and species of nitrogen into the matrix of carbon. The evaluation of electrochemical performance in a three- electrode cell configuration reveals the enhanced specific capacitance, exceptional rate capability, and significant cyclic stability relative undoped activated carbon. The findings show that Ag-doped activated carbon produced through urea-assisted alternations is a viable electrode material for next-generations supercapacitors providing a cost-effective and scalable solution for energy storage application.

References:

1. X. Wu, J. Liu, Y. Wang, Y. Zhao, G. Li, and G. Zhang, Chem. Eng. J., 512 (2025) 162487.
2. T. Manimekala, R. Sivasubramanian, M. A. Dar, and G. Dharmalingam, RSC Adv., 15 (2025) 2490–2522.
3. A. Jain, M. Michalska, A. Zaszczyńska, and P. Denis, J. Energy Storage, 54 (2022) 105367.
4. R. Wang, X. Li, Z. Nie, Q. Jing, Y. Zhao, H. Song, and H. Wang, J. Energy Storage, 51 (2022) 104364.

$InVO_4$ / RGO Nanocomposite for Hybrid Supercapacitor Application

Surya Sathiyamoorthy, and Balaji Manavaimaran*

Chemical Vapor Deposition Lab, Department of Materials Science,

University of Madras, Guindy Campus, Chennai - 600 025, India

***Corresponding author e-mail:** drbalajimaran@gmail.com

ABSTRACT

Energy storage plays a crucial role in meeting global energy demands and supporting economic development. Supercapacitors are promising candidates for energy storage applications due to their high-power density and long cycle life [1,2]. Transition metal orthovanadates and graphene-based materials have emerged as attractive two-dimensional (2D) semiconducting materials for electrochemical energy storage applications. In this work, high-quality indium vanadate ($InVO_4$) and graphene oxide (GO) were synthesized using facile hydrothermal and Hummers' methods, respectively. $InVO_4$/RGO nanocomposites containing 5, 10, and 15 wt.% RGO were successfully prepared via an ultrasonication process [3,4]. A high-performance supercapacitor electrode was fabricated using the $InVO_4$/RGO nanocomposite. Structural characterization using X-ray diffraction (XRD) and Raman spectroscopy confirmed the successful formation of $InVO_4$, RGO, and their nanocomposites. UV-visible diffuse reflectance spectroscopy (DRS) revealed bandgap energies of 2.3 eV for $InVO_4$, 1.6 eV for RGO, and 2.2-1.9 eV for the $InVO_4$ / RGO nanocomposites. Field-emission scanning electron microscopy coupled with energy-dispersive X-ray analysis (FESEM-EDAX) confirmed the uniform incorporation of RGO nanosheets onto the surface of $InVO_4$ nanoflake structures. The electrochemical performance of $InVO_4$, RGO, and $InVO_4$/RGO electrodes was evaluated using a three-electrode system in 1 M KOH electrolyte. Cyclic voltammetry exhibited hybrid capacitive behavior with quasi-rectangular profiles, while galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS) further demonstrated the enhanced charge storage performance of the $InVO_4$ / RGO nanocomposite electrode.

Keywords: $InVO_4$; RGO; nanocomposites; hybrid capacitance; supercapacitors

References:

1. S. Sharma and P. Cha, Results Chem., 5 (2023) 100885.
2. J. Zhang, M. Gu, and X. Chen, Micro Nano Eng., 21 (2023) 100229.
3. B. Subramanian, M. Veerappan, K. Rajan, Z. Chen, C. Hu, F. Wang, F. Wang, and M. Yang, Global Challenges, 4 (2020) 2000002.
4. D. Ma, Y. Zhang, M. Gao, Y. Xin, J. Wu, and N. Bao, Appl. Surf. Sci., 353 (2015) 118–126.

EN-017

Synergistic Bi_2WO_6/PANI Nanocomposites: Toward Sustainable and Efficient Energy Storage

Dinesh. B and T. Vijayakumar*

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** vijayakt1@srmist.edu.in

ABSTRACT

The development of high-performance supercapacitors has garnered significant attention due to the growing demand for sustainable and efficient energy storage systems. In this context, Bi_2WO_6/Polyaniline (PANI) nanocomposites have emerged as promising electrode materials, leveraging the synergistic properties of both components. Bi_2WO_6, a layered perovskite-type semiconductor, provides excellent electrochemical stability, high redox activity, and fast charge transport. Meanwhile, PANI, a conducting polymer, enhances conductivity and boosts the composite's capacitance through its pseudocapacitive behaviour. The Bi_2WO_6/PANI hybrid structure offers an expanded surface area, improved ion diffusion pathways, and enhanced charge-storage capacity. Studies like X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Fourier-transform infrared spectroscopy (FTIR) confirm the successful integration of Bi_2WO_6 and PANI, while electrochemical tests including cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) have demonstrated that this composite exhibit high specific capacitance, excellent cycling stability, and superior rate capability, making it a competitive candidate for next-generation supercapacitors.

References:

1. V. D. Nithya, R. K. Selvan, D. Kalpan, L. Vasylechko, and C. Sanjeeviraj, Electrochim. Acta, 109 (2013) 720–731.
2. A. Chelladurai et al., Mater. Sci. Eng. B, 313 (2025).
3. M. Jayachandran, A. Rose, T. Maiyalagan, N. Poongodi, and T. Vijayakumar, J. Mater. Sci.: Mater. Electron., 32 (2021) 6623–6635.
4. A. C. Hu, K. H. Chang, M. C. Lin, and Y. T. Wu, Nano Lett., 6 (2006) 2690–2695.
5. Q. Qu et al., J. Phys. Chem. C, 113 (2009) 14020–14027.

Superhydrophilic-Underwater Superoleophobic Cluster-Like TiO_2 Coated Mesh, a Tool for Oily Wastewater Treatment

Mihir Paul[1]*, Debarun Dhar Purkayastha[2]

[1]*North Eastern Regional Institute of Science and Technology, Nirjuli, Arunachal Pradesh, India, 791109*

[2]*National Institute of Technology, Chumukedima, Nagaland, 797113*

***Corresponding author e-mail:** mpl@nerist.ac.in

ABSTRACT

The rapid expansion of industrialization has resulted in the generation of oily wastewater, which poses a serious threat to ecological systems and necessitates urgent treatment solutions. In this study, cluster-like TiO_2 structures were grown on a stainless-steel mesh using solvothermal method followed by annealing. Contact angle measurements demonstrated that the fabricated mesh exhibits superhydrophilic and underwater superoleophobic characteristics. XRD analysis confirmed the presence of the anatase phase of TiO_2, while FESEM images revealed a cluster-like morphology of TiO_2. Due to its excellent water affinity and strong oil-repellent behavior, the modified mesh effectively separates various oil–water mixtures. The mesh achieved a separation efficiency of approximately 98% along with a high permeation flux. Moreover, owing to efficient charge separation ability of TiO_2, the mesh successfully degraded the organic pollutants present in the water. These results indicate that the fabricated mesh is a promising multifunctional material for oily wastewater treatment.

Keyword: Oil-water separation, Photocatalytic activity, Cluster-like TiO_2, underwater superoleophobic

References:

1. Changhui Fu, Guangyi Tian, Shiping He, Li Yao,* and Zhiguang Guo, ACS Appl. Mater. Interfaces 16 (2024) 37757−37769.
2. Fengzhen Zhang, Ranhao Wu, Huanhuan Zhang, Yuling Ye, Zhong Chen, and Aiai Zhang, ACS Omega 9 (2024), 16303-16310.

EN-019

One-Pot Carbonization of Zn-Based Deep Eutectic Solvent for High-Performance Carbon Anodes in Aqueous Zinc-Ion Batteries

Nishanth Sudarsanan, and Vijayakumar.T*

Futuristic Materials Research Centre for Planetary Exploration, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur campus, Chengalpattu-603203, Chennai, Tamil Nadu, India

***Corresponding author e-mail:** vijayakt1@srmist.edu.in

ABSTRACT

A novel one-pot carbonization method using Zn-based deep eutectic solvents (DES) produces a zinc-doped carbon anode material for high-performance zinc-ion batteries (ZIBs), where the DES acts solely as a carbon precursor without serving as the electrolyte. The Zn-DES, composed of zinc salts like $ZnCl_2$ mixed with urea or ethylene glycol, undergoes direct pyrolysis to yield a porous carbon matrix with embedded Zn species, providing zincophilic sites, high electrical conductivity, and structural stability for reversible Zn^{2+} plating/stripping. This approach avoids multi-step processes, enabling scalable production of binder-free anodes with enhanced dendrite suppression and cycling stability over traditional Zn metal anodes. Electrochemical evaluations in standard aqueous ZIB electrolytes demonstrate superior rate capability and capacity retention, attributed to the DES-derived carbon's ability to guide uniform Zn deposition and mitigate corrosion. This green, cost-effective strategy advances sustainable anode design for aqueous energy storage systems [1,2].

References:

1. M. Xue, J. Bai, M. Wu, Q. He, Q. Zhang, and L. Chen, Energy Storage Mater., 62 (2023) 102940.
2. W. Zheng, L. Zhu, H. Huang, Z. Sun, H. Zhou, and K. Zhang, ACS Sustain. Chem. Eng., 12 (2024) 8070–8082.

Synthesis and Characterisation of Bio Hosted PCM for Thermal Management Application

Krishna Kumar. M[1], Rithikaa. T[1], MullaiMalar. A[1], Manikandan. S[2], Jeyalakshmi. R[1]*

[1]*Department of Chemistry, CET, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*Department of Mechanical Engineering, CET, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** jeyalakr@srmist.edu.in

ABSTRACT

Phase change materials (PCMs) offer significant potential for thermal management applications, yet challenges including leakage, low thermal conductivity, and structural instability limit their widespread adoption. This study presents a comprehensive computational investigation of bio-hosted lauric acid-palmitic acid (LA-PA) eutectic PCM (ePCM) composites using COMSOL Multiphysics® software. Three composite systems were developed and characterized: (1) neat eutectic PCM (ePCM), (2) ePCM with geopolymer matrix and reduced graphene oxide (rGO) nanofiller, and (3) ePCM with SiO_2 matrix and rGO nanofiller. All three composite systems were bio-hosted using sodium alginate and calcium chloride crosslinking to create sustainable, leakage-proof bio-based capsules. Comprehensive characterization through Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and Differential Scanning Calorimetry (DSC) was performed to evaluate chemical compatibility, structural properties, and thermal behavior of the developed composites. COMSOL Multiphysics® software model analysis was implemented to validate the thermal characteristics of the bio-hosted PCM composites through heating-cooling cycle simulations, revealing temperature distribution patterns, heat transfer rates, and energy storage-release behavior under realistic operating conditions. Numerical simulation will provide comprehensive validation of experimental findings, enable prediction of thermal performance under diverse thermal management scenarios beyond laboratory testing capabilities including electronic cooling systems and temperature-critical applications, and facilitate optimization of bio-hosted PCM composite design parameters for enhanced heat dissipation and temperature regulation across various thermal management systems.

Keywords: COMSOL Multiphysics; Phase change materials; lauric-palmitic acid; bio-hosting; geopolymer; thermal simulation; building insulation.

References:

1. X. Chen, Z. Duan, J. Li, M. Xu, W. Qiu, J. Zhang, and W. Xu, J. Therm. Anal. Calorim., 149 (2024) 14175–14185.
2. S. Dora, F. Kuznik, and K. M. Mini, J. Energy Storage, 105 (2025) 114625.

A Novel $NiMn_2O_4$@TiO_2 Core shell structure as a high-performance electrode for supercapacitor material

Archanadevi Balamurugan, Vijayakumar T*

Futuristic Materials Research Centre for Planetary Exploration, Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Chengal pattu, Tamilnadu, India, 603203

***Corresponding author e-mail:** Vijayakt1@srmist.edu.in

ABSTRACT

A novel Nickel Manganite ($NiMn_2O_4$) Core shell structure synthesised via Two step hydrothermal method as an excellent electrode material for supercapacitor application. The $NiMn_2O_4$@TiO2 was characterized by XRD, XPS, SEM, TEM. The "core" $NiMn_2O_4$ and "Shell" TiO_2 are both active materials and both participate in faraday redox reaction to facilitate $NiMn_2O_4$@TiO_2 electrode to obtain more excellent electrochemical characteristics. The internal $NiMn_2O_4$ nanoparticles provide a good electron transport path for electrochemical reaction. Subsequently, the electrochemical performance of both $NiMn_2O_4$ and NiMn2O4@TiO2 was evaluated via CV, GCD and EIS in 1M KOH as an electrolyte solution. The remarkable electrochemical performance of the $NiMn_2O_4$@TiO_2 nanocomposites electrode is attributed to the synergistic effect and enhanced interfacial connection between $NiMn_2O_4$ and TiO_2, which facilitate rapid electron and ionic transport. This work significantly contributes to the advancement of composite materials for energy storage applications, particularly in high-performance supercapacitors.

References:

1. P. E. Saranya, A. Arulraj, R. V. Mangalaraja, V. Siva, and R. O. M. U. Jauhar, Mater. Lett., — (2025) 139515.
2. P. N. Thonge, S. D. Dhas, S. D. Waghmare, A. H. Patil, T. M. Patil, M. A. Yewale, and D. Kim, ACS Appl. Nano Mater., 7 (2024) 18579–18589.
3. K. C. Lee, Y. S. Hsiao, M. Y. Sung, Y. L. Chen, N. J. Wu, J. H. Huang, and S. C. Hsu, J. Environ. Chem. Eng., 11 (2023) 110762.

α-MnO_2@C Nanospheres Cathode with Enhanced Electrochemical Characteristics for Aqueous Zinc-Ion Battery Applications

Rohan Santosh Zoting[1] and K. Thirukkumaran[1]*

[1]*Department of Physics, National Institute of Technology, Tiruchirappalli, Tamil Nadu, India*

***Corresponding author e-mail:** *kkumaran@nitt.edu*

ABSTRACT

Aqueous electrolyte-based zinc-ion batteries (ZIBs) are developing as a viable alternative over conventional lithium-based energy storage systems due to its inherent safety, environment compatibility, and low manufacturing costs. Among various cathode materials, the Alpha-Manganese dioxide (α-MnO_2) has been extensively utilized in ZIBs due to its high theoretical specific capacity, low environmental impact, and higher operating voltage. However, pristine α-MnO_2 has a limited rate capability and a rapid capacity degradation, rendering it unsuitable for practical applications. In this study, pitch carbon-coated α-MnO_2 nanospheres were synthesized in two steps: the solvothermal approach and the carbonization method. The α-MnO_2 nanospheres show homogeneous particle sizes (250-700 nm), mesoporous morphology, and distinct α-MnO_2 diffraction peaks, indicating the formation of a tunnel structure suitable for ZIBs. The coin cells (CR2032) were used to perform electrochemical testing on pristine MnO_2 nanospheres and pitch carbon-coated MnO_2 nanospheres using a 2M $ZnSO_4$ and 0.1M $MnSO_4$ aqueous electrolyte. The pristine MnO_2 nanosphere cathode showed an initial discharge capacity of 300 mAh/g at 0.1 A/g and retained around 50 mAh/g at a 1C rate. The pitch carbon coated MnO_2 achieved an initial specific capacity of ~340 mAh/g for 0.1C rate and retained ~140 mAh/g at a 0.1C rate. The carbon coated α-MnO_2 nanosphere shows the long-term cycling at 0.1 A g-1 stable performance with enhanced capacity retention as compared to the pristine nanosphere. Cyclic voltammetry demonstrated different redox behavior associated with consecutive H+ and Zn2+ insertion, while EIS confirmed lower charge-transfer resistance upon activation. This study explores the use of carbon-coated α-MnO_2 nanosphere electrodes in aqueous ZIB applications, leading develop high-performance eco-friendly batteries.

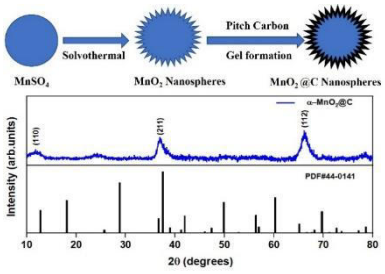


Fig.1. (a) Schematic diagram of synthesis processes of carbon coated α-MnO_2 nanosphere (b) X-ray diffraction pattern of carbon coated α-Mno_2 nanospheres.

Keywords: Zinc-ion batteries; MnO_2 nanospheres; Enhanced capacity; Energy storage system

References:

1. X. Wang, Z. Zhang, B. Xi, W. Chen, Y. Jia, J. Feng, and S. Xiong, ACS Nano, 15 (2021) 9244–9272.
2. S. Islam, M. H. Alfaruqi, J. Song, S. Kim, D. T. Pham, J. Jo, S. Kim, V. Mathew, J. P. Baboo, Z. Xiu, and J. Kim, J. Energy Chem., 26 (2017) 81.

$NaFePO_4$ as a Cathode Material for Sodium-ion Batteries

Suprap Paritkar [1,2] *

[1]*COEP Technological University, Pune, Maharashtra, India, 411005*

[2]*C-MET, Pune, Maharashtra, India, 411008*

***Corresponding author e-mail:** paritkarss24.meta@coeptech.ac.in

ABSTRACT

Sodium-ion batteries (SIBs) have been considered as a prospective energy storage solution in the near future due to the abundance and wide distribution of sodium resource on the earth. The exploration of high-performance cathode materials is the key to the practical application of advanced SIBs. Among various SIB cathode materials, NaFePO4 possesses the advantages of abundant reserve, low cost and safety, which make it an ideal positive electrode material for SIBs. This paper provides a comprehensive research on progress and future prospect of NaFePO4 positive electrode material. Firstly, introduction to batteries have been discussed, how the battery works and performance parameters. Then Li-ion battery is compared with Na-ion battery giving their advantages and disadvantages. Theoretical studies on different cathode and anode materials have been summarized in details. After coating there is fast ionic diffusion of Na+ ions and electron movement. The good electrochemical performances are attributed to the NaFePO4 nanoparticles after coating. After solid state synthesis we have performed various operations on the given material to predict their properties. XRD, FE-SEM, doping, coating, electrode making and testing have been performed on NaFePO4 material. This paper also aims to provide a material which is cost effective, highly scalable and safer to use. This research aims to provide insights into the rational design of high-performance NaFePO4 cathode materials and to accelerate the practical application of NaFePO4 in SIBs.

References:

1. Duan Wang, Yuanbo Wu, Jinmeng Lv, Rongrong Wang, Sailong Xu, Colloids and Surfaces A, 583 (2019) 123957.
2. Fangyu Xiong, Qinyou An, Lixue Xia, Yan Zhao, Liqiang Mai, Haizheng Tao, Yuanzheng Yue, Nano Energy, 57 (2019) 608–615.
3. Bingqiu Liu, Qi Zhang, Lu Li, Lingyu Zhang, Zhanshuang Jin, Chungang Wang, Zhongmin Su, Chemical Engineering Journal, 405 (2021) 126689.
4. Huanyi Liao, Zhi Zhang, Yifan Zheng, Yihua Gao, Energy Storage Materials, 65 (2024) 103157.

Design of Zn-MOF/Ni–Co Bimetallic Oxide Hybrid Electrodes for Enhanced Asymmetric Supercapacitor Performance

Arun Tamilselvan[1]*, K. Aravinth[1], P. Balaji Bhargav[1]

[1]*Department of Physics, SSN Research centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakam, Tamilnadu 603110, India.*

***Corresponding author e-mail:** arunt@ssn.edu.in

ABSTRACT

Bimetallic oxide composites have attracted significant interest as electrode materials for high-performance supercapacitors owing to their rich redox activity, excellent electrochemical stability, mixed ionic-electronic conductivity, and cost effectiveness. In contrast, metal-organic frameworks (MOFs) offer exceptionally high surface areas, well-defined porosity, and tunable redox-active sites, but their practical application is often hindered by poor electrical conductivity and limited structural robustness. To overcome these limitations, a Zn-MOF decorated $NiCo_2O_4$ (ZNCO) nanocomposite was synthesized via a facile hydrothermal approach. Comprehensive structural, morphological, and electrochemical characterizations confirmed the strong synergistic interaction between the MOF and bimetallic oxide components. As an electrode material, ZNCO delivered a high specific capacitance of 550.6 F g-1 at 1 A g^{-1} in an aqueous electrolyte. Furthermore, an asymmetric supercapacitor assembled using activated carbon as the anode and ZNCO as the cathode achieved a remarkable energy density of 20.94 Wh kg^{-1} at a power density of 800.2 W kg^{-1}. The device also demonstrated excellent cycling stability, retaining 95 % of its initial capacitance with a coulombic efficiency of % after charge-discharge cycles at 5 A g^{-1}. These findings highlight the effectiveness of MOF decoration in enhancing bimetallic oxide electrodes and underscore the strong potential of ZNCO nanocomposites for next-generation energy storage systems.

Keywords: Bimetalic; MOF; Energy density; supercapacitor

References:

1. Subramani, S., Tamilselvan, A., Rajamanickam, G., & Karuppannan, A. 140, 11901, (2025).
2. Karthigaimuthu, D., Priya, V. N., Arun, T., & Florence, S. S.), 113097. (2025).

EN-025

Electrodeposited Binder-Free Bi-Metallic Oxide Nanostructures and Vertical Graphene Nanosheets Hybrid Electrodes for Supercapacitor Applications

S R Polaki*, and Sumithra K

Surface and Sensors Studies Division, Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam, TN 603102, A CI of Homi Bhabha National Institute (HBNI)

***Corresponding author e-mail:** polaki@igcar.gov.in

ABSTRACT

Recently, bi-metallic oxides AB_2O_4 type spinel oxides have garnered significant attention due to their remarkable properties, including high specific capacitance resulting from multiple redox states, excellent electrical conductivity, large surface area, and the synergistic effects of the constituent metals. Conventionally, growth of bi-metallic oxide supercapacitor electrodes involves conducting substrates and polymer binders. Usage of the polymer binders limits the energy storage performance of the bi-metallic oxide supercapacitor electrodes by impeding their electrochemical active surface area. Development of scalable growth process for the fabrication of binder-free bi-metallic oxide supercapacitor electrodes is of great importance in order to realize their full potential for practical applications. Herein, binder-free growth of bi-metallic oxide (MCo2O4, where M=Fe or Ni) directly on highly conducting Vertical Graphene Nanosheets (VGNs) by electrodeposition technique is demonstrated. Influence of microstructure and morphology, cation distribution and valance state, and charge transfer kinetics are elucidated. The areal capacitance of FeCo2O4/VGNs and NiCo2O4/VGNs hybrid electrodes are 61 and 55 mF/cm2, respectively @ 20 mV/s. Finally, the fabrication and testing of asymmetric supercapacitor device using the bi-metallic oxide and VGNs hybrid electrodes is demonstrated to realize its potential for practical applications.

Keywords: Supercapacitor, bi-metallic oxide, Vertical Graphene Nanosheets, electrodeposition

References:

1. X Zhong, et. al., J. Energy Storage 73 (2023) 2
2. Peng Tan, et. al., J. Electrochem. 166 (2019) 3448
3. Madhav Kumar V, et. al., J. Energy Storage 79 (2023) 110160

EN-026

Biomass-Derived Activated Carbon of Citrus Limon Derived Activated Carbon for Ultracapacitors Performance

B.H. Poornima[1], T. Vijayakumar[2]*

[1]*Department of Physics, Mohan Babu University, Sree Sainath Nagar, Tirupati- 517102, Andra Pradesh India.*

[2]*Futuristic Materials Research Centre for Planetary Exploration, Department of Physics and Nanotechnology, College of Engineering and Technology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603203, Kancheepuram, Tamil Nadu, India*

***Corresponding author e-mail address:** vijayakt1@srmist.edu.in

ABSTRACT

The Citrus Limon is most abundant and environmentally friendly substitutes for synthetic fillers or carbon-dense products such as biochar, which is extended durations, contributing to the reduction of atmospheric CO_2 levels leads to beneficial for various energy storage devices. Hence, we described in the current study, synthesis of porous structure carbon from the Citrus Limon Shell, which are chemically activated with KOH. The creation of porous structure carried out at different activation temperatures and optimized. A comprehensive analysis of the surface storage process is provided, along with an examination of the stability of the synthesized samples.

Keywords: Citrus Limon, porous carbon, ultracapacitors, energy density, power density.

References:

1. T. Yue, C. Xia, X. Liu, Z. Wang, K. Qi, and B. Y. Xia, ChemElectroChem, 8 (2021) 1021–1034.

EN-027

Ternary Nanocomposite of Polypyrrole/Graphener Oxide - MoO_3 for High-Performance Supercapacitor Electrode

Bharathi B, Jagannathan K*

Department of Physics, SRM Institute of Science and Technology, Vadapalani Campus, No.1, Jawaharlal Nehru Salai, 100ft Road, Vadapalani, Chennai – 600026, TN, India

***Corresponding author e-mail:** kjagan81@gmail.com

ABSTRACT

This study proposes the development and electrochemical evaluation of a ternary Polypyrrole/Graphene Oxide/Molybdenum Trioxide (PPy/GO–MoO_3) nanocomposite for use as a high-performance supercapacitor electrode. The composite was prepared by a sequential chemical route: polypyrrole (PPy) was synthesized via chemical oxidative polymerization, graphene oxide (GO) was prepared using the modified Hummer's method, and the hydrothermal method was used to synthesize the MoO_3. Finally the ternary composite was prepared by chemical oxidative polymerization method. The structures and morphology of the resulting ternary nanocomposites were characterized by using Fourier transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy, and energy-dispersive X-ray spectroscopy. In a three-electrode aqueous electrolyte system, the electrochemical investigations were carried out. The specific capacitance, rate capability, cycling stability, and charge-transfer kinetics were analyzed for the prepared PPy/GO-MoO_3 electrode.

Keywords: Supercapacitor, Ternary Nanocomposite, Polymerization, Electrochemical, Specific Capacitance.

EN-028

Design of Succinonitrile (SCN)-Modified LATP–PVDF-HFP Nanofiber Hybrid Electrolytes for High-Performance Flexible All-Solid-State Batteries

Vijaysingh Velu, Ananthakumar Ramadoss*

Advanced Research School for Technology and Product Simulation (ARSTPS), School for Advanced Research in Petrochemicals (SARP), Central Institute of Petrochemicals Engineering and Technology (CIPET), Chennai- 600 032, India.

***Corresponding author e-mail: ananth.**cipet@gmail.com

ABSTRACT

The growing demand for electric vehicles necessitates the development of energy storage systems that offer high safety, fast charging, and elevated energy density. Conventional lithium-ion batteries are constrained by safety concerns arising from flammable liquid electrolytes. Solid-state batteries provide a safer alternative through the use of non-flammable solid electrolytes that function as both lithium-ion conductors and separators. Among various candidates, NASICON-type LATP ceramic electrolytes are promising due to their high ionic conductivity, wide electrochemical stability window, cost-effectiveness, and excellent ambient stability; however, their intrinsic brittleness limits flexible device applications. In this work, LATP ceramic powders were incorporated into a flexible polymer matrix via electrospinning to construct a ceramic–polymer nanofibrous framework. To enhance ionic transport and interfacial compatibility, the porous membrane was infiltrated with lithium salt solutions containing an SCN plasticizer. The SCN plasticizer plays a crucial role in improving polymer chain mobility, electrolyte uptake, and electrode–electrolyte interfacial contact, thereby facilitating efficient lithium-ion conduction. The structural, morphological, thermal, and interfacial characteristics of the composite electrolytes were systematically examined using XRD, FTIR, FESEM, DSC, TGA, flammability, and contact angle analyses. Ionic conductivity was evaluated by electrochemical impedance spectroscopy (EIS). Therefore, LATP-based nanofiber hybrid electrolytes are promising candidates for flexible all-solid-state lithium battery applications.

Keywords: LATP Ceramic, Hybrid Electrolyte, Electrospinning, Solid-State Batteries.

References:

1. X. Ye et al., Adv. Funct. Mater., 35 (2025) 2413205.

Hydrothermally Synthesized Li-KNN And PVDF Based Flexible Composites for Piezoelectric Energy Harvesting

Piyush[1], Babita Sharma[1], Arijit Chowdhuri[2], Reema Gupta[3], Monika Tomar[4*]

[1]*Department of Physics and Astrophysics, University of Delhi, 110009*

[2]*Acharya Narendra College, University of Delhi, 110019*

[3]*Hindu College, University of Delhi, 110009*

[4]*Miranda College, University of Delhi, 110009*

***Corresponding author e-mail:** monikatomar@gmail.com

ABSTRACT

Self-powered nanoscale energy harvesters have gained significant attention from researchers due to their capacity for next-generation sustainable power in wearable electronics, biomedical sensors, and IoT devices without relying on external energy sources [1][2], particularly through piezoelectric nanogenerators that convert ambient mechanical energy into electrical output. Amongst all, Potassium Sodium Niobate (KNN) being the environment friendly along with the feature of large piezoelectricity, high Curie temperature and good ferroelectricity have been utilized for the piezoelectric energy harvesting. So, present work describes the preparation of Lithium (Li) doped KNN ceramic with varying concentration of Li in KNN from 0-10% using hydrothermal method. Further, Polyvinyldene Fluoride (PVDF) was used as a polymer matrix to prepare flexible composite sheets of Li-KNN/PVDF through solution-casting. The influence of Li-KNN concentration on structural, morphological and piezoelectric performance of PVDF has been investigated. The Fourier transform infrared spectroscopy (FTIR) studies revealed the fraction of β-phase enhancement from 27.9 to 48.3 % which is 73.1% higher as compared to the pristine PVDF film with incorporation of these nanofillers. The composite sheets show a maximum value of polarization of 1.896 μC/cm2 at a voltage of 10V with the fixed frequency of 50Hz. The as-prepared nanogenerator exhibits the open-circuit voltage up to 22.06 V under external weight of 0.98N with power density of 4.06 (μW/cm2) across 1MΩ load resistance. The output performances of Li doped KNN based device indicates that it can be a potential candidate for mechanical energy harvesting under various human body motions as well as for wearable piezoelectric sensor applications.

References:

1. A. Zanella, N. Bui, A. Castellani, L. Vangelista, and M. Zorzi, IEEE Internet Things J., 1 (2014) 22–32.
2. S. M. R. Islam, D. Kwak, M. H. Kabir, M. Hossain, and K.-S. Kwak, IEEE Access, 3 (2015) 678–708.

EN-030

Development of PVDF-HFP/Guar Gum Based Composite Polymer Electrolyte for Proton Conducting Battery Applications

M. Tamilarasi, K. Jagannathan*

Department of Physics, SRM Institute of Science and Technology, Vadapalani Campus, No.1, Jawaharlal Nehru Salai, 100ft Road, Vadapalani, Chennai – 600026, TN, India

***Corresponding author e-mail:** kjagan81@gmail.com

ABSTRACT

The energy storage devices require safe and efficient electrolytes with high ionic conductivity. This work aims to develop a PVDF-HFP based polymer electrolyte for proton conducting batteries. The polymer electrolyte film was prepared using PVDF-HFP, ammonium thiocyanate and graphene oxide. Here the polymer electrolyte film was prepared using poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and guar gum as the polymer matrix, ammonium thiocyanate (NH_4SCN) as the proton salt, and graphene oxide as a conductive filler. The electrolyte films were fabricated by the solution casting method. The structural and molecular interactions were analyzed using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR). The scanning electron microscopy (SEM) revealed homogeneous filler dispersion, while thermogravimetric analysis (TGA) shown the composite electrolyte was more stable at high temperatures. The Electrochemical Impedance Spectroscopy (EIS) was employed to investigate proton transport behaviour and a DC polarization study confirms the ionic conduction. The linear sweep voltammetry (LSV) demonstrated the electrochemical stability of the electrolyte. The charge–discharge and cyclic voltammetry (CV) analyses revealed the stable electrochemical performance and good reversibility, confirming effective proton transport within the electrolyte. The PVDF-HFP/guar gum-based composite polymer electrolyte is a viable option for proton-conducting energy storage devices of the future.

Keywords: Nanocomposites; Dielectric properties; Thermal stability; Electrochemical stability; Batteries.

EN-031

Hydrothermal Synthesis and Energy Related Performance of Vanadium Doped BaO Containing Layered Double Hydroxide Nanomaterials

G Vignesh*, Xavier Gama

St Joseph's University, Bengaluru, Kittel Science College, Dharwad, India

***Corresponding author e-mail:** vignesh.g@sju.edu.in

ABSTRACT

Vanadium doped, barium containing layered double hydroxides (LDHs) are promising precursors to BaO rich mixed oxides for electrocatalysis and energy conversion. LDHs are tunable anionic clays whose nanosheet morphology, mixed metal composition, and post calcination oxides have been widely exploited in catalysis and energy devices1,2. Vanadium incorporation in transition metal LDHs modifies the electronic structure, generates defect sites, and enhances charge transfer kinetics, yielding improved oxygen evolution and related electrochemical performance3,4,5. Barium containing LDHs such as Ba(II)–Fe(III) systems demonstrate that Ba can be integrated into layered frameworks and subsequently transformed into BaO containing mixed oxides with altered basicity and interfacial behavior6. Hydrothermal crystallization offers a robust route to compositionally homogeneous, highly ordered LDH nanosheets with controllable defect densities, superior to simple coprecipitation for dopant controlled synthesis7,8. In this work, a practical hydrothermal procedure is developed to synthesize V doped Ba containing LDH nanomaterials via controlled coprecipitation (pH ≈ 10–11) followed by autoclave treatment, yielding nanosheets/nanoplates with tailored Ba/M/V ratios. Structural, compositional, and textural properties are correlated using XRD, FT IR, XPS, TGA, BET, and electron microscopy, while electrochemical measurements evaluate activity toward alkaline oxygen evolution, super capacitive charge storage, and photo/electrocatalytic water splitting. The study highlights how BaO domains derived from the LDH and V induced electronic modulation act cooperatively to tune activity and stability in emerging energy conversion electrodes.

Keywords: layered double hydroxide; BaO containing mixed oxides; vanadium doping; hydrothermal synthesis; nanosheets; oxygen evolution reaction; electrocatalysis; supercapacitors; photo electrocatalytic water splitting; energy conversion materials.

References:

1. F. Xianghong, Z. Ruikun, et al., RSC Adv., 15 (2025).
2. D. Wang, et al., Nat. Commun., 10 (2019) 3899.
3. R. Keyikoglu, et al., Chem. Eng. J., 430 (2022) 132785.
4. Y. Hu, et al., ACS Sustain. Chem. Eng., 7 (2019) 14401–14409.
5. T. Das, et al., Inorg. Chem., 61 (2022) 12768–12781.

EN-032

Engineering $NiMn_2O_4/NiMoO_4$ Heterobimetallic Oxides as Efficient Electrode Materials for Asymmetric Supercapacitors

Esaithendral Thangadurai[1], Arun Tamilselvan[2], Srinivasan Manickkam[2], Radha Sankararajan[1]*

[1]*Department of Electronics and Communication Engineering, Sri Sivasubramaniya Nadar College of Engineering, Kalavakam, Tamilnadu 603110, India.*

[2]*Department of Physics, SSN Research centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakam, Tamil Nadu 603110, India.*

***Corresponding author e-mail:** radhas@ssn.edu.in

ABSTRACT

Transition metal oxide-based nanomaterials are widely recognized as promising electrode candidates for high-performance supercapacitors (SCs), owing to their intrinsic redox activity, strong electrochemical stability, mixed ionic-electronic conductivity, cost-effectiveness, and environmental friendliness. In this work, a heterobimetallic $NiMn_2O_4/NiMoO_4$ (NMO/NMoO) nanocomposite was successfully synthesized via a simple hydrothermal method. The electrochemical performance, morphology, and structural features of the synthesized composite were systematically evaluated. The NMO/NMoO electrode delivered an excellent specific capacitance of 493 F g^{-1} at 1 A g^{-1} in aqueous electrolyte. Furthermore, an asymmetric supercapacitor device assembled using activated carbon (AC) as the anode and NMO/NMoO as the cathode achieved a high energy density of 18.5 Wh kg^{-1} at a power density of 802 W kg-1. The device also demonstrated outstanding cycling durability, retaining 94.6 % of its initial capacitance with a coulombic efficiency of 97.5 % after 10,000 charge-discharge cycles at 3 A g^{-1}. Overall, these results highlight the synergistic electrochemical behavior of the heterobimetallic oxide system and underscore its strong potential for next-generation energy storage applications.

Keywords: Supercapacitor; $NiMn_2O_4$; $NiMoO_4$; Asymmetric; Heterobimetallic oxides; Energy density

References:

1. H. Jia, Z. Zhang, S. Li, M. Han, Y. E, C. Liu, Q. Wang, and W. Liu, ACS Appl. Nano Mater., 7 (2024) 15387–15394.
2. P. Simon and Y. Gogotsi, Nat. Mater., 7 (2008) 845–854.

An Alternative Aluminum-Copper Galvanic Cell Model for Aluminum Ion Battery Systems Using Fe_2O_3 Nanoparticles in Acidic Mixture Electrolyte

M. Vishnu Devan*

Department of Chemistry, Government Arts College (Autonomous), Kaur, Tamilnadu, India, 639005

***Corresponding author e-mail:** devan70@rediffmail.com

ABSTRACT

A Novel Al-Cu galvanic cell in high chloride acidic aqueous electrolyte has been developed for an alternative to already existing Aluminium ion battery systems. An acid electrolyte aqueous system with 3% NaCl and 1000 ppm Fe_2O_3 Nanoparticles (NPs) (synthesized by chemical precipitation) was chosen, and the performance of the galvanic cell was evaluated by measuring its internal electrolytic resistance, specific capacity, and cell potential. These cell parameters were then compared with Fe_2O_3 NPs unmixed and uncharged electrolytic systems. Due to the anodic depolarization effect of Fe_2O_3 NPs, which lowers the speed of aluminium ion dissolution at the anode, the presence of Fe_2O_3 NPs in this electrolyte improved the overall cell performance of both the charged three pair of cell series connected system and uncharged single pair system by increasing cell potential, specific capacity, and lowering cell internal electrolytic resistance.

References:

1. M.-C. Lin, M. Gong, B. Lu, et al., Nature, 520 (2015) 324.
2. S. Das, S. S. Manna, and B. Pathak, ACS Omega, 6 (2021) 1043.
3. B.-E. Jia, A. Q. Thang, C. Yan, C. Liu, C. Lv, Q. Zhu, J. Xu, J. Chen, H. Pan, and Q. Yan, Small, 18 (2022) 2107773.
4. J. Zhao, Y. Chen, Z. An, M. Zhang, W. Wang, Q. Guo, Y. Li, S. Han, and L. Zhang, Green Chem., 26 (2024).

EN-034

Design of Zn–Sr–Ni Trimetallic Nanocomposites for Environmental Remediation and Energy Storage

P. Naga Nandhini[1], J. Helen Ratna Monica[1]*, S. Stephen Rajkumar Inbanathan[2], M. Jeevaraj[3]

[1]*PG & Research Department of Chemistry, The American college, Madurai, Tamilnadu.*

[2]*PG & Research Department of Physics, The American college, Madurai, Tamilnadu.*

[3]*Institute of Physics and Technology,Ural Federal University, Yekaterinburg, Russia-620002.*

***Corresponding author e-mail:** helenrmonica@americancollege.edu.in

ABSTRACT

The development of multifunctional materials with enhanced physicochemical properties has attracted considerable interest for environmental remediation and energy storage applications. In this study, a Zn–Sr–Ni trimetallic nanocomposite was successfully synthesized via a suitable chemical route. The incorporation of three distinct metal components is expected to generate synergistic effects, resulting in improved catalytic activity, efficient charge transport, and enhanced electrochemical stability. The synthesized Zn–Sr–Ni material was comprehensively characterized using standard analytical techniques to elucidate its structural, morphological, and compositional features. The photocatalytic performance of the trimetallic nanocomposite was evaluated through the degradation of organic dye pollutants under light irradiation. The results revealed significantly enhanced photocatalytic efficiency compared to mono- and bimetallic systems. This improvement can be attributed to effective charge separation, suppressed recombination of photogenerated electron–hole pairs, and the combined influence of Zn, Sr, and Ni ions. Furthermore, the electrochemical properties of the Zn–Sr–Ni nanocomposite were investigated for supercapacitor applications using cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy. The trimetallic electrode exhibited high specific capacitance, excellent rate capability, and long-term cycling stability, demonstrating its suitability for energy storage devices. The superior supercapacitor performance arises from the redox-active nature of Ni, enhanced electrical conductivity, and the structural integrity imparted by Zn and Sr. Overall, this study highlights the Zn–Sr–Ni trimetallic nanocomposite as a promising multifunctional material for simultaneous photocatalytic environmental remediation and advanced supercapacitor applications. The findings underscore the potential of trimetallic systems as efficient and sustainable candidates for next-generation energy and environmental technologies.

Keywords: Trimetallic nanomaterial; Zn–Sr–Ni; Photocatalytic degradation; Supercapacitor; Energy storage; Environmental remediation

References:

1. A. Fujishima, X. Zhang, and D. A. Tryk, Surf. Sci. Rep., 63 (2008) 515.
2. P. Simon and Y. Gogotsi, Nat. Mater., 7 (2008) 845.
3. J. Wang and S. Kaskel, J. Mater. Chem., 22 (2012) 23710.

Synthesis of Carbon-Based Materials for Positive Electrode Fabrication in Energy Storage Devices

Suganya Subramaniyan[1], Archana Jayaram[1]*

[1] *Centre of Excellence in Materials for Advanced Technologies (CeMAT), SRM Institute of Science and Technology, Kattankulathur Campus, Chengalpattu District, Tamil Nadu-603203.*

***Corresponding author e-mail:** archanaj@srmist.edu.in

ABSTRACT

The continuous consumption of fossil fuels and the associated environmental concerns have accelerated research into environmentally benign and sustainable energy storage technologies. Among various energy storage devices, supercapacitors have attracted significant attention due to their superior power density, fast charge–discharge rates, and long operational lifespan. Notably, the electrochemical performance of supercapacitors is strongly dependent on the properties of electrode materials, making their development a key research focus. Carbon-based materials such as activated carbon, graphene, carbon nanotubes, and carbon aerogels exhibit exceptional electrical conductivity, high specific surface area, and porous architectures, facilitating rapid ion transport and efficient electric double-layer formation, which collectively enable efficient charge storage and long-term cycling performance, thereby making them ideal electrode materials for supercapacitor applications. The structural characteristics and phase formation of synthesized carbon material was investigated by XRD analysis, and its morphological features was studied using SEM analysis. Further, their electrochemical evaluations were carried out in a three-electrode system employing cyclic voltammetry and galvanostatic charge–discharge techniques. The fabricated electrode demonstrated superior electrochemical behavior with an extended discharge time, reflecting enhanced charge storage efficiency.

Keywords: Supercapacitors, Carbon materials, Surface area

References:

1. Vivek, E., Arulraj, A., Khalid, M. and Potheher, I.V., Journal of Alloys and Compounds, 908 (2022) 164541.
2. Mehtab, A., Alshehri, S.M. and Ahmad, T., ACS Applied Nano Materials, 5 (9) (2022) 12656-12665.

EN-036

Hybrid Bio-leaching and AI-Assisted Optimization for REE Recovery from PCB and NdFeB E-Waste

Prabhakaran Arjunan[1], Poovammal E[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** poovamme@srmist.edu.in

ABSTRACT

Rare earth elements (REEs) such as neodymium, dysprosium, praseodymium, and terbium are essential for electric vehicles, renewable energy technologies, and advanced electronic systems. Increasing supply constraints and environmental concerns associated with primary mining have intensified interest in electronic waste as a secondary resource for REE recovery. Printed circuit boards (PCBs) and NdFeB permanent magnets represent two major e-waste streams with significant REE potential but complex material compositions that challenge conventional extraction routes. This work examines bio-leaching-based approaches for the recovery of REEs from PCB and NdFeB magnet waste, with particular emphasis on hybrid process strategies aimed at improving recovery efficiency and selectivity. Microbial and organic-acid-mediated leaching mechanisms are discussed in terms of dissolution behavior, process kinetics, and environmental performance. The limitations of stand-alone bio-leaching, including incomplete extraction, slow reaction rates, and co-leaching of impurities, are critically evaluated. To overcome these challenges, hybrid routes integrating bio-leaching with hydrometallurgical separation techniques, solvent extraction, and electrochemical recovery are reviewed. To address process variability and optimization challenges, this study further proposes an AI-assisted process optimization framework for bio-leaching systems. Machine-learning-based models are suggested to correlate key operational parameters—such as pH, temperature, pulp density, leaching time, and microbial activity—with REE recovery efficiency and selectivity. The study demonstrates that combining hybrid bio-leaching routes with AI-assisted optimization provides a promising pathway toward environmentally sustainable and economically viable recovery of critical REEs from complex e-waste streams, supporting circular-economy-driven materials management.

References:

1. Tuncuk, A., Stazi, V., Akcil, A., Yazici, E. Y., Deveci, H., Minerals Engineering, 25 (2012) 28–37.
2. Brandl, H., Bosshard, R., Wegmann, M., Hydrometallurgy, 59 (2001) 319–326.
3. Cui, J., Zhang, L., Journal of Hazardous Materials, 158 (2008) 228–256.
4. Chakraborty, P., Selvaraj, S., Valsaraj, K. T., Roy, P. D., Chowdhury, A., Science of the Total Environment, 621 (2018) 930–938.
5. Tripathy, S. K., Sahoo, S. K., Sahu, S. N., Minerals Engineering, 76 (2015) 106–114.

Egg Shell Mediated Ni_5P_4/Polypyrrole Electrocatalyst for Sustainable Water Splitting

Nasrin Banu G, Bernaurdshaw Neppolian*

Energy and environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering and technology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, 603203, India.

***Corresponding author e-mail:** neppolib@srmist.edu.in

ABSTRACT

A systematically crafted synthesis methodology of hydrothermal reaction followed by oxidative polymerization was implemented to fabricate nickel phosphide (Ni_5P_4) particles intricately deposited onto eggshell powder (ES). This process strived to prevent agglomeration of Ni_5P_4 particles and was further reinforced with a polypyrrole (PPy) matrix, resulting in the formation of an integrated composite material known as Ni_5P_4@ES/PPy. This harmonious fusion of Ni_5P_4 particles with the ES and PPy matrix synergistically enhances the catalytic efficiency of the composite material, particularly in expediting the water-splitting process. The resultant Ni_5P_4@ES/PPy composite exhibits remarkable performance for both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) in 1 M KOH solution. Furthermore, the as prepared catalyst delivers exceptional performance, promoting overall water splitting at low cell voltage of 1.52 V to achieve a current density of 10 mA/cm^2. This achievement outperforms the benchmark system Pt-C/NF||RuO_2/NF, which typically demand a higher voltage of 1.60 V.

References:

1. S. Anantharaj, M. O. Valappil, K. Karthick, V. K. Pillai, S. Alwarappan, and S. Kundu, Catal. Sci. Technol., 9 (2019) 223.
2. X. Bi, J. Xu, W. Zhang, D. Tang, K. Zhang, S. Xin, and Z. Zhao, ChemistrySelect, 6 (2021) 9513.

Experimental and Computational Analysis of PCM Assisted Cooling for Solar Collectors

G. Om Prakash, M. Bala Chennaiah, M Sumalatha, T. Akshai, P. Satish

Department of Mechanical Engineering, Siddhartha Academy of Higher Education (Deemed to be University), VR Siddhartha School of Engineering, Vijayawada, India-520007.

***Corresponding author e-mail:** chennai303.mech@vrsiddhartha.ac.in

ABSTRACT

The efficiency and longevity of photovoltaic (PV) solar panels are greatly influenced by working temperature, since high heat lowers energy conversion efficiency and accelerates material degradation. This study focuses on enhancing the thermal management of PV panels by integrating phase change material (PCM), namely paraffin wax, which can take up and retain surplus heat during phase change and give it out during cooling periods.

An experimental setup was designed to study the thermal and electrical performance of a PCM-incorporated PV system under actual outdoor conditions. Temperature distribution, power generation, and efficiency were measured and compared with a traditional PV panel to assess the cooling effectiveness of the PCM layer. Supplementing the experimental efforts, a computational analysis was conducted utilizing ANSYS Fluent to simulate the heat transfer behaviour within the PCM and PV structure. Radiation boundary conditions were imposed on the upper surface to simulate solar heating, and parameters like temperature distribution and fraction of melt were examined to investigate the behaviour of PCM during charging and discharging processes. The findings show that the integration of paraffin wax consistently reduces the peak operating temperature of the PV panel, encourages consistent heat distribution, and enhances efficiency. The analysis of melt fraction verified successful phase change and latent heat uptake during peak irradiance times. Therefore, the passive cooling system using PCM improves panel reliability and extends operational duration. The integrated experimental and computational study verifies the applicability of paraffin wax as a cheap, effective, and renewable thermal control material for photovoltaic applications.

References:

1. A. Hasan, S. J. McCormack, M. J. Huang, and B. Norton, Sol. Energy, 84 (2010) 1601.
2. M. A. Kareem and K. S. Reddy, Renew. Energy, 119 (2018) 91.
3. S. Rajput and S. C. Kaushik, (2017).

Synthesis and Characterization of Transition Metal (M = Co, Cu, Ni, Zn) Doped $SrTiO_3$ for Enhanced Photocatalytic Hydrogen Evolution

Umashankar S[1], Siva Chidambaram [1]*

[1]*Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** sivac@srmist.edu.in

ABSTRACT

The development of efficient and stable photocatalysts for solar-driven hydrogen evolution is critical for sustainable energy production. Strontium titanate $SrTiO_3$, a classic perovskite, is a promising candidate due to its excellent chemical stability and suitable band edge positions for water splitting. However, its large bandgap (~3.2 eV) limits its activity primarily to the ultraviolet region. In this study, we report the synthesis and characterization of $SrTiO_3$ doped with 5% concentrations of transition metals, specifically Cobalt (Co), Copper (Cu), Nickel (Ni), Zinc (Zn), and, to enhance its visible-light response and photocatalytic efficiency. The resulting nano cubic morphology and phase purity were confirmed through X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM), Fourier-Transform Infrared Spectroscopy (FTIR) and X-ray Photoelectron Spectroscopy (XPS) verified the successful lattice integration and oxidation states of the dopants. UV-Vis Diffuse Reflectance Spectroscopy (DRS) revealed a significant redshift in the absorption spectra, indicating modified band states. The photocatalytic performance across all samples underwent quantification via Gas Chromatography (GC). Doping with 5% transition metals effectively enhanced H_2 evolution rates compared to pristine $SrTiO_3$. These results indicated that the metallic dopants acted as sites for charge trapping, thereby reducing recombination and facilitating proton reduction. This work demonstrated that hybridizing $SrTiO_3$ with transition metal dopants provided a strategic avenue to engineer high-performance photocatalytic systems for sustainable energy applications.

Keywords: $SrTiO_3$; transition metal doping; Gas Chromatography; Hydrogen Evolution Reaction; photocatalysis.

References:

1. M. Lamhani, Z. Chchiyai, and A. Hasnaoui, Inorg. Chem., 62 (2023)
2. K. Kaiya, Y. Ueki, H. Kawamoto, and A. Kudo, J. Mater. Chem. A, 12 (2024)

EN-040

Deciphering the Contribution of Quantum and Faradaic Capacitance in Er_2O_3 Decorated MXene Hybrid Composites for Supercapacitor Electrodes

Yeshwanth H Reddy[1], Ambika M R[1]*, Subramanian K R V[2], Hemalatha Krishna Naik[3], Basavaraja B M[3], Srilakshmi B P[1], Nagaiah N[4]

[1]*Department of Physics, M S Ramaiah Institute of Technology, Bengaluru-560054, India*

[2]*Department of Mechanical Engineering, M S Ramaiah Institute of Technology, Bengaluru-560054, India*

[3]*Department of Science & Humanities, PES University, Bengaluru-560085, India*

[4]*Department of Physics, Bangalore University, JB Campus, Bengaluru-560056, India*

***Corresponding author email ID:** ambikamr@msrit.edu

ABSTRACT

MXenes, a novel class of 2D transition metal nitrides and/or carbides, have sparked intense scientific concern owing to their unique properties which make them ideal candidates for standalone electrode materials but also allow seamless integration with other functional compounds to form high-performance composites. In this study, a hybrid material was designed by coupling Ti_3C_2 MXene with Erbium oxide (Er_2O_3), a rare-earth metal oxide known for its redox-active behavior. The layered Ti_3C_2 sheets were synthesized via selective chemical etching, followed by hydrothermal technique for composite formation with Er_2O_3. In the three-electrode setup, pristine MXene demonstrated a specific capacitance of 476.19 F g^{-1} with 77.4% retention. Upon integrating Er_2O_3, the hybrid system showcased a remarkable boost in electrochemical performance, reaching an outstanding capacitance of 2758 F g^{-1} at 1 A g^{-1} with 85.99% stability. This substantial improvement stems from the synergistic harmony between MXene's high conductivity and Er_2O_3 pseudocapacitive contribution, which collectively enhance charge storage and cycling durability. In addition, asymmetric supercapacitor ended up with a magnificent specific capacitance of 1870 F g^{-1} at 0.5 A g^{-1} of current density, delivering an energy density of 113.13 Wh kg^{-1} upholding the power density to 659.03 W kg^{-1}. Moreover, Quantum capacitance was assessed from reported DOS and DFT data to support theoretical charge storage insights. The individual benefactions of double layer and redox capacitance were further quantified via power-law analysis and Trasatti's method. This synergy opens up new avenues for tailoring MXene hybrids in integrating efficient and durable energy storage devices tailored for next-generation technologies.

Keywords: MXene, MXene/Er_2O_3, Energy storage, Supercapacitor.

EN-041

Sustainable Marine Algae-Derived Carbon/MXene/$HoFeO_3$ Nanohybrid for Photocatalytic Degradation of Persistent Agrochemical Pollutants in Water

Aswini Ravi[1], Ganesh Kumar V[1]*

[1]*Centre for Ocean Research, Sathyabama Institute of Science and Technology, Chennai-600119, India*

***Corresponding author e-mail:** ganeshkumar@sathyabama.ac.in

ABSTRACT

The persistent presence of agrochemical pesticides in water poses a significant environmental challenge due to their chemical stability, toxicity, and resistance to conventional treatment methods. Herein, a sustainable ternary nanohybrid photocatalyst comprising marine algae-derived nitrogen-doped porous carbon, $Ti3C2T_x$ MXene, and holmium orthoferrite (HoFeO3) is developed for efficient solar-driven degradation of persistent pesticide contaminants. The bio-derived carbon is obtained via controlled pyrolysis of marine biomass, MXene is prepared through selective etching and delamination of the corresponding MAX phase, and HoFeO3 is synthesised using a low-temperature solid-state route. The nanohybrid is assembled through in situ growth to ensure strong interfacial coupling and efficient charge transfer. Comprehensive structural, morphological, and surface characterisation using XRD, FTIR, Raman, SEM–EDX, TEM, XPS, UV–Vis DRS, and BET analyses confirms successful hybrid formation and favourable electronic interactions. The nanohybrid exhibits enhanced visible-light absorption and suppressed charge recombination, enabling rapid and efficient photocatalytic degradation of chlorpyrifos under simulated solar irradiation, with high mineralisation efficiency. Mechanistic studies employing LC-MS, TOC, and ESR analyses indicate that hydroxyl and superoxide radicals dominate the degradation pathway. Furthermore, the photocatalyst demonstrates excellent structural stability and reusability over multiple cycles. This study offers a promising solution for sustainable water purification and environmental remediation.

References:

1. A. Borzyszkowska, A. Fiszka, A. Sulowska, P. Czaja, A. Bielicka-Giełdoń, I. Zekker, and A. Zielińska-Jurek, RSC Adv., 13 (2023) 25529.
2. S. Chen, S.-Z. Zhang, and H. Jiang, ACS ES&T Water, 4 (2024) 531.
3. A. Grzegórska, I. Wysocka, P. Głuchowski, J. Ryl, J. Karczewski, and A. Zielińska-Jurek, Chemosphere, 308 (2022) 136191.
4. Z. Wu, Y. Liang, X. Yuan, D. Zou, J. Fang, L. Jiang, H. Yang, and Z. Xiao, Chem. Eng. J., 394 (2020) 124921.
5. H. Wang, W. Li, D. Song, X. Wang, W. Wang, X. Xing, G. Li, J. Wang, and F. Gao, Chem. Eng. J., (2025) 164853.

EN-042

Preparation and Characterisation of the Nano-Enhanced Phase Change Material for Battery Thermal Management Applications

G.V. N. Trivedi[1], R. Parameshwaran[2], Veerakumar Chinnasamy[1]*

[1]*Centre for Interdisciplinary Research, SRM University AP, Andhra Pradesh, India, 522240*

[2]*Department of Mechanical Engineering, Birla Institute of Technology and Science, Pilani, Hyderabad Campus, Telangana, India,500078*

***Corresponding author e-mail:** veerakumar.c@srmap.edu.in

ABSTRACT

Phase change materials (PCMs) have the ability to store and release thermal energy by undergoing a phase change from solid to liquid or vice versa. PCMs lack thermal conductivity and exhibit supercooling that hinders their applications in engineering systems. Nano-enhanced PCMs overcome these challenges and can be utilised for battery thermal management applications [1]. This study focuses on the preparation and characterisation of the iron oxide nanoparticle based tetradecanol PCM for battery thermal management applications. The iron oxide nanoparticles were synthesised from iron (II) sulphate heptahydrate through a co-precipitation method. The synthesised nanoparticles were embedded in tetradecanol for the preparation of Nano-PCM and characterised using FESEM, EDS, XRD, DSC, TGA, and a thermal conductivity analyser. The differential scanning calorimetry test results, as shown in Fig. 1, illustrate that the phase change material has a latent heat of 230 J/g, with an onset melting temperature of 35.9 °C and an onset freezing point of 36.3 °C. The thermal stability studies show that the PCM has an onset decomposition temperature of around 170 °C. Furthermore, the Incorporation of iron oxide nanomaterials into tetradecanol, as shown, improved both thermal conductivity and thermal properties of the PCM. In total, enhanced thermal properties and high thermal energy storage potential make the Nano-PCM a potential candidate for battery thermal management applications

Keywords: Phase change materials, iron oxide nanoparticles, differential scanning calorimetry

References:

1. Tang, J. Pan, D. Xia, T. Cai, Q. Zhang, G.A. Tenkolu, Y. Jin, Int. J. Heat Mass Transf. 224 (2024) 125389.

EN-043

One-Step Synthesis of a Dual Metal Chalcogendies Heterojunction Encapsulated in Carbon Nanotubes for High-Performance Supercapacitors

Dhanasekaran Vikraman[1], Anandhavelu Sanmugam[2], Arumugam Shanmugam[2], Zulfqar Ali Sheikh[3,4], Sajjad Hussain[3,4], K. Karuppasamy[5,6], Zafar Abbas Syed[3,4], JongwanJung[3,4], AkramAlfantazi[5,6], Hyun-Seok Kim[1]*

[1]*Division of Electronics and Electrical Engineering, Dongguk University-Seoul, Seoul 04620, Republic of Korea.*

[2]*Department of Applied Chemistry, Sri Venkateswara College of Engineering, Pennalur, Sriperumbudur 602117, India.*

[3]*Department of Nanotechnology and Advanced Materials Engineering, Sejong University, Seoul 05006, Republic of Korea.*

[4]*Hybrid Materials Center (HMC), Sejong University, Seoul 05006, Republic of Korea.*

[5]*Emirates Nuclear Technology Center (ENTC), Khalifa University of Science and Technology, Abu Dhabi, 127788, United Arab Emirates.*

[6]*Department of Chemical and Petroleum Engineering, Khalifa University of Science and Technology, Abu Dhabi, 127788, United Arab Emirates.*

***Corresponding author e-mail:** hyunseokk@dongguk.edu

ABSTRACT

The energy sector is on the brink of transformative change by harnessing the power of renewable sources like geothermal, solar, and wind energy. 2D transition metal dichalcogenides are emerging as promising candidates for energy storage devices due to their unique physicochemical properties. This study presents a facile one-step synthesis of carbon nanotube-encapsulated WS_2-$MoSe_2$ heterostructures (WS_2-$MoSe_2$@CNT), which serve as high-performance electrodes for supercapacitors. This hybrid architecture has been meticulously designed to tackle the inherent challenges associated with WS_2 and $MoSe_2$, particularly their susceptibility to rapid capacity decay and suboptimal rate capability. The selectively engineered attributes of the optimized WS2-$MoSe_2$@CNT electrode demonstrate an impressive specific capacitance of 828 F g^{-1} at a current density of 2 A g^{-1}, coupled with outstanding cycling stability, showcasing a remarkable 97.8% capacitance retention and 100% Coulombic efficiency after an extensive 10,000 charge/discharge cycles. For the assembled asymmetric supercapacitor device, the system achieves an energy density of 88 Wh kg^{-1} at a power density of 45,000 W kg^{-1}, with a notable 97.1% capacitance retention after prolonged cycling. This work not only underscores a potent strategy for advancing transition metal chalcogenide-based heterostructures but also highlights the critical role of concurrent defect engineering and meticulous nanostructural control in enhancing performance. The remarkable performance of the WS_2-$MoSe_2$@CNT is attributed to a synergistic interplay of several key factors including thermodynamic stability and electrochemical surface area, providing more favorable conditions for electrochemical reactions.

Synergistic Composite Engineering of 0D Halide Perovskite in Cuse Enables Ultra-Low Thermal Conductivity and High Thermoelectric Performance

C.N. Dhivya Mahalakshmi[1], K.P. Mohamed Jibri[1], J. Archana[2], M. Navaneethan[1,2]*

[1] *Nanotechnology Research Centre (NRC), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, India, 603203*

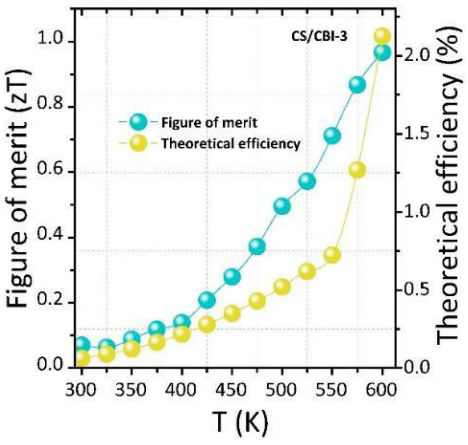
[2] *Centre of excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, India, 603203*

***Corresponding author e-mail:** m.navaneethan@gmail.com

ABSTRACT

The metal inorganic halide perovskites offer its advantages over various applications include solar cells and optoelectronics. However, its potential path in the waste heat management system still lies in its infant stage. In this work, we integrate the potential 0D metal halide perovskite $Cs_3Bi_2I_9$ as a composite material in CuSe matrix through simple chemical synthesis. The 0D perovskite characterized by its isolated $[Bi2I9]^{3-}$ units and anti-bonding states act as phonon scattering centers. The structural analysis confirms that the incorporation of Cs3Bi2I9 creates local lattice strain and bond softening there by decreasing the total thermal conductivity of 0.8 $Wm^{-1}K^{-1}$ for CS/CBI-3 at 600 K. The Debye-Callaway modeling, supported by Mathiessen's rule analysis, reveals multiple phonon scattering events such as dislocation cores, dislocation scattering (dominant below 15 THz) and point defects contribute synergistically, while Umklapp scattering is suppressed in the composites. The HR-TEM confirms dense edge dislocations and moire fringes at CS/CBI interfaces, arising from lattice mismatch. Concurrently, bonding heterogeneity reduces elastic moduli and sound velocity, promoting glass-like thermal transport. Despite a modest drop in electrical conductivity, the drastic κ_lat suppression elevates the peak figure of merit (zT) to ~0.9 at 600K for CS/CBI-3. Thus, the composite engineering strategy establishes CS/CBI composites as promising mid-temperature thermoelectric compound.

Keywords: anti bonding states, bond softening, moire fringes, glass-like thermal transport, composite engineering.



References:

1. C. N., D. M., and K. P., M. J., Appl. Phys. Lett., 126 (2025).
2. J. Li, L. Wei, Z. Ti, L. Ma, Y. Yan, G. Zhang, and P.-F. Liu, Phys. Rev. B, 108 (2023) 224302.

Design of a Carbon-Modified $ZnMn_2O_4$ Cathode for High-Performance Aqueous Zinc-ion Batteries

Nithya Chadrasekaran[1]*, Subashree Murugesan[1]

[1]*Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore – 641 004, India*

***Corresponding author e-mail:** nithyajcs@gmail.com

ABSTRACT

The development of high-performance cathode materials remains a major challenge for aqueous zinc-ion batteries (ZIBs), primarily due to their limited specific capacity, unsatisfactory rate performance, and poor cycling stability. Among various candidates, manganese-based cathode materials have attracted considerable attention owing to the natural abundance and low cost of manganese, along with the structural diversity, multiple phases, and flexible stoichiometries of manganese oxides. Nevertheless, their practical application is hindered by low intrinsic electrical conductivity and slow Zn^{2+} diffusion kinetics. In this study, a $ZnMn_2O_4$/C composite cathode is successfully synthesized to address these limitations through the integration of conductive carbon within the active material. The incorporated carbon significantly enhances electronic conductivity, promotes ion transport, and alleviates structural degradation during repeated charge–discharge cycles. Comprehensive structural and compositional characterizations confirm the formation of a well-defined composite architecture with high phase purity. Electrochemical evaluations reveal that the $ZnMn_2O_4$/C cathode exhibits markedly improved specific capacity, superior rate capability, and enhanced cycling stability compared to pristine $ZnMn_2O_4$. These results demonstrate that the $ZnMn_2O_4$/C composite is a promising cathode material for high-performance aqueous zinc-ion batteries.

Keywords: Aqueous zinc-ion batteries, $ZnMn_2O_4$/C composite, Manganese-based cathode, Carbon modification

References:

1. M. Shi, B. Wang, Y. Shen, J. Jiang, W. Zhu, Y. Su, M. Narayanasamy, S. Angaiah, C. Yan, Q. Peng, Chem. Eng. J. 399, (2020), 125627.
2. X. Gao, H. Wu, W. Li, Y. Tian, Y. Zhang, H. Wu, L. Yang, G. Zou, H. Hou, X. Ji, Small 16, (2020)1905842.

EN-046

Electrochemical Investigation of Hydrothermally Synthesized $MnMoO_4$-Co-MOF Composite for Supercapacitor Applications

Kaaviyapriya S S, Abinash Kumararaj, Pavithran Ravi, Geetha Arunachalam*

Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India

***Corresponding author mail id:** geethaa@srmist.edu.in

ABSTRACT

Manganese molybdate was synthesized using a hydrothermal technique and integrated with a cobalt-based metal-organic framework to enhance its efficacy as a supercapacitor electrode. Powder X-ray diffraction validated the effective synthesis of the composite, while Fourier-transform infrared spectroscopy and Raman studies elucidated the functional groups and vibrational properties [1]. Transmission electron microscopy confirmed crystal clarity, whereas scanning electron microscopy demonstrated a porous, interconnected morphology. X-ray photoelectron spectroscopy determined the oxidation states of the elements. Electrochemical investigations employing cyclic voltammetry, galvanostatic charge-discharge, electrochemical impedance spectroscopy, and cycling stability assessments demonstrated hybrid capacitance characteristics with advantageous charge storage and enhanced ion transport. The electrode maintained substantial capacitance and superior Coulombic efficiency after five thousand cycles, suggesting that the manganese molybdate–cobalt metal–organic framework composite is a viable material for high-performance supercapacitor applications.

Keywords: Manganese molybdate; Cobalt metal–organic framework; Hydrothermal synthesis; Hybrid capacitance; Supercapacitor.

References:

1. T. A. Sundaram, K. Kowsuki, R. Nirmala, Y. H. Ra, and R. Navamathavan, J. Alloys Compd., 1039 (2025) 183218.

Compositing NiFe Layered Double Hydroxide (LDH)/MXene for electrocatalytic water splitting application

Atchaya K, Tamilselvan Appadurai*

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail:** tamilsea3@srmist.edu.in

ABSTRACT

Owing to the escalating energy crisis and economic concerns, sustainable and carbon-free hydrogen production via water splitting has attracted considerable attention as a promising energy conversion technology. Water splitting involves two critical electrochemical half-reactions: the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode, respectively. Efficiently driving these reactions requires the development of an electrocatalyst with high reactivity. In developing water-splitting devices, designing efficient semiconductor electrodes remains a major challenge. In these contexts, layered double hydroxides (brucite- like structure $M_{1-x}^{2+}M_x^{3+}(OH)_2{}^{q+}\,A_{\frac{q}{n}}^{n-}.yH_2O$ where M^{2+}= divalent; M^{3+}= trivalent; OH -= Hydroxide ions and A= interlayer anions) serve as the outstanding candidate for water splitting. These unique layered structures, compositional flexibility, and abundant active sites facilitate changes in oxidation state, directly linked to the catalysts. However, they suffer from poor electrical conductivity. Therefore, significant efforts focus on structural engineering, which led us to the incorporation of MXene ($M_{n+1}X_nT_x$(n=1-3), M=Ti, X= Carbon and T= terminal functional groups)[2], a highly conductive 2D material, to improve the catalytic performance. In this work, we have synthesized NiFe LDH/MXene compounds with different ratios and studied their crystal structure by PXRD. Then, the composite materials have been subjected to electrochemical studies, such as CV, LSV and Tafel by coating active materials on Ni foam electrodes. Further analysis in electrochemical studies such as two-electrode system, will be discussed in detail.

References:

1. L. Peng et al., Angew. Chem. Int. Ed., 60 (2021) 24612.
2. D. S. Abraham, M. Vinoba, and M. Bhagiyalakshmi, ACS Appl. Nano Mater., 7 (2024) 5791.

EN-048

SnO_2 Quantum Dots: A New Frontier in Ultrafast Photocatalysis

Pawan Chetri*

Department of Physics, North Eastern Regional Institute of Science and Technology, (NERIST) Nirjuli, Arunachal Pradesh, India, 791109

***Corresponding author e-mail:** chetripawan2009@gmail.com

ABSTRACT

Enhancing the efficiency of pure metal oxide photocatalysts for the removal of hazardous pollutants from the industrial wastewater is a significant challenge in contemporary research. In this study, we have developed an ultrafast and cost-effective pure SnO_2 quantum dot photocatalyst through modifications introduced during the annealing process synthesized via a hydrothermal-assisted, simple sol-gel technique. This SnO_2 quantum dot photocatalyst is employed for the degradation of model pollutants commonly released into natural water bodies by textile, agricultural, and pharmaceutical industries under natural sunlight. Experimental results demonstrate the formation of ultra-small SnO_2 nanoparticles (NPs) with enhanced optical and structural properties compared to conventional SnO_2 NPs. Sunlight-driven photocatalytic tests reveal that the SnO_2 quantum dot photocatalyst efficiently degrades 97.48%, 62.90%, and 57.69% of methyl orange, 2,4-D, and levofloxacin, respectively, within just one minute of sunlight exposure, outperforming standard SnO2 NPs. Furthermore, in-situ radical capture experiment indicates that superoxide radicals are the primary reactive species responsible for the photocatalytic degradation of methyl orange. This study highlights the potential of pure SnO_2 photocatalysts for the effective treatment of wastewater contaminated by various industrial pollutants.

Keywords: SnO_2, Photocatalysis, Dye, 2,4-D, Levofloxacin, Sunlight.

Design and Synthesis of Phenothiazine based Materials for Dye-Sensitized Solar Cells

G. R. Divya Praba* and S. Sambathkumar

PG and Research Department of Chemistry, Vivekanandha College of Arts and Sciences for Women (Autonomous), Elayampalayam, Namakkal 637 205, Tamil Nadu, India

***Corresponding author e-mail:** sambathtacw@gmail.com

ABSTRACT

Over the past decade, dye sensitized solar cells (DSC's) based on nanocrystalline mesoporous metal oxides (typically TiO_2) have been intensively studied and developed as a promising, low-cost alternative to conventional silicon photovoltaic devices. As a critical component in DSC's, the sensitizer plays a vital role in the light harvesting efficiency providing electron injection in to the conduction band of the semiconductor upon light excitation and they usually possess the structure of Donor - π Bridge -Acceptor (D- π-A). In the present case, special consideration has given to the design of the molecular structure to determine its correlation to the performance of DSC's, a series of novel organic materials, whose structures has slightly different from one to another has been synthesized based on phenothiazine with an additional donor and characterized with various spectroscopic techniques. The Optical and electrochemical properties of the synthesized materials were analyzed systematically. In order to understand the geometrical properties associated with the synthesized materials, theoretical studies have been performed. This contribution brings further credit to these molecular designs as efficient sensitizers for DSCs, en route for a cheap and less toxic substitute to ruthenium based sensitizers and silicon based photovoltaics as potential eco-friendly energy candidates for the development of sustainable materials and technologies.

Keywords: Dye sensitized solar cells, phenothiazine, electron injection, sensitizer, sustainable materials

Samarium-doped Ni-Co Ferrite based Systems for Improved Magnetic and Electrochemical Properties

B. S. Maharnavar[1,2], A Yengantiwar[1]*, R. J. Deokate[3]*

[1]*Department of Physics, Fergusson College (Autonomous), Savitribai Phule Pune University, Pune, PIN 411004, India*

[2]*Department of Physics, Dada Patil Mahavidyalaya, Karjat, Dist-Ahmednagar, MH, India*

[3]*Department of Physics, Vidya Pratishthan's Arts Science and Commerce College Baramati (MS), India.*

***Corresponding author e-mail:** rjdeokate@gmail.com

ABSTRACT

Samarium doped Ni-Co ferrites ($Ni_xCo_{1-x}Sm_yFe_{2-y}$) were synthesized using sol-gel auto-combustion technique with Sm3+ doping concentrations varying as y = 0.025, 0.050, 0.075, 0.100 and 0.125 with simultaneously variation with Ni-Co as x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0. The prepared nanomaterials were examined using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Field Emission Scanning electron microscopy (FE-SEM), and vibrating sample magnetometer (VSM). The XRD analysis verified the pure spinel phase of all samples with no impurity peak. The FTIR analysis for spinel molecules formation identified two frequency bands at the octa and tetrahedral sites. The FE-SEM analysis confirmed the shape, size and distribution of prepared nanoparticles. (what changed size or remained constant. The different dielectric properties were analysed with a frequency necessary range and the impact of doping was also studied simultaneously. Magnetic properties of prepared materials were investigated at room using the VSM. Electrochemical studies write the obtained values Electrochemical Impedance studies (EIS) revealed distinct pseudocapacitive behaviour, low internal resistance, and enhanced specific capacitance for Sm- doped Ni-Co Ferrite. The enhanced performance arises from synergistic effects of mixed transition metal ions, rare-earth substitution, and optimized nanostructure, highlighting their potential for supercapacitor applications.

Keywords: Nanomaterial, ferrite, supercapacitor, magnetic study etc.

Ni-Doped TiO_2/rGO Nanocomposites as High-Performance Electrode Materials for Supercapacitor Applications

K.P Subadinesh[1], S. Mohammed Hanif[1], Naveenkumar N[1], D. V. Sridevi[2] and V. Ramesh[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

[2]*Centre for Materials Research, Centre for Advanced Materials Research, Department of Chemistry, Rajalakshmi Institute of Technology, Kuthambakkam, Thiruvalur, Tamil Nadu, India, 600124*

***Corresponding author e-mail:** rameshv@srmist.edu.in

ABSTRACT

TiO_2/Ni/rGO nanocomposites with nickel doping concentrations of 1, 3, 5, 7, and 9% were synthesized and evaluated as electrode materials for supercapacitor applications. The composite integrates the structural stability of TiO_2, the redox activity of Ni species, and the high electrical conductivity of reduced graphene oxide (rGO), resulting in enhanced charge storage behavior. X-ray diffraction confirmed the presence of the crystalline TiO_2 phase with successful Ni incorporation. Scanning and transmission electron microscopy revealed uniformly dispersed nanoparticles with average particle sizes of ~20-35 nm, well anchored on crumpled rGO sheets, forming a porous and interconnected architecture that facilitates efficient ion diffusion and rapid electron transport. Electrochemical measurements conducted in an alkaline electrolyte demonstrated that Ni doping significantly improves the capacitive performance of TiO_2/rGO electrodes. The optimally doped TiO_2/Ni/rGO electrode delivered a high specific capacitance of ~680 F g^{-1} at 1 A g^{-1}, with good rate capability, retaining ~85% capacitance at 10 A g^{-1}. The assembled supercapacitor achieved an energy density of ~38 Wh kg^{-1} at a power density of ~800 W kg^{-1} and maintained ~24 Wh kg^{-1} at ~5000 W kg^{-1}. Additionally, the electrode exhibited excellent cycling stability with over 92% capacitance retention after 5000 charge–discharge cycles. These results confirm that Ni-doped TiO_2/rGO nanocomposites are promising candidates for high-performance and durable supercapacitor applications.

Keywords: TiO_2/Ni/rGO nanocomposites, Energy storage, Supercapacitor, Specific capacitance, Electrolytes, and Electrochemical measurements

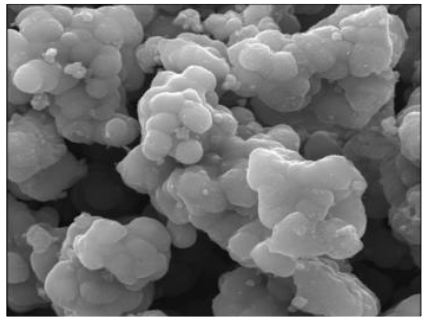


Fig. Depicts the SEM image of TiO_2/Ni Nanoparticles

References:

1. S. H. Samson, V. A. F. Raj, M. V. A., and J. M., Mater. Today Sustain., 28 (2024) 100972.

EN-052

Synthesis of Substituted Carbazole based Materials for Dye Sensitized Solar Cells

G. Roseline Stephina* and S. Sambathkumar

PG and Research Department of Chemistry, Vivekanandha College of Arts and Sciences for Women (Autonomous), Elayampalayam, Namakkal 637 205, Tamil Nadu, India

***Corresponding author e-mail:** sambathtacw@gmail.com

ABSTRACT

Over the past decade, dye sensitized solar cells (DSC's) based on nanocrystalline mesoporous metal oxides (typically TiO_2) have been intensively studied and developed as a promising, low-cost alternative to conventional silicon photovoltaic devices. As a critical component in DSC's, the sensitizer plays a vital role in the light harvesting efficiency providing electron injection in to the conduction band of the semiconductor upon light excitation and they usually possess the structure of Donor - π Bridge -Acceptor (D- π-A). In the present case, special consideration has given to the design of the molecular structure to determine its correlation to the performance of DSC's, a series of novel organic materials, whose structures has slightly different from one to another has been synthesized based on carbazole with an additional donor and characterized with various spectroscopic techniques. The Optical and electrochemical properties of the synthesized materials were analyzed systematically. In order to understand the geometrical properties associated with the synthesized materials, theoretical studies have been performed. This contribution brings further credit to these molecular designs as efficient sensitizers for DSCs, en route for a cheap and less toxic substitute to ruthenium based sensitizers and silicon based photovoltaics as potential eco-friendly energy candidates for the development of sustainable materials and technologies.

Keywords: Dye sensitized solar cells, carbazole, electron injection, sensitizer, sustainable materials

Facile Hydrothermal Synthesis of Bi_2O_3/MoS_2 (1:1) Heterostructure Electrodes with High Capacitance and Long-Term Stability for Supercapacitors

Naveenkumar N[1], Nivin T S[1], Sridevi D V[2], Premanand G[1], Karthigeyan Annamalai[1], and Ramesh V[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

[2]*Centre for Materials Research, Centre for Advanced Materials Research, Department of Chemistry, Rajalakshmi Institute of Technology, Kuthambakkam, Thiruvalur, Tamil Nadu, India, 600124*

***Corresponding author e-mail:** rameshv@srmist.edu.in

ABSTRACT

Bismuth oxide (Bi_2O_3)/molybdenum disulfide (MoS_2) composites with a one-to-one mass ratio were synthesized via a facile hydrothermal method to develop high-performance supercapacitor electrodes. The optimized Bi_2O_3/MoS_2 heterostructure features a porous nanosheet architecture with abundant active sites and intimate interfacial contact, thereby facilitating efficient ion diffusion and rapid electron transport. Morphological and structural analyses by X-ray diffraction, scanning electron microscopy, and transmission electron microscopy confirm the formation of a uniform Bi_2O_3/MoS_2 hybrid. Electrochemical measurements in 1 M KOH reveal a high specific capacitance of 630.52 F g^{-1} at 1 A g^{-1} and an excellent rate of capacitance, retaining 92% at 10 A g^{-1}. Furthermore, the device maintains around 92% of its initial capacitance after 2500 cycles with nearly 100% coulombic efficiency, highlighting its outstanding cycling stability. The synergistic combination of redox-active Bi_2O_3 and conductive MoS_2 layers enhances charge storage kinetics and structural robustness. The facile synthesis, superior capacitive performance, and long-term stability of the Bi_2O_3/MoS_2 (1:1) composite underscore its potential for scalable, durable energy storage applications. This study offers new insights into designing binary metal oxide/sulfide electrodes with tailored compositions for next-generation electrochemical energy storage devices that exhibit high efficiency.

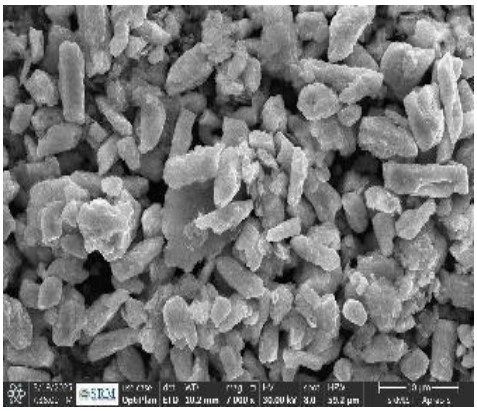


Fig. HR-SEM Images of Bi_2O_3/MoS_2 nanocomposite synthesized by the hydrothermal route.

Keywords: Bi_2O_3/MoS_2 nanocomposite, Hydrothermal synthesis, Supercapacitor electrodes, Specific capacitance, and Cycling stability

Reference:

1. M. Ismail, K. B., M. Arun Kumar, R. Jayavel, M. Arivanandhan, and M. A. Mohamed Ismail, RSC Adv., 13 (2023) 24272–24285.

Cr-Doped $NiCo_2O_4$ Nanoparticles Synthesized by a Hydrothermal Route for High-Performance Supercapacitor Applications

Mohammed Hanif S[1], Subadinesh K P[1], Naveenkumar N[1], Sridevi D V[2] and Ramesh V[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

[2]*Centre for Materials Research, Centre for Advanced Materials Research, Department of Chemistry, Rajalakshmi Institute of Technology, Kuthambakkam, Thiruvalur, Tamil Nadu, India, 600124*

***Corresponding author e-mail:** rameshv@srmist.edu.in

ABSTRACT

Cr-doped $NiCo_2O_4$ nanoparticles with chromium concentrations of 1, 2, 3, 4, and 5% were synthesized via a hydrothermal method at 400 °C for 3-hrs, followed by annealing at 100 °C for 10 h, and investigated as electrode materials for supercapacitor applications. X-ray diffraction confirmed the formation of phase-pure spinel $NiCo_2O_4$ with successful Cr incorporation. Scanning and transmission electron microscopy revealed uniformly distributed nanoparticles with average particle sizes in the range of 25-30 nm, forming porous and interconnected clusters that provide abundant electroactive sites and facilitate efficient ion diffusion and electron transport. Electrochemical measurements performed in an alkaline electrolyte demonstrated that Cr doping significantly enhances the capacitive performance of $NiCo_2O_4$ electrodes. The optimally doped Cr–$NiCo_2O_4$ sample exhibited a high specific capacitance of approximately 950-1100 F g^{-1} at 1 Ag^{-1}, with good rate capability and reduced charge-transfer resistance compared to pristine $NiCo_2O_4$. The assembled supercapacitor delivered an energy density of about 40 Wh kg^{-1} at a power density of ~1 kW kg^{-1} and maintained ~25 Wh kg^{-1} at ~5 kW kg^{-1}. In addition, the electrode showed excellent cycling stability with over 90% capacitance retention after 5000 charge–discharge cycles. These results demonstrate that Cr-doped $NiCo_2O_4$ nanoparticles are promising electrode materials for high-performance supercapacitor energy storage systems.

Keywords: $NiCo_2O_4$ nanoparticles, Cr doping, Hydrothermal synthesis, Supercapacitor, Energy density and Power density.

References:

1. R. Ahmed and G. Nabi, J. Energy Storage, 33 (2021) 102115.

EN-055

Thermal Reliability of Graphene-Based Nanofluid Heat Pipes for Next – Generation Electronic Cooling

Aruna Veerasamy[1]*, Kanimozhi Balakrishnan[1]

[1]*Centre of Excellence for Additive Manufacturing, Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India, 600119.*

[1]*Department of Mechatronics, Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India, 600119.*

***Corresponding author e-mail:** arunaveer@gmail.com, aruna.irc@sathyabama.ac.in

ABSTRACT

The high heat generated during operation reduces the lifespan or deteriorates performance for most electronic devices and gadgets. One of the common and effective passive cooling methods to get around this issue involves the use of heat pipes. This study, therefore, explores how heat pipes efficiently transport heat from heat-generating components with the aim of prolonging the life of an electronic device. Graphene nanofluid was used as the working fluid in an attempt to enhance the thermal properties of the working fluid. Besides the effects brought about by changing heat inputs under one certain filling ratio, the performance of the heat pipe was investigated through the use of inclination angles of 20°, 40°, 60°, and 80°. Some of the significant parameters considered are thermal resistance, the overall thermal performance, and temperature distribution between the condenser and evaporator. The optimal inclination angles and increased heat input that result from such factors tend to result in an enhanced thermal performance, characterized by reduced thermal resistance together with a reduced temperature difference between the condenser and the evaporator. These results shown indicate that HPs can successfully be employed in electronic systems in order to reduce excessive heating. HPs are often suggested for electronic heat management applications due to their low maintenance and passive operating conditions.

EN-056

Room-Temperature Magnetic Response in Co-Doped $Na_{0.5}Bi_{0.5}TiO_3$: A Lead-Free Perovskite System

Nilesh Kumar Prasad[1], Satya Prakash pati[1]

[1] *North -Eastern Hill University, Shillong, Meghalaya*

***Corresponding author e-mail:** nileshprasad700@gmail.com

ABSTRACT

Cobalt-doped sodium bismuth titanate, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT), ceramics with compositions $Na_{0.5}Bi_{0.5}TiCo_xO_3$ (x = 0.02-0.10) were synthesized via the sol-gel method. X-ray diffraction analysis combined with Rietveld refinement confirmed a single-phase perovskite structure with tetragonal symmetry (space group P4mm) for both undoped and Co-doped samples, indicating structural stability upon doping. The refined lattice parameters (a = 5.173 Å and c = 3.9073 Å) were slightly larger than standard values, suggesting lattice distortion due to Co incorporation [1]. Crystallite size and microstrain were estimated using the Debye–Scherrer and Williamson–Hall methods, revealing nanoscale crystallinity. FTIR spectra exhibited characteristic bands at ~633 and 834 cm, confirming Ti-O vibrational modes of the perovskite lattice. Thermogravimetric analysis showed good thermal stability with weight loss below 4%. Magnetic measurements at 300 K revealed predominantly paramagnetic behavior with weak ferromagnetic characteristics, exhibiting a remanent magnetization of 0.001247 emu/gm and coercivity of 1.68 Oe [2]. The Curie temperature was observed near room temperature, indicating potential for lead-free multifunctional applications.

References:

1. Fan, Pengyuan, et al. Journal of Materiomics 7.3 (2021): 508-544.
2. Cao, W. P., et al. Ceramics International 40.7 (2014): 9273-9278.

Hydrothermal Engineering of Ni–Co Layered Double Hydroxides for High-Performance Supercapacitor Electrodes

Amol R. Pardeshi, Mahesh S. Bhadane*

Department of Physics, Rayat Shikshan Sanstha's Dada Patil Mahavidyalaya Karjat, Dist-Ahilyanagar, MH, INDIA-414402

***Corresponding author e-mail:** mbhadane24@gmail.com

ABSTRACT

Nickel–cobalt layered double hydroxide (NiCo-LDH was synthesized via a hydrothermal route and comprehensively characterized for supercapacitor applications. X-ray diffraction analysis confirmed the formation of a well-crystallized hexagonal LDH phase with prominent reflections indexed to the (003), (006), (012), (015), and (113) planes and an interlayer spacing of ~9.5 Å. The average crystallite size calculated from the (003) plane was approximately 2–3 nm, indicating nanoscale crystallinity. FTIR spectroscopy revealed characteristic O–H stretching, interlayer water vibrations, and metal–oxygen bonding, while XPS confirmed the coexistence of mixed Ni^{2+}/Ni^{3+} and Co^{2+}/Co^{3+} oxidation states. Scanning electron microscopy showed a porous, interconnected nanosheet morphology favorable for ion transport. Electrochemical evaluation demonstrated battery-type behavior with a specific capacity of ~1100–1300 F g^{-1} at a current density of 2 A g^{-1}, along with good rate capability and stable cycling performance, retaining over ~90% capacitance at higher current densities. The enhanced electrochemical performance is attributed to the layered structure, mixed-valence redox activity, and porous nanosheet architecture, highlighting NiCo-LDH as a promising electrode material for advanced energy storage devices.

Keyword: Ni-Co LDH; Hydrothermal synthesis; Nanosheet architecture; Mixed oxidation states; Supercapacitor electrode.

EN-058

Synthesis of Flexible Carbon-Based Electrodes for Supercapacitors through the Resistive Heating Method

Vijayan M[1], Ramesh R[1]*

[1]*Periyar University, Periyar Palkalai Nagar, Salem, India, 636011*

***Corresponding author e-mail:** rameshphys@gmail.com

ABSTRACT

Carbon-based materials are widely used as electrode materials for energy storage devices due to their high electrical conductivity, large surface area, and mechanical flexibility. However, conventional methods for synthesizing nanocarbon materials have several limitations, including poor scalability, complex processing steps, and long processing time. To address these issues, a simple and efficient resistive heating method is employed. In this method, nanocarbon materials are prepared under various pulse-width modulation (PWM) conditions and power levels. The structural and morphological characteristics of the synthesized materials are investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy, confirming the formation of conductive nanocarbon frameworks with favourable crystallinity and controlled defect characteristics. Furthermore, the electrochemical performance of the prepared flexible nanocarbon electrodes was evaluated, demonstrating efficient charge storage behaviour along with long-term cyclic stability.

Keywords: Nanocarbon; Supercapacitor; Resistive Heating

References:

1. Zhu, Sheng, et al. ACS Materials Letters 4.10 (2022): 1863-1871.
2. Yuan, Jiahui, et al. Journal of Materials Chemistry C (2024).
3. Huang, Pengfei, et al Journal of Environmental Science and Health, Part A 57.1 (2022): 33-44.
4. Raj, Rishi et al. J. European Ceramic Society (2012), 32.10, 2293-2301.
5. Wyss, Kevin M., et al. Carbon 174 (2021): 430-438.

Metal-Free g-C_3N_4/Nitrogen-Doped Carbon Dots Nanocomposite for Enhanced Photocatalytic Hydrogen Generation

Anbarasan E [1], Ramesh R[1]*

[1]*Department of Physics, Periyar University, Salem-636 011, Tamilnadu, India.*

***Corresponding author e-mail:** rameshphys@gmail.com

ABSTRACT

Graphitic carbon nitride g-C_3N_4 (GCN) loaded with nitrogen-doped carbon dots (NCDs) has recently emerged as a promising metal-free photocatalyst for sustainable hydrogen (H2) production under visible light irradiation. Although such hybrid systems have demonstrated significantly enhanced photocatalytic performance. In this work, N-doped carbon dots were synthesized and successfully hybridized with GCN to construct a GCN/NCDs nanocomposite photocatalyst, aiming to elucidate the synergistic effects between the two components. Comprehensive characterization results (XRD, SEM and TEM) confirmed the effective incorporation of NCDs into the GCN. The GCN/NCDs nanocomposites exhibited enhanced visible-light absorption compared to pristine GCN, which can be attributed to the light-harvesting capability of the NCDs. Moreover, transient photocurrent response, and electrochemical impedance spectroscopy analysis revealed that the introduction of NCDs significantly suppressed the recombination of photogenerated electron hole pairs and promoted efficient charge separation and transfer. Notably, the 0.1 wt% of NCDs loaded GCN exhibited optimal performance, achieving a high photocurrent rate approximately 3.5 times higher than that of pristine g-C_3N_4 (GCN).

Keywords: Graphitic carbon nitride, Carbon Dots, Photocatalyst, H2 generation

References:

1. S. Zhang, M. Gao, Y. Zhai, J. Wen, J. Yu, T. He, Z. Kang and S. Lu, J. Colloid Interface Sci., 2022, 622, 662–674.
2. S. Lv, Y. Li, K. Zhang, Z. Lin and D. Tang, ACS Appl. Mater. Interfaces 2017, 9, 44, 38336–38343.
3. S. Asadzadeh-khaneghah, A. Habibi-yangjeh and M. Abedi, Sep. Purif. Technol., 2018, 199, 64–77.
4. V. D. Dang, T. Annadurai, A. Pradiprao, J. Lin, J. Adorna, W. Yu, B. Pandit, T. Viet and R. Doong, Appl. Catal. B Environ., 2023, 320, 121928.
5. F. Wang, P. Chen, Y. Feng, Z. Xie, Y. Liu, Y. Su, Q. Zhang, Y. Wang, K. Yao, W. Lv and G. Liu, "Applied Catal. B, Environ., 2017, 207, 103–113.

EN-060

Bimetallic (NiFe) Metal-Organic Framework for High Electrochemical Performance for Supercapacitor Applications

*Pavithran Ravi [1], Abinash Kumararaj [1], Kaaviyapriya. S. S [1], Geetha Arunachalam [1]**

[1]Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Tamil Nadu - 603203, India.

***Corresponding author e-mail:** geethaa@srmist.edu.in

ABSTRACT

A bimetallic nickel–iron metal–organic framework (NiFe-MOF) was successfully synthesized via a facile hydrothermal method and explored as an advanced electrode material for supercapacitor applications. The synergistic interaction between Ni and Fe ions significantly enhances the electrical conductivity and electrochemical activity compared to their monometallic counterparts. Its structure and morphology were confirmed by X-ray diffraction, Fourier-transform infrared spectroscopy, field-emission scanning electron microscopy, and X-ray photoelectron spectroscopy. Electrochemical measurements reveal that the (NiFe)-MOF electrode delivers a high specific capacitance, excellent rate capability, and a 2-electrodes supercapacitor device exhibits high energy density and power density, as well as good cycling stability after five thousand charge–discharge cycles. These results demonstrate that bimetallic (NiFe)-MOFs is promising candidates for high-performance supercapacitor applications, providing a feasible strategy for designing advanced MOF-based energy storage materials.

Keywords: Bimetallic MOF; NiFe-MOF; Supercapacitor; Electrochemical performance; Energy storage.

EN-061

Electrochemical Nitrate Reduction to Ammonia by $NiFe_2O_4/Fe_2O_3$

Abdurrahman, N V Nagarjun, Muhammed Iyas M I, Swaroop, G M Madhu*, Dr. Nagaraju Kottam , Santhosh C R

Chemical Engineering Department, Ramaiah Institute of Technology, Bengaluru, India, 560054

*Corresponding author e-mail: gmmadhu@msrit.edu

ABSTRACT

Nitrate contamination in water, mainly from agricultural and industrial sources, is a serious environmental issue. This research work presents a sustainable approach to tackle this problem by converting nitrate into ammonia through electrochemical reduction. We synthesized a novel catalyst made of $NiFe_2O_4$ using a simple hydrothermal method. Xray diffraction confirmed that the catalyst contains a mixture of $NiFe_2O_4$ and Fe_2O_3 phases, which contribute to its effectiveness. The catalyst was coated onto a working electrode and tested electrochemically using techniques like chronoamperometry and linear sweep voltammetry. Ammonia produced during the reaction was measured with the indophenol method and UV-Vis spectroscopy, Results showed that the catalyst is highly selective for ammonia production and effectively suppresses unwanted side reactions such as hydrogen evolution. The best performance was observed at -1.6 V, achieving a Faradaic efficiency of around 76%. This study demonstrates that Ni Fe_2O_4 is a promising, low-cost catalyst for turning harmful nitrate pollutants into valuable ammonia, supporting both environmental cleanup and resource recovery. Future work will aim to further improve the catalyst's performance by combining it with other materials

Hydrophobic Concrete Using Admixtures and Industrial By-Products

Vishnuvardhan.Ch, Vedantham H V V Ranganadha Aatreya, Nirmala.R*, Priyadharshini B

Sathyabama Institute of Science and Technology, Chennai, Tamilnadu, India, 600119

***Corresponding author e-mail:** nirmala.civil@sathyabama.ac.in

ABSTRACT

The building and construction sector is facing increasing pressure to adopt sustainable practices and reduce its environmental impact. One promising approach is the development of eco-friendly concrete by utilising admixtures as a partial replacement for the regular component. This study focuses on the development of hydrophobic concrete using a combination of chemical and mineral admixtures to enhance durability and water resistance. Silane and siloxane admixtures, ranging from 0.5% to 3% by weight of cement, are incorporated to impart hydrophobicity to the concrete matrix and 1% polyvinyl alcohol (PVA) fibres. Additionally, cement is partially replaced with 10% silica fume, 2% and Titanium Dioxide (TiO2). Key performance indicators, such as Quality Control and Testing, Compressive Strength, Workability, Water Absorption, Rapid Chloride Penetration (RCPT), Microscopic Analysis, and Durability, are evaluated. The outcome of the study is to assess the feasibility and effectiveness of this sustainable substitution approach in developing high-performance hydrophobic concrete.

References:

1. L. Falchi, E. Zendri, U. Muller, and P. Fontana, Cem. Concr. Compos., 59 (2015) 107–118.
2. Y. Huang, D. K. Sarkar, and X. Grant Chen, Appl. Surf. Sci., 356 (2015) 1012–1024.
3. G. Li, J. Yue, C. Guo, and Y. Ji, Constr. Build. Mater., 169 (2018) 1–7.
4. F. Wang, M. Zhang, S. Lei, J. Ou, and W. Li, Appl. Phys. A, 125 (2019) 1–8.
5. X. Kong, Y. Shen, J. Shi, N. Zhang, R. Kang, and Y. Fu, Colloids Surf. A Physicochem. Eng. Asp., 684 (2024) 2435–2447.

High Performance Electrospun Niobium Nitride Carbon Nanofibre Electrodes for Enhanced Lithium-ion Battery Efficiency

Shruti Kannan[1], Indu M Santhakumari[2], Manikoth M. Shaijumon[2], Ananthakumar Ramadoss[1]*

[1]*Advanced Research School for Technology and Product Simulation (ARSTPS), School for Advanced Research in Petrochemicals (SARP), Central Institute of Petrochemicals Engineering and Technology (CIPET), Chennai- 600 032, India.*

[2]*School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram, Vithura, Thiruvananthapuram, Kerala 695551, India*

***Corresponding author e-mail:** ananth@cipet.gov.in

ABSTRACT

Persistent societal challenges have spurred the expansion of advanced energy storage devices. Lithium-ion batteries (LIBs), being an optimal energy storage device, are desired due to their greater energy density, and their electrochemical efficiency is mainly dependent on their rate performance, cycle life and stability of the electrode materials used. Among these, the development of an improved anode material is considered significant as it directly influences the capacity and energy density of the device. In this context, the present study focuses on the electrospinning of a carbon nanofibre (CNF) framework to host niobium-based electroactive material onto it. Though utilising a niobium-based material reduces the volume expansion of the electrode during cycling, their constrained capacity and conductivity limit their application. Henceforth, the niobium-based CNF was nitrided via vapour phase deposition as a subsequent step to enhance its electrochemical performance. The synergistic interaction of the CNF with niobium nitride renders the electrode with a greater surface-to-volume ratio, reduced ion diffusion distance and conductivity, which is considered vital for improving the electrochemical performance of the LIBs. The physicochemical studies, such as XRD, FE-SEM, EDX, and XPS, uncovered the formation and consistent presence of niobium nitride over the CNF. The electrochemical analysis of the as-prepared electrode exhibited a specific capacity of 330 mAh/g at 0.1 A/g and showed stable rate performance, proving the potential of niobium-based anode materials for LIBs.

Keywords: Lithium-ion Batteries; Electrospinning; Carbon Nanofibre; Anode; Niobium Nitride.

References:

1. D. Mandal, J. Y. Jeong, B. S. Singu, S. Lee, W. J. Mun, and H. Kim, J. Energy Storage, 48 (2022) 104031.
2. F. Ma, Z. Chen, K. Srinivas, Z. Zhang, Y. Wu, D. Liu, H. Yu, Y. Wang, X. Li, M.-Q. Zhu, Q. Wu, and Y. Chen, J. Energy Chem., 88 (2024) 260–271.
3. M. Akter, I. Hossain, M. Howlader, F. Shahriar, and U. H. Saima, Energy Technol., 13 (2025) 2401426.

Boosting Energy Density in Hybrid Supercapacitors with Fe MOF@GO Decorated Ni Nanoparticle Electrodes: A Robust Anode Electrode Material

Aiswarya. R[1] & Kalaivani. T[1]*

[1]*Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Tamil Nadu 603203, India.*

***Corresponding author e-mail:** kalaivat@srmist.edu.in

ABSTRACT

Hybrid supercapacitors have emerged as promising energy storage devices by combining the high power density of supercapacitors with the enhanced energy density of battery-type electrodes. In this work, we report the rational design of a robust anode electrode based on nickel nanoparticles decorated with iron-based metal–organic framework anchored on graphene oxide Fe MOF@GO/Ni. The synergistic integration of highly conductive Ni nanoparticles, redox-active Fe MOF, and graphene oxide with a large surface area significantly enhances charge storage kinetics and electrochemical stability. The Fe MOF@GO decoration prevents nanoparticle agglomeration and provides abundant electroactive sites, while the Ni framework facilitates rapid electron transport. As a result, the Fe MOF@GO/Ni anode exhibits a high specific capacitance, excellent rate capability, and long-term cycling durability. When assembled into a hybrid supercapacitor device, the electrode delivers a markedly improved energy density without compromising power performance. This work demonstrates an effective strategy for engineering multifunctional composite electrodes toward next-generation high-energy hybrid supercapacitors.

Keywords: Hybrid supercapacitors, Metal–organic frameworks, Graphene oxide, Nickel nanoparticles, Energy density enhancement

References:

1. R. Batool, S. D. Dhas, A. C. Mendhe, A. Ghazal, I. Kim, and D. Kim, J. Mater. Chem. A, 12 (2024) 21230–21242.
2. A. Gowdhaman, S. A. Kumar, D. Elumalai, C. Balaji, M. Sabarinathan, R. Ramesh, and M. Navaneethan, J. Energy Storage, 61 (2023) 106769.
3. M. A. Al-Tahan, B. Miao, S. Xu, M. Hou, M. R. Shatat, M. Asad, Y. Luo, A. E. Shrshr, and J. Zhang, Colloids Surf. A Physicochem. Eng. Asp., 682 (2024) 132899.

EN-065

Sustainable and Scalable Low-VOC Inorganic Aqueous Coatings for Passive Daytime Radiative Cooling

To-Yu Wang[1], Ming-Wei Chen [1], Hsin-Yu Fan [1], Hsiu-Mei Yao [1], Chao-Wei Huang [1]*

[1]*Department of Engineering Science, National Cheng Kung University, Tainan, Taiwan, 701012*

***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

Passive daytime radiative cooling (PDRC) technology provides an energy-free cooling approach by reflecting solar radiation and emitting thermal radiation through the mid-infrared atmospheric window (8-13 μm) [1]. It has emerged as a promising solution for mitigating global warming and reducing energy consumption in buildings. However, most paint-based PDRC coatings utilize organic polymer binders, which necessitate the use of large amounts of volatile organic solvents during fabrication, leading to excessive VOC (volatile organic compound) emissions, poor mechanical stability, and limited outdoor durability [2].

To address these limitations, we developed a low-VOC inorganic aqueous BM-ZrO_2/Na_2SiO_3 radiative cooling coating through a simple and scalable aqueous-based process. The coating combines ball-milled ZrO_2 particles with a Na_2SiO_3 matrix, achieving a solar reflectance of 91.39%, mid-infrared emissivity of 0.89, and a VOC content of only 86 g/L. Under high solar irradiance (933 W/m^2) and humidity (65.37%), it achieves a temperature reduction of 5.8°C, while maintaining excellent mechanical robustness, hydrophobicity, and anti-contamination properties. This environmentally friendly inorganic coating demonstrates great potential for energy-efficient and low-carbon building applications.

Keywords: Passive radiative cooling coating, Ball-milling method, ZrO_2 particles, Inorganic aqueous coating, Na_2SiO_3 matrix, and Low-VOC content

References:

1. Zhai, H.; Fan, D.; Li, Q. Sol. Energy Mater. Sol. Cells 245 (2022) 111853.
2. Huang, W.; Chen, Y.; Luo, Y.; Mandal, J.; Li, W.; Chen, M.; Tsai, C.-C.; Shan, Z.; Yu, N.; Yang, Y. Adv. Funct. Mater. 31 (2021) 2010334.

Carrier Modulation and Glassy Thermal Transport in Cu, Sb Co-Doped Ag_8SnSe_6 PGEC system

Nivin Thulasibai Sasidharan[1,4], Vijay Vaiyapuri[2], Karvannan Elamurugan[1], Rajesh Kumar[4], Navaneethan Mani [2,3]*, Karthigeyan Annamalai[1]*

[1] *Hydrogen Storage Materials and Nanosensors Laboratory, Department of Physics and Nanotechnology SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India*

[2] *Centre of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur 603 203, India*

[3] *Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603 203, India*

[4] *Materials and Device Laboratory, Department of Physics, Indian Institute of Technology Indore, Simrol 453552, India*

***Corresponding author e-mail:** karthiga@srmist.edu.in, navaneem@srmist.edu.in

ABSTRACT

Ag-based argyrodites (Ag_8SnSe_6) are superionic materials known for their liquid-like cation mobility and dynamic ion interactions, yet their potential is often constrained by inherently poor electrical properties [1,2]. Cu and Sb were successfully introduced into Ag8SnSe6 bulk materials, prepared through a combination of ball milling and melting in vacuum-sealed quartz ampoules. The crystallinity, defect density, and porosity were effectively controlled through systematic doping. Enhanced carrier concentration and mobility contributed to improved electrical transport properties, with electrical conductivity increasing from 39.58 S/m to 263.73 S/cm at 703 K. Meanwhile, the reduction of lattice thermal conductivity from 0.639 to 0.276 W/mK at 303 K was achieved by tuning the phonon mean free path via engineered porosity and defects. As a result, a maximum ZT value of 1.31 was obtained at 703 K for the $Ag_{7.95}Cu_{0.05}Sn_{0.99}Sb_{0.01}Se_6$ sample.

References:

1. Shen, X.; et al. Adv. Funct. Mater. 30 (2020) 2000526.
2. Zhao, X.; et al. Adv. Funct. Mater. (2025) 2421449.

EN-067

Visible-Light-Driven Green Hydrogen Production Using 2D–2D WO_3/G-C_3N_4 Heterostructured Photocatalysts

V. S Manikandan[1], Ali Akbari-Fakhrabadi[2], Arun Thirumurugan[1]

[1]*Sede Vallenar, Universidad de Atacama, Av. Costanera # 105, Vallenar, 1612178, Chile.*

[2]*Advanced Materials Laboratory, Department of Mechanical Engineering, University of Chile, Santiago, Chile*

***Corresponding author e-mail:** manikandasiva88@gmail.com

ABSTRACT

The growing global demand for sustainable energy has intensified research interest in green hydrogen (H_2) production using renewable energy–driven photocatalytic systems. In this context, WO_3/g-C_3N_4 two-dimensional (2D) composite photocatalysts were synthesized via a simple co-precipitation method followed by ultrasonication and evaluated for visible-light-driven H_2 generation. Structural and optical characterizations (XRD, UV–vis, PL, FESEM, and XPS) confirmed the successful anchoring of monoclinic WO_3 nanoparticles (5–80 nm) onto g-C_3N_4 nanosheets with intimate interfacial contact. Photoelectrochemical and electrochemical impedance studies revealed enhanced charge separation and transfer in the composite system. The optimized WO_3/g-C_3N_4 photocatalyst containing 25 mg of g-C_3N_4 exhibited a maximum H_2 evolution rate of 2917 μmol h^{-1} g^{-1}, significantly outperforming pristine WO_3. The enhanced activity is attributed to improved visible-light absorption, efficient electron–hole separation, and suppressed charge recombination. Additionally, the composite achieved 93% degradation efficiency toward Rhodamine B, demonstrating its multifunctional photocatalytic performance.

EN-068

Copper-based Oxy selenide: Pioneering Single-Material Solution for Integrated Green Hydrogen Production and Environmental Remediation

Pavithra Rajaethirajlu [1], Bernaurdshaw Neppolian [1]*

[1]*Energy and Environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu 603203, India.*

***Corresponding author e-mail:** neppolib@srmist.edu.in

ABSTRACT

Copper-based oxy-selenide (CBOS), an unexplored p-type oxychalcogenide semiconductor and earth-abundant material, is introduced as a multifunctional platform for clean energy production and environmental remediation. It is synthesized via a simple and low-cost solution process, and shows strong near-infrared light absorption and broad spectral response for efficient sunlight utilization. Herein, we report CBOS as a standalone photocathode, which generated a photocurrent density of -2.68 mA cm^{-2} at 0 VRHE without any added co-catalysts or complex heterostructures. CBOS also drive overall water splitting at 10 mA cm^{-2} using only 1.5 V applied voltage, and matches the leading benchmark catalysts. Additionally, it worked effectively as a dual-purpose electrocatalyst for hydrogen and oxygen evolution reactions, marking its first electrocatalytic application. CBOS further achieved 80% photocatalytic removal of the antibiotic pollutant sulfathiazole under natural sunlight, an unprecedented result for this material. These findings position CBOS as a versatile solution for sustainable hydrogen generation and environmental remediation.

Effect of Annealing Temperature on the Structure and Electrochemical Performance of Nickel Vanadate/Nitrogen-Doped Graphene Oxide (NiV_2O_6/N-GO) Nanocomposites

Shikha Dubey, Nutan Mangate, Kalawati Chute, Sushama Giripunje*

Visvesvaraya National Institute of Technology, Nagpur, Maharashtra, India, 440010

***Corresponding author e-mail:** sushamagiripunje9@gmail.com

ABSTRACT

In this work, Nickel Vanadate/ nitrogen-doped graphene oxide (NiV_2O_6/N-GO) nanocomposites were successfully synthesized via a facile hydrothermal strategy. Graphene oxide (GO) was prepared using the modified Hummers' method, followed by hydrothermal nitrogen doping to obtain N-GO. The resulting nanocomposites effectively integrate the high electrical conductivity, large surface area, and abundant defect sites of N-GO with the intrinsic pseudocapacitive behavior of NiV_2O_6 leading to significantly enhanced electrochemical performance. To investigate the synergistic interaction between N-GO and NiV_2O_6, the nanocomposites were annealed at different temperatures, and their electrochemical properties were systematically evaluated. Among the prepared samples, the GN3 composite (NiV_2O_6/N-GO annealed at 400°C) exhibited outstanding electrochemical performance. It delivered a high specific capacitance of 2110.17 F g^{-1} at a scan rate of 5 mV s^{-1}, along with excellent rate capability. Notably, GN3 demonstrated exceptional cycling stability, retaining 100% of its initial capacitance after 5000 charge–discharge cycles, indicating robust structural integrity and efficient charge transfer kinetics. Furthermore, a symmetric supercapacitor (SSC) device was assembled using NiV_2O_6/N-GO nanocomposites as both positive and negative electrodes. The fabricated device achieved a remarkable energy density of 120.75 Wh kg^{-1} at a power density of 2700 W kg^{-1} and maintained 75% capacitance retention after 5000 cycles. These results demonstrate that NiV_2O_6/N-GO nanocomposites are promising electrode materials for high-performance supercapacitor applications.

References:

1. Wei Hau Low, Poi Sim Khiew, Siew, J. Alloys and Compounds, 768 (2018) 995-1005
2. Mayuri G. Magadum, Umesh V. Shembade, , J. Solid State Chemistry 335 (2024) 124697

Asymmetric $CuFe_2O_4$ and Holey Reduced Graphene Oxide Electrodes for High-Performance Capacitive Deionization of NaCl and Heavy Metals

Lavanya S, G. Bharath*

SRM Institute of Science and Technology, Kattankulathur, Tamilnadu – 603203

***Corresponding author e-mail:** sribharath7@gmail.com & bharathg4@srmist.edu.in

ABSTRACT

Capacitive deionisation (CDI) is a promising technology for removing salts and heavy metal ions from brine and industrial wastewater. This study presents an asymmetric electrode configuration with 2D $CuFe_2O_4$ incorporated holey reduce graphene oxide ($CuFe_2O_4$/h-RGO) as anode and highly porous carbon as cathode. The $CuFe_2O_4$/h-RGO nanoarchitecture features high crystallinity, hierarchical pores and an enhanced higher electrocatalytic active surface area, facilitating efficient interaction with salt and heavy metal ions. The asymmetric CDI (a-CDI) configured with $CuFe_2O_4$/h-RGO as anode and porous activated graphene as cathode for performing the removal of NaCl and heavy metal ions such as Pb^{2+}, Cd^{2+}, and Cr^{3+}. This a-CDI exhibits remarkable ion removal performance, driven by a synergistic balance of electric double-layer capacitance and faradaic charge storage mechanisms. The electrodes successfully removed heavy metal ions like Pb^{2+}, Cd^{2+}, and Cr^{3+} and demonstrated a high salt adsorption capacity for NaCl under mild working conditions. The a-CDI is also demonstrated excellent cycling stability under prolonged charge-discharge cycles. This asymmetric configuration offers a sustainable and scalable solution for addressing water scarcity and contamination, advancing next-generation CDI systems.

Keywords: Ferrites; Asymmetric electrodes; Capacitive deionisation; NaCl removal; wastewater removal

References:

1. Bharath, G et.al. Environmental Research 197 (2021): 111110.
2. Bharath, G et.al. Chemosphere 266 (2021): 129048.
3. Bharath, G et.al., Electrochimica Acta 337 (2020): 135668.

EN-071

Binary-Ternary Complex Oxide Nanoflower: Pulse Reverse Electrodeposited Electrode for Designing Supercapacitor Prototype

Nikita Ahlawat[1], Rajesh Kumar[1,2,*]

[1]*Materials and Device Laboratory, Department of Physics, Indian Institute of Technology Indore, Simrol-453552, India*

[2]*Centre for Advanced Electronics, Indian Institute of Technology Indore, Simrol-453552, India.*

***Corresponding author e-mail:** rajeshkumar@iiti.ac.in

ABSTRACT

Tailoring electrode materials' architecture through deposition strategy is a critical route toward achieving materials with enhanced electrochemical performance for energy applications. Here, nanodimensional nickel cobaltite ($NiCo_2O_4$)- manganese oxide (MnO_2) complex (NCMO) based electrodes, prepared using three distinct electrodeposition recipes, have been studied, and their electrochemical energy storage properties have been evaluated. Films prepared by constant electrodeposition (CED), pulse potential (PP), and pulse reverse potential (PRP) exhibit distinctly different morphologies and energy storage properties, with the PRP electrode showing the best performance. The CED mode yields a non-uniform film composed of large agglomerates, while PP produces a more homogeneous nano-flake structure. On the other hand, PRP mode results in a fully interconnected flake–flower-like nanostructured network. It delivers a high specific capacitance of 596 mF/cm^2, outperforming the other two electrodes. An asymmetric supercapacitor device prepared using this electrode exhibits performance suitable for practical applications, retaining 92% of its capacitance over more than 4500 charge-discharge cycles. A prototype device could operate a multipurpose digital display for several minutes, underscoring its practical viability for usage in appliances. The study offers a recipe for designing and fabricating a solid-state supercapacitor for actual application as a next-generation energy storage system.

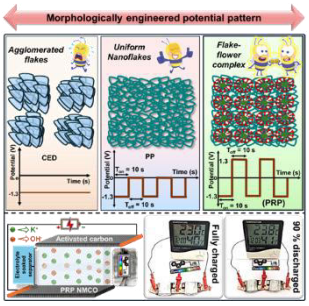


Fig. 1 TOC graphics of the morphological engineered prepare electrode material and device application.

Keywords: metal oxide composite; pulse reverse potential; supercapacitor; specific capacitance; energy density

References:

1. N. Ahlawat, P. S. Rout, L. Bansal, B. Sahu, D. K. Rath, S. Srivastava, S. Kumar, S. Singh, A. S. Shekhawat, S. K. Saxena, S. K. Chondath, R. Kumar, Adv. Mater. Technol. n/a, e02300.

EN-072

Bayesian Reliability Analysis of Mineral-Tallow Oil Blends for Sustainable Dielectric Cooling in Electrochemical Energy Systems

Rahul Somnath S, Sowmmiya U*, Nithya C, Preetha Roselyn J, Vikraman Ganesh Moorthi

Department of Chemistry, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 6032035

*Corresponding author e-mail: sowmmiyu@srmist.edu.in

ABSTRACT

The rapid expansion of high-power rechargeable batteries and supercapacitors necessitates sustainable dielectric cooling fluids that ensure electrical insulation and thermal stability under non-uniform thermal loads. This study evaluates buffalo tallow methyl ester (TOME), a bio-derived natural ester, as a renewable thermofluids to partially replace mineral oil in liquid-cooled energy-storage modules. TOME was synthesized via controlled transesterification and blended with mineral oil at 0%, 20%, 40%, 60%, 80%, and 100%. Blends were characterized for dielectric strength, dissipation factor, resistivity, viscosity, density, acidity, moisture content, and interfacial tension following IEC 60156 and 60296 standards. Due to strong property-to-property coupling and inherent uncertainties, a Bayesian probabilistic framework was implemented to quantify the likelihood that each blend simultaneously satisfies all operational constraints, accounting for measurement variability, composition drift, and batch effects. The resulting joint reliability index provides a rigorous, uncertainty-aware metric for compositional suitability beyond deterministic thresholds. Results reveal that TOME blends containing 20–40% maintain high joint reliability (>0.95), with breakdown voltages of 65–68 kV, dissipation factor <0.01, and stable thermophysical properties (viscosity 11–12 mm^2/s, density 0.88–0.90 g/cm^3), suitable for passive cooling channels and dielectric barriers in energy-storage modules. Higher ester fractions (≥60% TOME) show substantial dielectric deterioration: breakdown voltage decreases to 52 kV (T60) and 34 kV (T100), dissipation factor rises to 0.02–0.05, reducing joint reliability to 0.582 and 0.163, despite retaining acceptable viscosity and fire-safety margins. This study delivers two key contributions: (i) a validated composition window (20–40% TOME) for bio-derived dielectric cooling fluids, and (ii) a scalable, probabilistic methodology for screening sustainable thermofluids under uncertainty. These findings provide actionable guidance for integrating renewable esters into high-voltage energy-storage systems while maintaining operational safety and performance.

Keywords: sustainable insulating fluids, Mineral–tallow blends, Bayesian reliability, Bio-based insulating fluids.

References:

1. U. Mohan Rao et al., IEEE Access, 7 (2019) 184552–184571.

High-Performing Nickel Sulfide Nanoparticles Decorated 2D Mxene Electrocatalysts for the Valorization of Furfural

Divyabharathi S, Bharath G*

Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu – 603203

***Corresponding author e-mail:** sribharath7@gmail.com & bharathg4@srmist.edu.in

ABSTRACT

Furfural, an emerging biomass-derived bio-oil compound, is essential for carbon neutrality through biomass valorization. This valorization can be done using electrochemical hydrogenation (ECH), offering efficient conversion of furfural into valuable chemicals when compared to traditional methods. Optimizing the electrode type and reaction mechanisms for producing value-added chemicals is a challenging task for the ECH of furfural. This work investigates the morphology dependency on the precursor concentration of nickel sulfide (NiS) nanoparticles synthesized by ethylenediamine-tetraacetic acid decorated on 2D MXene. The influence of precursor concentration was analyzed using SEM and HRTEM, revealing that the nanoparticles resemble sphere-like structures composed of nanosheets deposited on 2D MXene nanosheets, enhancing the electrocatalytic activity towards the conversion of furfural. This study also examines various parameters, including electrolyte concentration and applied potential and their influence on conversion efficiency, product yield, and selectivity. The results demonstrated that the NiS/MXene nanocatalyst offered enhanced furfural conversion into value-added bio-fuels with high selectivity and yield under mild operating conditions. The significance of this study highlighted the impact of morphology and electrolyte concentration for effective hydrogenation of furfural.

Keywords: Electrochemical hydrogenation, sustainable bio-fuels, furfural, value-added chemicals, biomass valorization.

References:

1. Bharath al., ACS applied materials & interfaces 13 (21), 24643-24653
2. Karthikeyan, R. et al., Dalton Transactions 43.46 : 17445-17452

Synergistic Catalytic Effect of Pt-Ni_2P/rGO Composite for Efficient Ammonia Oxidation Toward Greener Hydrogen Production

Prasanth S, G. Bharath*

SRM Institute of Science and Technology, Kattankulathur, Tamilnadu – 603203

***Corresponding author e-mail:** sribharath7@gmail.com & bharathg4@srmist.edu.in

ABSTRACT

Hydrogen gas (H_2) is difficult to store and transport because of its very low volumetric density, which forces the use of high-pressure cylinders or cryogenic systems. In contrast, ammonia (NH_3) contains 17.8 wt% hydrogen higher than most hydrides and alcohol-based hydrogen carriers and can be liquefied under relatively mild conditions (-33 °C or 8-10 bar), allowing safe, economical storage and long-distance transport. Therefore, storing hydrogen as ammonia is a better and cheaper way to handle it than managing it directly. Furthermore, when required, the hydrogen can be extracted from the ammonia easily. Herein, a ternary Pt-Ni_2P/rGO composite was successfully produced and tested as a high-efficiency electrocatalyst for the hydrogen evolution reaction (HER), the oxygen evolution reaction (OER), and the electrochemical ammonia oxidation reaction (AOR). Electrochemical studies show that the Pt-Ni_2P/rGO catalyst is substantially more active for HER, OER, and AOR activity than pure Pt, Ni_2P, and binary Pt-Ni_2P catalysts. It has a low overpotential, high peak current density, high stability, low cell voltage, and a higher turnover frequency in alkaline medium. These studies indicate that the Pt-Ni_2P/rGO composite is an excellent electrocatalyst for efficient hydrogen production via ammonia oxidation and also give significant insights for the strategic development of multifunctional catalysts for future energy applications.

Keywords: Ammonia oxidation reaction, Hydrogen production, Nickel phosphide, Pt-Ni_2P/rGO composite, Hydrogen evolution reaction, Oxygen evolution reaction.

References:

1. C. Jo et al., Chem. Eng. J., 463 (2023) 142314.
2. H.-Y. Sun et al., J. Energy Chem., 47 (2020) 234–240.
3. A. Paliwal et al., ACS Appl. Mater. Interfaces, 17 (2025) 3383–3392.

To Improve Strength and Durability of Concrete with Biopolymer Additives and Sisal Fiber Reinforcement Concrete

G.Great Antony Aaship[1]*, Mr.J.Vanjinathan[1]

[1] *Sathyabama Institute of Science and Technology, Chennai, Tamilnadu, India, 600119*

***Corresponding author e-mail:** antonygreataaship@gmail.com

ABSTRACT

This study investigates the mechanical and durability performance of concrete modified with lignosulfonate as a partial cement replacement and reinforced with sisal fibers as natural reinforcement. Lignosulfonate, an eco-friendly byproduct of the paper industry, was incorporated at replacement levels of 2%, 4%, 6%, and 8%, improving workability, reducing water demand, and enhancing microstructural densification. Sisal fibers, with tensile strength ranging from 660 MPa and modulus of elasticity between 15 GPa, were used as discrete reinforcement. To Experimental investigations were conducted to assess compressive strength, split tensile strength, flexural strength, and durability aspects such as water absorption and chloride resistance. Analytical modeling using ANSYS Workbench was employed to simulate the flexural behaviour of sisal fiber and lignosulfonate-modified concrete beams under static loading. The simulations provided insights into stress distribution, crack propagation, and deflection patterns. Combining experimental results with computational analysis enabled a deeper understanding of the structural performance. Overall, the study highlights the potential of sisal fiber and lignosulfonate in producing eco-friendly, durable, and high-performance concrete composites.

References:

1. Naraganti, S. R.; Pannem, R. M. R.; Putta, J. Constr. Build. Mater. 2019.
2. Gao, C.; Fu, Q.; Huang, L.; Yan, L.; Gu, G. Polymers (Basel) 2020.
3. Sridhar, J. J. Nat. Fibers 2023, 20.
4. Pagella, G.; et al. Constr. Build. Mater. 2018.
5. Ren, G.; Yao, B.; Huang, H.; Gao, X. Constr. Build. Mater. 2021.

EN-076

Modulation of the Interfacial Lithium-Ion Transport within Lithium-Ion Batteries: Insights from Multi-Scale Simulations

Chi-cheng Chiu[1,2,3,4]*

[1]*Department of Chemical Engineering, National Cheng Kung University, Tainan 701, Taiwan*

[2]*Center for Resilience and Intelligence on Sustainable Energy Research (RiSER), National Cheng Kung University, Tainan 701, Taiwan*

[3]*Program on Smart and Sustainable Manufacturing, Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University, Tainan 701, Taiwan*

[4] *Fire Protection and Safety Research Center, National Cheng Kung University, Tainan 711, Taiwan*

***Corresponding author e-mail:** ccchiu2@gs.ncku.edu.tw

ABSTRACT

Interfacial lithium-ion (Li^+) transport critically governs the rate capability, impedance, and long-term stability of lithium-ion batteries (LIBs), yet its molecular origins remain insufficiently understood due to the complex coupling between chemistry, electrostatics, and structure across multiple length scales. In this work, we utilize a multi-scale simulation framework that integrates molecular dynamics (MD) and kinetic Monte Carlo (kMC) methods to systematically elucidate Li^+ transport mechanisms at key battery interfaces, including electrolyte–cathode and polymer–ceramic boundaries in composite polymer electrolytes (CPEs), as well as electrode–binder–electrolyte systems. MD simulations were employed to resolve the interfacial structure, ion coordination, and electric double-layer behavior induced by different polymer binders, ranging from conventional poly(vinylidene difluoride) to Li^+-coordinating, negatively charged, and zwitterionic polymers. The results reveal that binder charge characteristics strongly regulate local ion distributions and electrostatic potential profiles, leading to pronounced differences in Li^+ mobility and interfacial resistance. Negatively charged binders enhance Li^+ accumulation near Li^+-depleted cathode surfaces, whereas zwitterionic binders suppress excessive ion polarization and mitigate interfacial bottlenecks. To bridge molecular insights with device-relevant transport, kMC simulations under non-equilibrium conditions were conducted using MD-derived descriptors. These simulations demonstrate how binder-induced electrostatic landscapes translate into distinct ion flux responses and impedance characteristics. In parallel, strategies for mitigating polymer–ceramic interfacial resistance in CPEs, such as ceramic surface functionalization and crystallinity modulation, are evaluated. Overall, this work highlights how targeted interfacial chemistry and charge engineering can be leveraged to rationally design next-generation LIB materials with improved ionic transport and performance.

References:

1. H.-S. Liu, Chen, K.-Y. Chen, C.-E. Fang, and C.-c. Chiu, Electrochimica Acta, 2021, 375, 137915
2. Tsao, C.-H. et al. ACS Applied Materials & Interfaces, 2021, 13, 9846–9855.
3. P.-Y. Wang, T.-H. Chiu, and C.-c. Chiu, Polymers, 2024, 16, 319.

EN-077

Experimental and Computational Analysis of PCM Assisted Cooling for Solar Collectors

G. Om Prakash, M. Bala Chennaiah, M Sumalatha, T. Akshai, P. Satish

Department of Mechanical Engineering, Siddhartha Academy of Higher Education (Deemed to be University), VR Siddhartha School of Engineering, Vijayawada, India-520007.

***Corresponding author e-mail:** chennai303.mech@vrsiddhartha.ac.in

ABSTRACT

The efficiency and longevity of photovoltaic (PV) solar panels are greatly influenced by working temperature, since high heat lowers energy conversion efficiency and accelerates material degradation. This study focuses on enhancing the thermal management of PV panels by integrating phase change material (PCM), namely paraffin wax, which can take up and retain surplus heat during phase change and give it out during cooling periods.

An experimental setup was designed to study the thermal and electrical performance of a PCM-incorporated PV system under actual outdoor conditions. Temperature distribution, power generation, and efficiency were measured and compared with a traditional PV panel to assess the cooling effectiveness of the PCM layer. Supplementing the experimental efforts, a computational analysis was conducted utilizing ANSYS Fluent to simulate the heat transfer behaviour within the PCM and PV structure. Radiation boundary conditions were imposed on the upper surface to simulate solar heating, and parameters like temperature distribution and fraction of melt were examined to investigate the behaviour of PCM during charging and discharging processes. The findings show that the integration of paraffin wax consistently reduces the peak operating temperature of the PV panel, encourages consistent heat distribution, and enhances efficiency. The analysis of melt fraction verified successful phase change and latent heat uptake during peak irradiance times. Therefore, the passive cooling system using PCM improves panel reliability and extends operational duration. The integrated experimental and computational study verifies the applicability of paraffin wax as a cheap, effective, and renewable thermal control material for photovoltaic applications.



Fig : 1 (front view of experimental model)

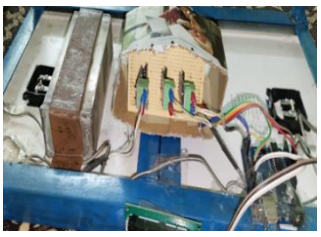


Fig : 2 (backside view of model)

References:

1. A. Hasan, S. J. McCormack, M. J. Huang and B. Norton, Sol. Energy, 2010, 84, 1601–1613.
2. M. A. Kareem and K. S. Reddy, Renewable Energy, 2018, 119, 91–101.
3. S. Rajput and S. C. Kaushik, Appl. Therm. Eng., 2017, 115, 1001–1012.

EN-078

Visible-Induced Photocatalysis by Cr Doped Fe_2O_3 Nanoparticles on Methylene Blue

Neha Joseph[1], Anjali Sharma[2], I.V Asharani[1], B Karthikeyan[2]*

[1]*Vellore Institute of Technology, Vellore, Tamilnadu, India, 632014*

[2]*National Institute of Technology, Tiruchirappalli, Tamilnadu, India, 620015*

***Corresponding author e-mail:** bkarthik@nitt.edu

ABSTRACT

Environmental pollution from the discharge of organic dyes like Methylene Blue (MB) in water bodies caused by industries is one of the major concerns. Among the various water treatment methods, photocatalytic degradation using semiconducting nanoparticles has gained attention due to their low cost, tunable bandgaps, and high efficiency. Hematite (α-Fe_2O_3) has been widely explored in this area, yet its photocatalytic efficiency is limited by fast electron-hole recombination. To overcome these limitations, transition metal doping has been studied.

In this work, we synthesized Cr^{3+}-doped iron (III) oxide (Fe_2O_3) nanoparticles (NPs) via a simple co-precipitation method to improve efficiency and to study their photocatalytic efficiency by the degradation of Methylene Blue under white-light irradiation. The Cr^{3+} ions are incorporated into the lattice, causing defects and modifying the band gap of the Fe^2O^3, thus enhancing the photocatalytic degradation efficiency. The NPs were characterized using XRD, UV, FTIR, and FESEM analysis for their phase purity, crystallinity, optical properties, functional groups, and morphology, respectively.

As compared to pure α-Fe_2O_3, Cr^{3+}-doped Fe_2O_3 showed more degradation efficiency due to enhanced electron-hole separation in the doped sample. This study highlights the potential of Cr^{3+}-doped Fe^2O^3 as a visible-light-activated catalyst in wastewater treatment.

References:

1. M. Mishra and D.-M. Chun, Appl. Catal. A: Gen., 2015, 498, 126–141.
2. T. Wang, J. Cao, J. Li, J. Li, D. Li, S. Wang and Z. Ao, Environ. Sci.: Nano, 2024, 11, 2415–2427.
3. P. Yadav, N. Dhariwal, M. Kumari, V. Kumar and O. P. Thakur, Chemosphere, 2023, 343, 140208.
4. N. Dhariwal, P. Yadav, M. Kumari, A. Sanger, Y. K. Mishra, V. Kumar and O. P. Thakur, Sci. Rep., 2024, 14, 19916.

Performance Evaluation of GGBS and Nano-Titanium Modified Concrete Beams Under Flexural Loading

C. Sathish*, R. Padmapriya

Sathyabama Institute of Science and Technology, Chennai, Tamilnadu, India, 600119

***Corresponding author e-mail**: sathishsekar031199@gmail.com

ABSTRACT

High strength concrete is increasingly recognized as a superior option for constructing robust and durable structures. In this project, we conducted a thorough investigation into the durability and strength properties of M80 grade high strength concrete (HSC) mixes. Various levels of Ground Granulated Blast-furnace Slag (GGBS) were used as replacements for cement at rates of 10%, 20%, 30%, and 40%. Additionally, the optimum percentage of GGBS was held constant while we explored different sand replacement levels, including 10%, 30%, 50%. To maintain consistency in our testing, GGBS percentages were fixed while incorporating varying levels of Titanium Dioxide (TiO2) as a cement substitute, specifically at 1%, 2% and 3%. The M40 concrete mix was designed in accordance with the BIS guidelines for selecting proportions for high strength concrete that includes Pozzolana Portland cement and other cementitious materials. Our findings reveal significant strength characteristics in the GGBS-based concrete mixes. Notably, the optimal combination of 20% GGBS, 50% GBS, and 3% TiO2 exhibited exceptional strength properties, outperforming conventional concrete mixtures.

References:

1. L. E. Copeland and R. H. Bragg, Anal. Chem., 1958, 30, 196–201.
2. A. Campillo, A. Guerrero, J. S. Dolado, A. Porro, J. A. Ibáñez and S. Goñi, Mater. Lett., 2007, 61, 1889–1892.
3. A. H. Shekari and M. S. Razzaghi, Procedia Eng., 2011, 14, 3036–3041.
4. H. L. Malhotra, Mag. Concr. Res., 1956, 8, 85–94.

EN-080

Waste-Derived Bacterial Cellulose Acetate Composite Membrane for high performance Microbial electrochemical Systems

Nishant Pandey[1] and Vipin Kumar[1]*

[1] *Laboratory of Applied Microbiology, Department of Environmental Science and Engineering, Indian Institute of Technology (Indian School of Mines), Dhanbad, Jharkhand-826004, India*

*** Corresponding author. e-mail**: vipinmicro1@iitism.ac.in

ABSTRACT

Bacterial cellulose (BC) is an attractive sustainable substrate for proton exchange membranes, but limitations in mechanical strength and ionic conductivity still constrain its use in bioelectrochemical systems. In this study, BC was produced by Stenotrophomonas sp. Isolated from orange pulp waste, transformed into bacterial cellulose acetate (BCA), and further developed into a composite membrane by incorporating 1 wt% graphene oxide and chitosan as functional additives. The resulting BCA/GO/chitosan membrane showed improved proton exchange membrane in dual-chambered microbial electrochemical system, where the cell delivered a maximum closed-circuit potential of 650 mV, reflecting robust bio- electrocatalytic performance. The membrane exhibited a tensile strength of 54 MPa, exceeding that of commercial Nafion, indicating superior mechanical durability suitable for prolonged operation. Collectively, this strategy valorizes citrus processing waste into a high-value, bio-derived proton exchange membrane, offering a promising materials pathway for sustainable energy and metal-recovery microbial electrochemical applications.

Keywords: Microbial Electrochemical System, Bacterial cellulose, Chitosan, composite membrane, proton-exchange membrane.

References:

1. G. Palanisamy et al., J. Energy Chem., 2023, 80, 402–431.
2. S. M. Ghaseminezhad, M. Barikani and M. Salehirad, Compos. Part B Eng., 2019, 161, 320–327.
3. U. F. Kandil, E. O. Taha, E. A. Mahmoud, N. O. Shaker, M. Mahmoud and M. R. Taha, Egypt. J. Pet., 2023, 32, 1–6.

EN-081

Structural and Catalytic Effect of Partial Substitution of Nickel by Niobium on the Hydrogen Storage Behaviour of Mechanically Alloyed Mg-Mg_2Ni Composites

Gorbel B[1], Ambuj Pathak[1], Anshul Gupta[2], Nitesh Kumar[1]*

[1]*Department of Materials Engineering, Indian Institute of Technology Jammu, Jammu, 181221, India*

[2]*Department of Metallurgical and Materials Engineering, National Institute of Technology Srinagar, Srinagar, 190006, India*

***Corresponding author e-mail:** nitesh.kumar@iitjammu.ac.in

ABSTRACT

Magnesium hydride (MgH_2) is widely recognized as a promising solid-state hydrogen storage material due to its high hydrogen capacity and cost-effectiveness; however, its practical application is limited by high absorption–desorption temperatures and slow reaction kinetics. In this study, a $Mg_2Ni_{0.8}Nb_{0.2}$ catalyst was synthesized by partially substituting Ni with Nb using the melt-spinning technique to enhance the hydrogen storage performance of MgH_2. The resulting catalyst was incorporated into Mg at 20 wt% to form Mg–$Mg_2Ni_{0.8}Nb_{0.2}$ composites through high-energy ball milling. These composites were subsequently hydrogenated for varying durations (10, 20, and 30 minutes) to evaluate the influence of hydrogenation time on their dehydrogenation behavior. Thermal analyses including differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and differential thermal analysis (DTA) were employed to investigate the decomposition characteristics of the hydrogenated composites. The onset of dehydrogenation for the optimized composite occurred at 225 °C, significantly lower than that of pure MgH_2. Furthermore, the activation energies associated with dehydrogenation were reduced to 126.35 kJ/mol, 131.66 kJ/mol, and 100.78 kJ/mol for hydrogenation times of 10, 20, and 30 minutes, respectively, compared with 275.52 kJ/mol for pristine MgH_2. These results demonstrate that the Mg–$Mg_2Ni_{0.8}Nb_{0.2}$ system exhibits strong catalytic activity, effectively functioning as a hydrogen pump within the MgH_2 matrix. The partial substitution of Ni with Nb improves thermodynamic behavior and significantly enhances dehydrogenation kinetics by facilitating Mg–H bond dissociation. Overall, the tailored catalyst–composite approach provides a promising pathway to overcome the limitations of conventional MgH_2 for hydrogen storage applications.

Keyword: Magnesium hydride, Hydrogen storage, Activation energy, Ball milling

EN-082

Tuning p-Type and n-Type Thermoelectric Transport in VFeSb Half-Heusler Alloys via Site-Specific Substitution

Yatin P. Desai[1], K. R. Priolkar[1,2]*

[1] *School of Physical and Applied Sciences, Goa University, Taleigao Plateau, Goa, 403206, India*

[2] *UGC DAE Consortium for Scientific Research, Khandwa Road, Indore, MP, 452001, India*

***Corresponding author e-mail:** krp@unigoa.ac.in

ABSTRACT

Half-Heusler alloys are promising materials for thermoelectric energy conversion due to their tunable electronic transport properties and structural robustness. In this work, we report a comparative study of site-specific substitution effects on the structural and thermoelectric transport properties of VFeSb-based Half-Heusler alloys. Polycrystalline samples of pristine VFeSb, Fe-site substituted $VFe_{0.9}Co_{0.1}Sb$, and V-site substituted $V_{0.9}Ti_{0.1}FeSb$ were synthesized and systematically characterized. X-ray diffraction analysis with Rietveld refinement confirms the dominant Half-Heusler phase in all samples with the presence of minor secondary phases in selected compositions. Electrical transport measurements reveal that pristine VFeSb exhibits negative thermopower, indicating intrinsic n-type conduction. Co substitution at the Fe site further enhances n-type behavior, leading to reduced electrical resistivity due to increased carrier concentration. In contrast, Ti substitution at the V site results in positive thermopower, signifying a transition to p-type conduction, accompanied by comparatively higher resistivity. Power factor analysis shows a strong temperature dependence for all compositions, with the highest values observed at 400 K. Notably, the p-type $V_{0.9}Ti_{0.1}FeSb$ sample exhibits a power factor at 400 K that is comparable to or slightly higher than that of pristine VFeSb, while the Co-substituted sample shows a lower power factor owing to its reduced thermopower. These results demonstrate that site-selective substitution enables effective control of carrier polarity and temperature-dependent thermoelectric performance in VFeSb-based Half-Heusler alloys.

References:

1. A. Yamamoto, T. Takeuchi, J. Electron. Mater., 46 (5) (2017) 3200–3206.
2. Y. Huang, K. Hayashi, Y. Miyazaki, Acta Materialia, 215 (2021) 117022.
3. Y. Huang, K. Hayashi, Y. Miyazaki, Chem. Mater., 32 (12) (2020) 5173–5181.
4. C.G. Fu, H.H. Xie, Y.T. Liu, T.J. Zhu, J. Xie, X.B. Zhao, Intermetallics, 32 (2013) 39–43.
5. L. Jodin, J. Tobola, P. Pecheur, H. Scherrer, S. Kaprzyk, Phys. Rev. B, 70 (18) (2004) 184207

Green Synthesis of CdS Nanostructures Using Plant Extracts and Their Morphological, Optical, and Photocatalytic Properties

Labhesh Baid[1]*, K. S. Ojha[1]

[1]*NIT Raipur, Raipur, Chhattisgarh, India, 603203*

***Corresponding author e-mail:** Labheshbaid777@gmail.com

ABSTRACT

CdS nanostructures were successfully synthesized via a hydrothermal method incorporating various green plant extracts. X-ray diffraction (XRD) analysis confirms the formation of a hexagonal phase with average crystallite sizes ranging from 7.43 nm to 9.59 nm for Hibiscus rosa-sinensis (Hibiscus/Gurhal), Citrus sinensis (Orange) peel, Azadirachta indica (Neem), Aloe barbadensis miller (Aloe vera) leaf capped CdS nanostructures. The synthesized nanostructures exhibit distinct morphological features, including snowflake-like, cauliflower-like, starflower-like, and sago-like formations, as confirmed by HRSEM. Elemental analysis via the EADX spectroscopic technique confirms the formation of pure CdS. Optical investigations reveal a variation in bandgap from 2.15 to 2.25 eV [1], and all samples exhibit a redshift compared to the bulk CdS. Photoluminescence spectra exhibit emission peaks in the UV, blue, and green-yellow regions centred at 371, 468, and 564 nm, respectively. Additionally, FTIR spectroscopy was employed to analyze the vibrational characteristics of the plant-extract-assisted CdS samples [2]. The photocatalytic performance of these nanostructures was explored for environmental remediation, demonstrating a promising degradation of acetaminophen with an efficiency of 91% in 140 min under visible light irradiation for Hibiscus rosa-sinensis extract-capped CdS nanostructure.

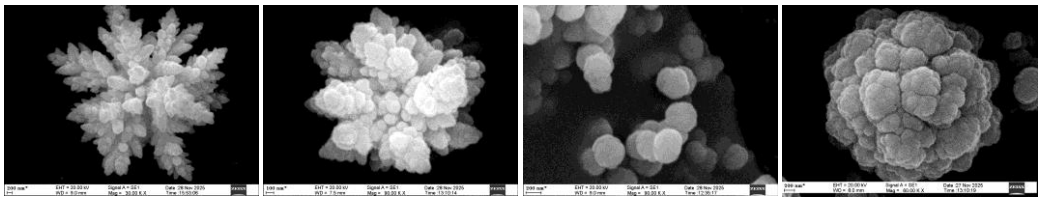


Fig. 1. SEM images of nanostructures

References:

1. M. H. K. Al-Mamoori, D. K. Mahdi and S. M. AlShrefi, AIP Conf. Proc., 2018, 1968, 030018.
2. B. S. M. Al Balushi et al., Appl. Surf. Sci., 2018, 457, 559–565.

EN-084

Polyaniline Coupled MoS_2-MoO_3 Heterostructures for High Performance Supercapacitors

Chandni A P[1], Binitha N Narayanan[1,2]*

[1]*Department of Chemistry, University of Calicut, Malappuram, Kerala, India, 673635*

[2] *Inter University Centre for Hydrogen & Energy Storage, University of Calicut, Malappuram, Kerala, India, 673635*

***Corresponding author e-mail:** binitha@uoc.ac.in

ABSTRACT

Supercapacitors are promising energy storage devices due to their high power density, rapid charge-discharge capability, and long cycle life. Polyaniline (PANI) is widely explored as a supercapacitor electrode material owing to its high theoretical capacitance and facile synthesis; however, its practical application is limited by structural degradation caused by repeated swelling and contraction during cycling.

To address these limitations, PANI was integrated with a MoS_2-MoO_3 hybrid via an in-situ polymerization strategy, enabling structural stabilization and the introduction of additional pseudocapacitive centres. The MoS_2-MoO_3 heterostructure provides multiple Mo oxidation states, offering abundant redox-active sites, while its layered architecture facilitates efficient electrolyte penetration. Strong synergistic interactions between PANI and the MoS_2-MoO_3 framework result in markedly enhanced electrochemical performance.

Structural and chemical analyses using XRD, FTIR, and Raman spectroscopy confirm successful nanocomposite formation. The optimized composite with an aniline/Mo ratio of ~14 exhibits the highest areal specific capacitance and excellent cycling stability. A symmetric pouch cell supercapacitor further demonstrates its practical viability.

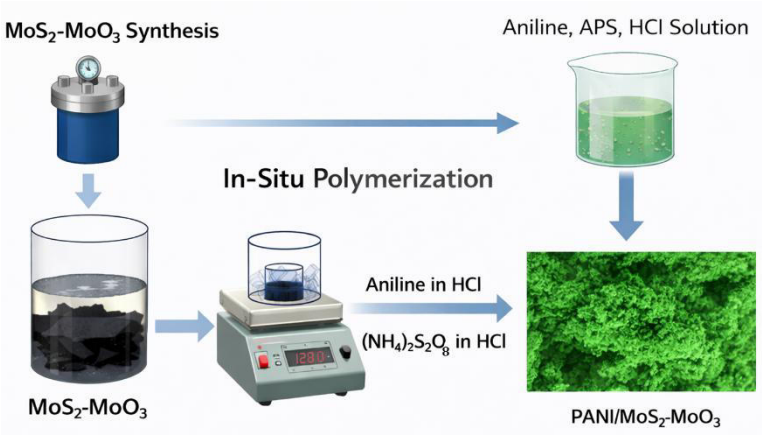


Fig 1. Schematic representation showing the formation of PANI/ MoS_2-MoO_3 nanocomposite.

References:

1. Raghu M. S., Yogesh Kumar K., Srilatha Rao, Aravinda T, Prasanna B. P., Prashanth M. K., Polym. Bull., 75 (2018) 4359–4375.

Hydrothermally Synthesized NiS Nanoparticles: Optical Properties and Electrocatalytic Performance for Hydrogen Evolution

Yogita Gendre[1], K. S. Ojha[1], Chinmaya Mahapatra[2]

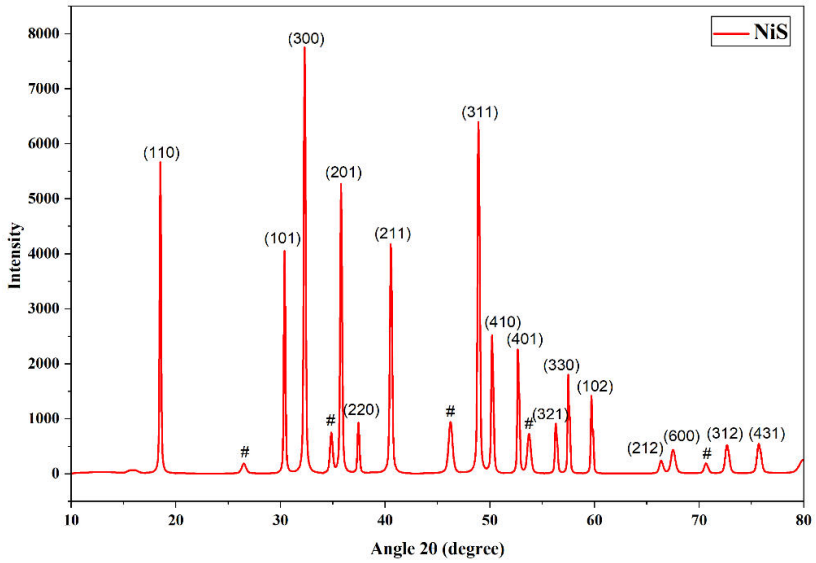
[1]*Department of Physics, National Institute of Technology Raipur, Raipur, Chhattisgarh*

[2]*Department of Biotechnology, National Institute of Technology Raipur, Raipur, Chhattisgarh*

***Corresponding author e-mail:** ygendre.phd2023.phy@nitrr.ac.in

ABSTRACT

In the present study, Nickel sulphide (NiS) nanoparticles have been synthesized via cost effective and facile hydrothermal method. The structural analysis of sample confirmed the formation of NiS nanoparticles with crystallite size 36 nm exhibiting hexagonal crystal structure. The formation of spherical like morphology is identified by field emission scanning electron microscopy (FESEM). The elemental composition is verified by energy dispersive X-ray (EDX) analysis. The synthesized sample's absorption and emission properties were examined using UV-vis and Photoluminescence (PL) spectroscopy. The molecular vibrations of synthesized sample were examined via Fourier transform infrared spectroscopy. The surface characteristics of prepared sample were examined using an X-ray photoelectron (XPS) spectroscopy. The performance of Hydrogen evolution reaction (HER) of the produced sample was determined by electrochemical evaluation comprising cyclic voltammetry (CV), linear sweep voltammetry (LSV), Tafel slope and electron impedance spectroscopy (EIS).



References:

1. M. Indhumathy, A. Prakasam, J. Clust. Sci., 31 (2020) 91–98.
2. W. Boughouiche, et al., Int. J. Hydrogen Energy, 162 (2025) 150757.

EN-086

Sol–Gel Auto-Combustion Synthesis and Photocatalytic Activity of 5% Co-Doped Bismuth Ferrite ($BiFe_{0.95}Co_{0.05}O_3$)

Aboorvaa L. B[1], S. Gokul Raj[1]*, S. Surya[1], G. Ramesh Kumar[2]

[1]*Department of Physics, Pondicherry University, Kalapet, Puducherry 605014, India*

[2]*Department of Science and Humanities, University College of Engineering Arni- Thatchur- (Anna University, Chennai), 632 326, India*

***Corresponding Author e-mail:** gokulraj@pondiuni.ac.in

ABSTRACT

Cobalt-doped Bismuth Ferrite ($BiFe_{0.95}Co_{0.05}O_3$) was synthesized through Sol Gel Auto Combustion method to investigate the effect of 5% Co substitution on the structural, optical, and photocatalytic properties of $BiFeO_3$. The synthesized samples were then calcined to various annealing temperatures to obtain single phase nature. Powder X-ray diffraction analysis confirmed the formation of a single-phase rhombohedral perovskite structure with successful incorporation of Co ions at the Fe site without detectable secondary phases. The photocatalytic performance was evaluated through the degradation of organic dye pollutants under visible-light irradiation, where $BiFe_{0.95}Co_{0.05}O_3$ exhibited significantly improved degradation efficiency compared to undoped $BiFeO_3$. The enhanced photocatalytic activity is due to reduced electron–hole recombination, defect-induced intermediate energy levels, and improved charge carrier mobility arising from addition of CO in Bismuth Ferrite. These findings demonstrate that 5% Co-doped $BiFeO_3$ is an efficient visible-light photocatalyst with strong potential for wastewater treatment and environmental remediation applications.

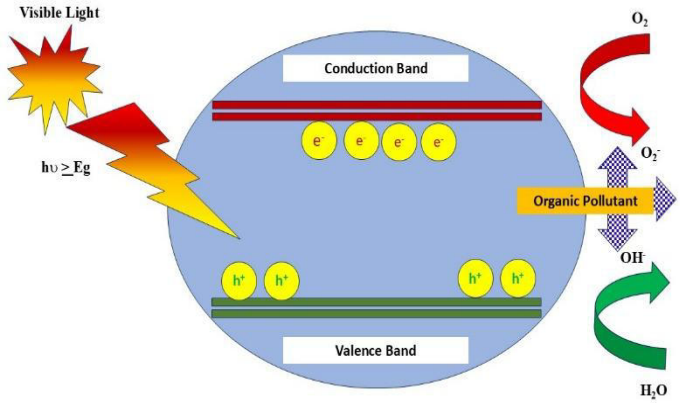


Fig. The photocatalytic behaviour mechanism in the visible light region

Keywords: Photocatalysis, Bismuth Ferrite, CO-doped BFO

References:

1. A. Haruna et al., Heliyon 6 (2020) e03237.
2. C. Ponraj et al., Environ. Nanotechnol. Monit. Manag. 7 (2017) 110–120.
3. Y. Nassereddine et al., Nanomaterials 14 (2023) 51.
4. S. Grover et al., Comput. Mater. Sci. 6 (2023) 2200673.
5. H. A. Mohd Azmy et al., J. Phys. Sci. 28 (2017) 85–103.

EN-087

Selective CO_2 Reduction to Formate using Copper Phosphide Based Electrocatalyst

Tanu Bagaria[1,2], Bharati Debnath[1,2]*

[1]*Research Institute for Sustainable Energy, TCG-CREST, Salt Lake, 700091, Kolkata, India*

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India*

***Corresponding author e-mail:** bharati.debnath@tcgcrest.org

ABSTRACT

The conversion of carbon dioxide (CO_2) into fuels or value-added chemical feedstocks driven by renewable electricity offers a sustainable pathway toward carbon neutrality and the mitigation of global climate change.[1] Electrochemical reduction of CO_2 (CO_2RR) has become an attractive approach for CO_2 conversion, benefiting from mild operating conditions, environmental friendliness, and high energy efficiency.[2] Among the various CO_2 reduction products, formate is highly attractive owing to its role as a chemical feedstock, hydrogen carrier, preservative, and fuel in direct formate fuel cells. Copper-based catalysts have been extensively studied for CO_2 reduction; however, achieving high selectivity toward formate while suppressing competing hydrogen evolution remains challenging.[3,4] In this work, we report a facile one-step electrodeposition strategy to fabricate a self-supported, dopant-engineered copper phosphide electrocatalyst. The incorporation of optimized % of d-block elements having empty 4d orbitals modulates the electronic structure, thereby enhancing CO_2 adsorption and activation. The optimized catalyst achieves a high impressive Faradaic efficiency of ~95% at -0.8 V vs. RHE, suppressing the competitive side reaction. Furthermore, it maintains excellent stability over 100 hours of continuous operation. This study provides valuable insights into catalyst design strategies for selective CO_2-to-formate conversion and highlights the potential of electrochemical CO_2 reduction as a promising approach for carbon utilization and sustainable chemical production.

References:

1. Z. Tao, Z. Wu, Y. Wu, H. Wang, ACS Catal., 10 (2020) 9271−9275.
2. H. M. Jeong, Y. Kwon, J. H. Won, Y. Lum, M. J. Cheng, K. H. Kim, M. H. Gordon, J. K. Kang, Adv. Energy Mater. 10 (2020) 1903423.
3. X. Ma, Y. Zhang, T. Fan, D. Wei, Z. Huang, Z. Zhang, Z. Zhang, Y. Dong, Q. Hong, Z. Chen, X. Yi, Adv. Funct. Mater., 33 (2023) 2213145.
4. T. H. M. Pham, J. Zhang, M. Li, T. H. Shen, Y. Ko, V. Tileli, W. Luo, A. Züttel, Adv. Energy Mater., 12 (2022) 2103663.

EN-088

Exploring the Thermoelectric Potential of $Bi_2Te_xSe_{3-x}$ Topological Insulators through Raman Thermometry and Theoretical Analysis

Sambit Kumar Prusty[1], Vipin Kurian Elavunkel[1], Prahallad Padhan[1,2]*

[1]*Department of Physics, Nanoscale Physics Laboratory, Indian Institute of Technology Madras, Chennai 600036, India*

[2]*Functional Oxides Research Group, Indian Institute of Technology Madras, Chennai 600036, India*

***Corresponding author e-mail:** padhan@iitm.ac.in

ABSTRACT

Thermoelectric (TE) materials enable the direct conversion of waste heat into electrical energy, offering a promising solution to meet growing energy demands. Among thermoelectric materials, chalcogenide compounds are attractive due to their favorable electronic properties and low lattice thermal conductivity at mid- to high temperatures. $Bi_2Te_xSe_{3-x}$ alloys are widely used in thermoelectric applications, as selenium (Se) substitution in Bi_2Te_3 enables tuning of electronic transport and phonon-mediated heat conduction. In this work, $Bi_2Te_xSe_{3-x}$ alloys were synthesized via a direct melt method in sealed quartz tubes, and their thermal transport and phonon behavior were investigated using experiment-informed analysis and first-principles calculations. Phase identification and lattice parameters were obtained using Rietveld refinement with FULLPROF. Temperature-dependent Raman spectroscopy was used to study phonon behavior, and Raman shifts and linewidths were analyzed via the bond-order–length–strength (BOLS) correlation to extract composition-dependent Grüneisen parameters (γ) and Debye temperature (θ_D). These parameters provide information on lattice anharmonicity. The derived γ and θ_D values were then used to estimate lattice thermal conductivity (κ_L) using the Slack equation, providing an experimentally informed evaluation of thermal transport. Phonon dispersion and thermal properties were computed using PHONOPY and PHONO3PY interfaced with Quantum ESPRESSO, treating atomic vibrations within the harmonic approximation and incorporating higher-order interactions through perturbation theory and the finite-displacement method. Theoretical results show good agreement with Raman-based analysis, and Se-rich compositions exhibit reduced lattice thermal conductivity, favorable for thermoelectric applications.

References:

1. D. Sharma, M.M Sharma, R.S Meena, V.P.S Awana, Physica B Condensed Matter 600 (2021) 412492.
2. A.Togo, I. Tanaka, Scr.Mater. 108 (2015) 1–5.
3. Vipin, K. E., P. Padhan, J.Mater. Chem. C 12 (2024) 7415−7425.
4. Vipin, K. E.; S.K. Das, P. Padhan, Phys.Chem. Chem. Phys. 25 (2023) 13577–13586.

EN-089

Improved Thermoelectric Performance of $SrTiO_3$-Based Entropy-Stabilized Perovskite Oxide for High-Temperature Waste Heat Recovery

Vivek Kumar* and Tanmoy Maiti

Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology, Kanpur, UP 208016, India

***Corresponding author e-mail:** vivek21@iitk.ac.in

ABSTRACT

Entropy stabilization has been proven to improve the thermoelectric performance of oxides by inherently reducing their thermal conductivity. It is attributed to multivalent cations and mass fluctuations present in the material, which leads to enhanced anharmonicity and phonon scattering, resulting in reduced lattice thermal conductivity. Here, we report a SrTiO3-based entropy-stabilized oxide, synthesized using the solid-state reaction route followed by spark plasma sintering. XRD analysis confirms the formation of a single-phase solid solution and SEM micrograph reveals a dense microstructure. Compositional study and defect chemistry have been examined using XPS analysis. Temperature-dependent thermal conductivity and electrical conductivity measurements have been studied to probe the material's thermoelectric performance. The temperature-dependent electrical conductivity shows manifold enhancement with an excellent Seebeck coefficient, achieving an enhanced power factor of 1052 μW/mK2 at 823 K. The lattice thermal conductivity has been found to reduce significantly with sub-nanometer phonon mean free path, reaching a minimum value of 2.75 W/mK at 1073 K. The thermoelectric figure of merit zT reached a maximum value of 0.27 at 1023 K. This work shows that entropy stabilization is a viable approach towards designing high-performance thermoelectric materials.

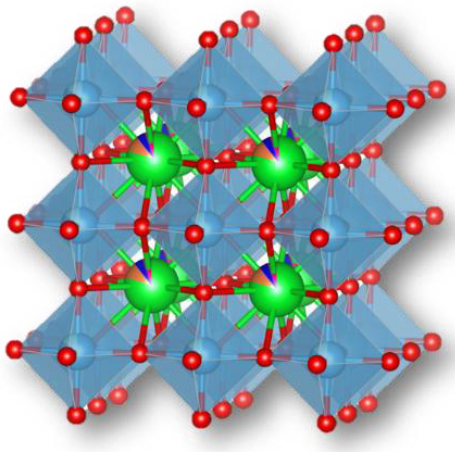


Fig. $SrTiO_3$ perovskite structure (red: O-site, green: Sr-site, and blue: Ti-site)

Water-in-Glass Additives: Synergistic Enhancement of Alkaline Hydrogen Evolution Reaction via Electrolyte Engineering

Jan Nisa Ahad*, Mallikarjuna Rao M., Sinorul Haque and Amarnath R. Allu

SRM University AP

*Corresponding author e-mail: jannisa_ahad@srmap.edu.in

ABSTRACT

Alkaline water electrolysis (AWE) is the industrial benchmark for hydrogen production, yet further kinetic enhancements are required to minimize energy consumption. Here, we present a novel electrolyte engineering strategy utilizing a water-soluble sodium alumino- phosphate-sulfate-glass ($28Na_2O$, $3.5Al_2O_3$, $28P_2O_5$, $12.5Na_2SO_4$, 28NaCl mol%) as a synergistic additive. We demonstrate that dissolving this functional glass into standard alkaline media (1 M KOH) fundamentally alters the interfacial kinetics of the Hydrogen Evolution Reaction (HER). The activity follows a Sabatier-type volcano trend, where a glass- to-alkali mass ratio (Rm) of 35% maximizes current density by restructuring the electrical double layer and facilitating the rate-determining water dissociation step. However, at higher loadings (Rm = 55%), performance declines due to competitive specific adsorption of multivalent anions (PO^{3-}, SO^{2-}), which sterically block active platinum sites. Long-term chronopotentiometry confirms that the optimized hybrid electrolyte maintains operational stability for over 24 hours, achieving a cathodic half-cell energy consumption corresponding to an overpotential of 425 mV at 100 mA cm^{-2}. This work establishes dissolved functional glasses as a versatile, scalable platform for designing next-generation electrolytes.

Keywords: Alkaline HER, Electrolyte engineering, Water in glass additive, Electrical double layer modulation.

Lattice Thermal Conductivity of $SrSnO_3$: A Combined Experimental and Theoretical Study

Santosh Kumar Sahu[1], Rasmi Ranjan Mohapatra[1]*, Sandip Kumar Padhi*[1], Prahallad Padhan[1,2]*

[1]*Department of Physics, Nanoscale Physics Laboratory, Indian Institute of Technology Madras, Chennai 600036, India*

[2]*Functional Oxides Research Group, Indian Institute of Technology Madras, Chennai 600036, India*

***Corresponding author e-mail:** sahusantosh860@gmail.com

ABSTRACT

Perovskite oxides are an important class of functional materials with applications in energy conversion and electronic devices, where efficient thermal management is essential. In this study, the lattice thermal conductivity (κ_l) of bulk strontium stannate ($SrSnO_3$) is systematically investigated through a combined experimental and theoretical approach. Temperature-dependent Raman spectroscopy was employed to probe phonon behavior and anharmonic interactions in SrSnO3. The observed phonon frequency shifts with temperature were analyzed using the Balkanski model to quantify anharmonicity and estimate the lattice thermal conductivity. Complementary first-principles calculations based on density functional theory were performed using the Phono3py framework to compute phonon dispersion relations, phonon lifetimes, and κ_l providing microscopic insight into phonon transport and scattering mechanisms. The theoretical results show good agreement with the Raman-based estimates, validating the reliability of the combined methodology. The relatively low lattice thermal conductivity of SrSnO3 compared to related perovskite oxides is primarily attributed to strong phonon anharmonicity and the presence of heavy atomic constituents, which enhance phonon scattering. This integrated experimental-theoretical investigation offers a comprehensive understanding of thermal transport in SrSnO3 and highlights its potential for applications requiring low thermal conductivity. The study also demonstrates the effectiveness of combining temperature-dependent Raman spectroscopy with first-principles phonon calculations as a robust framework for investigating lattice thermal transport in complex oxide materials.

References:

1. Masahiro Yasukawa, Kazushige Ueda, Satoru Fujitsu, Ceram. Int., 43 (2017) 9653-9657
2. E. Moreiraa, J.M. Henriques, D.L. Azevedo, J. Solid State Chem., 184 (2011) 921-928
3. Vipin Kurian Elavunkel, Prahallad Padhan, ACS Appl. Energy Mater., 8 (2025) 15241−15257
4. Muhammad Atif Sattar, Maamar Benkraouda, Physica B, 590 (2020) 412216

EN-092

Ca and Fe doping effect on Structural, Spectral and Dielectric properties of $Sr_{1-x}Ca_xTi_{1-y}Fe_yO_3$

K.Indu[1], N.Pavan kumar[2]

[1]*Department of Physics, Osmania University, Hyderabad 500 007, India*

[2]*Department of Physics, Matrusri Engineering College, Saidabad, Hyderabad, 500059, Telangana, India.*

ABSTRACT

This study investigates the dielectric and structural properties of calcium and iron co-doped strontium titanate ($Sr_{1-x}Ca_xTi_{1-y}Fe_yO_3$), a perovskite oxide with significant potential for thermoelectric and energy storage applications. Strontium titanate exhibits unique electrical, optical, and thermal-mechanical properties making it a model system for perovskite materials research. X-ray diffraction (XRD) analysis confirmed cubic crystal structure at room temperature in doped samples, with peak shifts attributing to lattice distortions caused by ionic radius differences of dopants. Fourier-transform infrared (FTIR) spectroscopy and Raman spectroscopy revealed significant structural modifications, including altered vibrational modes in the TiO_6 octahedra characteristic of the perovskite framework. Dielectric property measurements demonstrated that co-doped samples exhibit enhanced electrical energy storage capacity and reduced dielectric losses, with the CF-15 sample showing optimal polarization. Impedance spectroscopy indicated improved charge carrier mobility and reduced resistance with increasing frequency, particularly pronounced in samples with optimal doping concentrations. Results suggest that CF-15 exhibits superior dielectric properties with minimal energy dissipation, making it suitable for high-frequency applications. Comprehensive characterization using XRD, FTIR, and Raman spectroscopy provides valuable insights into how Ca and Fe co-doping modulates the lattice dynamics and electronic properties of strontium titanate, opening avenues for future thermoelectric generator development and advanced functional material applications.

Ideating at Interfaces: Enhancing the Performance and Longevity of Sustainable Energy Systems

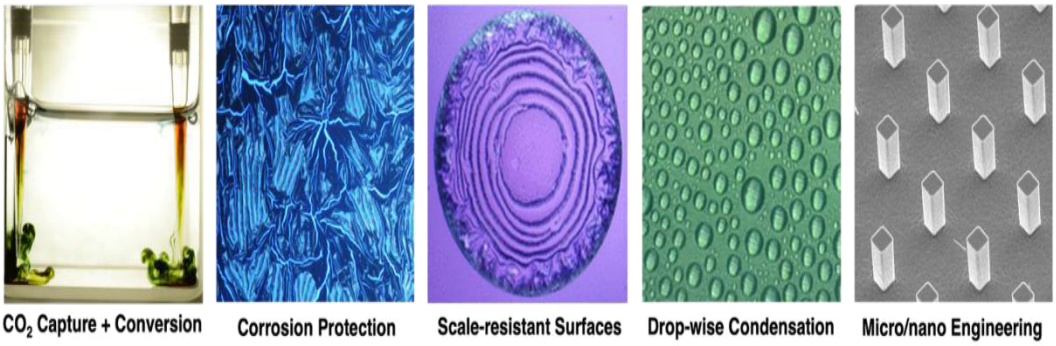
Sami Khan[1]*

[1]*Sustainable Energy Engineering, Simon Fraser University, Surrey, BC V3T0N1, Canada*

***Corresponding author e-mail:** s_khan@sfu.ca

ABSTRACT

Interfaces are decisive control points in sustainable energy systems, often limiting performance and durability through complex physicochemical interactions. In this talk, I will highlight how interfacial engineering can unlock new capabilities in three application areas. First, I will discuss strategies for soot removal in biomass combustion, where microtextured surfaces fabricated via laser ablation and sandblasting can promote self-cleaning and reduce fouling [1]. Second, I will present our recent work on carbon capture and conversion, showing how bubble-harnessing aerophilic surfaces enhance CO_2 dissolution and mass transfer for more efficient capture processes [2]. Third, I will describe our efforts to mitigate hydrogen embrittlement in pipeline steels using ultra-thin, self-healing liquid-like coatings that slow hydrogen ingress and provide superior long-term protection [3]. I will conclude by outlining a broader vision for how interfacial science and interfacial engineering can accelerate the transition to low-carbon energy systems and improve the longevity of clean energy technologies in the face of climate change.



References:

1. Oren O., McTaggart-Cowan G., Khan S., Sci. Rep., 14 (2024) 4247.
2. Nemir O., Refai R., Rodrigues R., Tiffin C., Fisher N., Yao-Bate L., Khan S., Appl. Phys. Lett., 127 (2025) 17.
3. Khan S., Toparli C., Yildiz B., Varanasi K.K., ACS Appl. Eng. Mater., 3 (2025) 654-661.

EN-094

Structural and Magnetic Properties of Rare Earth-Doped $Co_{0.8}Zn_{0.2}$ Ferrites Synthesized via Solid-State Reaction

Karne Mahesh, N.Pavan Kumar

Department of physics, Government City Collage, Hyderabad,500003, Telangana,India

Department of Sciences and Humanities, matrusri Engineering Collage, Hyderabad,500059, Telangana, India

ABSTRACT

A systematic series of cubic spinel ferrites were synthesized via solid-state ceramic reaction with progressive rare earth element (RE = Pr, Ho, Y) substitution to investigate structure-property relationships. Four compositions were prepared: the undoped reference $Co_{0.8}Zn_{0.2}Fe_2O_4$, singly doped $Co_{0.8}Zn_{0.2}Pr_{0.1}Fe_{1.9}O_4$, doubly doped $Co_{0.8}Zn_{0.2}Pr_{0.05}Ho_{0.05}Fe_{1.9}O_4$, and triply doped $Co_{0.8}Zn_{0.2}Pr_{0.03}Ho_{0.03}Y_{0.03}Fe_{1.9}O_4$. Powder X-ray diffraction (XRD) confirmed single-phase cubic spinel structures (space group Fd-3*m*) for all compositions with systematic lattice parameter modifications. Fourier transform infrared (FTIR) and Raman spectroscopy validated characteristic spinel metal-oxygen stretching modes. Scanning electron microscopy (SEM) revealed microstructural evolution and grain size refinement upon multi-dopant incorporation. Vibrating sample magnetometry (VSM) measurements demonstrated systematic variations in saturation magnetization, coercivity, and remanent magnetization with increasing rare earth dopant concentration. Elemental composition was confirmed via energy-dispersive X-ray spectroscopy (EDX). The multi-dopant system exhibited enhanced magnetic property tunability and refined grain morphology compared to single-dopant analogues, attributed to cooperative effects of Pr^{3+}, Ho^{3+}, and Y^{3+} substitution at iron sites. These findings demonstrate effective control of magnetic properties through strategic rare earth doping, with potential applications in high-frequency devices and tunable functional materials.

Numerical Investigation of High-Efficiency Two-Terminal Rb_1MAFA/In_2S_3 Tandem Perovskite Solar Cells

Ajay Kumar[1]*, Neha Gupta[2], Aditya Jain[3], Kaushal Kumar[4], and Amit Kumar Goyal[5]

[1]*ECE Department, Jaypee Institute of Information Technology, Noida, India, 201309.*

[2]*Department of Applied Sciences, GNIOT Group of Institutions, Uttar Pradesh, India, 201306.*

[3]*ECE Department, SIT, Symbiosis International (Deemed University), Pune, Maharashtra, India, 412115.*

[4]*ECE Department, Graphic Era Deemed to be University, Dehradun, Uttarakhand, India.*

[5]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104.*

***Corresponding author e-mail:** ajay.kumar@jiit.ac.in

ABSTRACT

Traditionally, silicon-based solar cells were widely used to produce solar energy. However, the efficiency of a solar cell is determined by its ability to convert solar energy directly into electricity, a process known as the photovoltaic effect [1]. This paper presents a comprehensive investigation of two-terminal tandem perovskite solar cells, highlighting their advantages in achieving better efficiency and performance compared to traditional single-terminal devices [2]. The proposed device structure consists of Rb1MAFA and In2S3 layers, stacked together to achieve higher efficiency. Simulations were performed using SCAPS-1D software under the AM1.5G solar spectrum and a temperature of 300 K [3]. By meticulously adjusting the thickness and other parameters of both layers, we achieved an efficiency of 32.46%, surpassing that of single-terminal devices. Additional parameters examined include current density, quantum efficiency, absorption coefficient, electric field, and IV characteristics such as Jsc=33.656 mA/cm2, Voc=1.2658 V, fill factor (FF) = 76.20%, and efficiency (η)=32.46%.

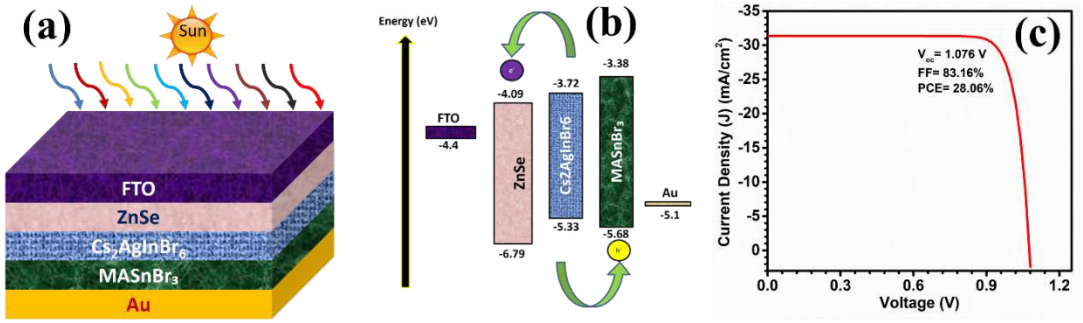


Fig. 1. (a) Device structure of 2T Tandem Solar Cells. (b) Current density 2T Tandem Solar Cells. (c) Quantum Efficiency 2T Tandem Solar Cells.

References:

1. Y. Yang et al., Sol. Energy Mater. Sol. Cells, 262, 112558 (2023).
2. P. Wang, Y. Zhao, and T. Wang, Appl. Phys. Rev., 7(3), 031303 (2020).
3. J. Werner, B. Niesen, and C. Ballif, Adv. Mater. Interfaces, 5(1), 1700731 (2018).

EN-096

Molarity Driven Electrochemical Optimization of Zn-Co LDH@CS Supercapacitor

Ariya K Vijayan[1], Arun Kumar Singh[2], Umisha Singh[3], Shoba Shukla[1,2,3], Sumit Saxena[1,2,3]*

[1]*Nanostructures Engineering and Modelling Laboratory, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology Bombay, Mumbai, MH 400076, India*

[2]*Centre for Research in Nanotechnology and Science, Indian Institute of Technology Bombay, Mumbai, MH 400076, India*

***Corresponding author e-mail:** sumit.saxena@iitb.ac.in

ABSTRACT

The pursuit for clean, renewable energy sources to meet the ever-increasing demand for energy has been catalyzed by the rapid depletion of fossil fuel resources. In this regard, it is crucial to develop effective energy storage technologies, such as supercapacitors (SCs), to store renewable energy. Zn-Co LDH is a potential electrode material for use in SCs due to its large surface area, layered structure, and multiple oxidation states. The charge storage capability, rate performance, and cycling stability of a supercapacitor are highly influenced by the type of electrode material used and the concentration (molarity) of the electrolyte, as these factors govern ion transport, electrical conductivity, and redox activity. In the present study, hybrid nanostructures of carbon spheres (CS) and Zn-Co LDH were synthesized to enhance their electrical conductivity and subsequently characterized. Since the electrolyte plays an important role in determining the electrochemical behaviour of SCs, their variation in specific capacitance with respect to different molar concentrations of electrolytes was systematically examined. Our results suggest that the molarity of electrolyte significantly influences the specific capacitance and overall performance of the SCs.

References:

1. John Peter I, Nav Deepak, Umisha Singh, Himanshu Soni, Shoba Shukla, Sumit Saxena, J. Power Sources 655 (2025) 237897.
2. Kumbhar, K. R., Redekar, R. S. & Tarwal, N. L. I, J. Energy Storage 146 (2026) 119854.

EN-097

Developing $Rh_{2-y}cr_yo_3$ Cocatalysts to Outperform Platinum in Semiconductor-Based Photocatalytic H_2 Evolution

Raveena P V, Logamithrai D, Anitha Christy Antonysamy, Debabrata Sarkar*

Applied Nanophysics Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and technology, Kattangulathur-603203, Chennai, Tamil Nadu

***Corresponding author e-mail:** deboo_phy@yahoo.com

ABSTRACT

The future of sustainable energy hinges on the ability to efficiently generate hydrogen via solar-driven photocatalysis, a pursuit that demands revolutionary advances in cocatalyst design to transcend the intrinsic limitations of semiconductor[1]. Traditionally, noble metal cocatalysts like Pt, Ru, and Rh, Ir etc.,—especially Platinum for its high work function—have excelled at facilitating water reduction, but their vulnerability to photooxidation and reverse water formation fundamentally limits efficiency and stability[2]. In regard with this, $Rh_{2-y}Cr_yO_3$ mixed oxide has emerged as an exciting alternative, uniting remarkable photocatalytic activity with exceptional stability and catalytic precision[3]. Here, we present the successful integration of $Rh_{2-y}Cr_yO_3$ cocatalysts onto oxide-based photocatalysts via facile impregnation method, producing a sophisticated core–shell motif. In this architecture, a catalytically potent Rh core facilities the proton reduction, while the Cr oxide shell acts as a guardian, effectively suppressing unwanted photooxidation and reverse water formation pathways that undermine efficiency. A systematic exploration reveals a critical dependence of photocatalytic performance on the Cr shell thickness, with an optimized layer dramatically amplifying hydrogen evolution rate. Surpassing Pt-based systems in both activity and durability, the $Rh_{2-y}Cr_yO_3$ mixed oxide demonstrates unrivaled potential as a durable, high-performance cocatalyst platform. This work not only highlights the pivotal role of controlled cocatalyst architecture but also charts a compelling path towards next-generation photocatalysts that marry exceptional efficiency with longevity for scalable solar fuel production

Keywords: Cocatalyst; $Rh_{2-y}Cr_yO_3$; Photocatalyst; Hydrogen evolution

References:

1. S. Chen, T. Takata, K. Domen, Nat. Rev. Mater. 2017, 2, 1.
2. A. Kudo, Y. Miseki, Chem. Soc. Rev. 2009, 38, 253.
3. K. Maeda, K. Teramura, H. Masuda, T. Takata, N. Saito, Y. Inoue, K. Domen, J. Phys. Chem. B 2006, 110, 13107.

EN-098

Investigation of WO_3 Nano-Structured Materials for Hydrogen Evolution Reaction

Jayakaushalya Manogaran, Karthik Dilly Rajan, Kiruthika Murugesan, Maheswaran Ratinam*

Department of Physics and Nanotechnology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur, Tamilnadu, 603 203, India

***Corresponding author e-mail:** *maheswar@srmist.edu.in*

ABSTRACT

Generation of clean fuel hydrogen from renewable energy source by using semiconductor and water is the most challenging target in the 21st century. Water electro splitting is one of the most promising ways of producing green hydrogen in large quantities when powered by renewables. In the present work WO_3 nanomaterial was successfully synthesized via simple hydrothermal method incorporating mild reducing agents like citric acid (WO_3 – C) and sodium chloride (WO_3 –N) and alongside a reducing-agent-free counterpart (WO_3) prepared by direct hydrothermal treatment of the metal precursor solution. The nano materials were analyzed by using various techniques such as X-ray diffraction, SEM - Scanning Electron Microscopy, TEM - Transmission Electron Microscopy characterization techniques, UV spectroscopy. Electrochemical measurements were performed on an electro chemical workstation using a typical three-electrode setup for Hydrogen evolution reaction in 1 M KOH as electrolyte. The WO_3 – C sample exhibits greater HER catalytic activity compared with other two WO_3, WO_3-N samples in 1M KOH electrolyte with an overpotential of 99.5 mV at 10mA/cm^2. Thereby stating that WO_3 – C promising electrocatalyst for the HER, with wide-ranging applications in the future.

References:

1. X. Wei et al., Chem. Commun., 55 (2019) 6515–6518.
2. W. Adamson et al., Catal. Today, 351 (2020) 44–49.

Enhanced Thermoelectric Performance in Mn-Doped $AgCrSe_2$: Synergistic Optimization of Carrier Concentration and Lattice Thermal Conductivity

A. Thameemul Ansari[1], K.P. Mohamed Jibri[1], J. Archana[2], M. Navaneethan[1*]

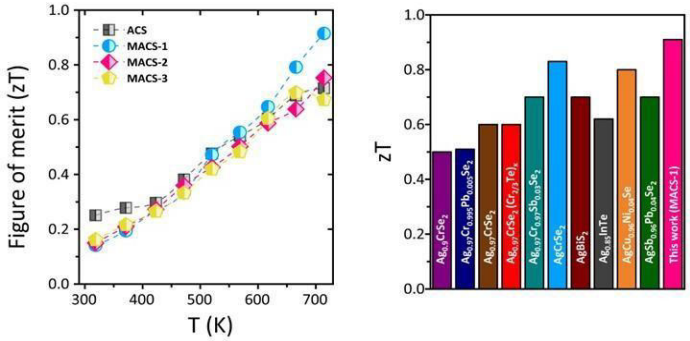
[1]*Nanotechnology Research Centre, SRM Institute of Science and Technology, KTR Campus, Chengalpattu Tamilnadu-603-203.*

[2]*Centre of Excellence in Materials and Advanced Technologies, SRM Institute of Science and Technology, KTR Campus, Chengalpattu Tamilnadu-603-203.*

***Corresponding author e-mail:** navaneem@srmist.edu.in

ABSTRACT

$AgCrSe_2$, a layered superionic conductor, has emerged as a promising thermoelectric material due to its intrinsically low lattice thermal conductivity and unique Phonon-Liquid Electron Crystal (PLEC) behavior. However, its poor electronic transport properties have remained a critical challenge. To overcome the, Mn doping at the Cr site was employed to optimize the charge carrier concentration and enhance electrical conductance. Notably, $AgCr_{0.99}Mn_{0.01}Se_2$ led to a substantial increase in electrical conductivity, reaching 517 S cm^{-1} at 317K, compared to 217 S cm^{-1} in the pristine sample, primarily due to an increase in carrier concentration from 10^{18} to 10^{19} cm^{-3}. Simultaneously, this composition maintained an ultra-low lattice thermal conductivity of 0.14 W m^{-1} K^{-1}, attributed to a notable reduction in transverse sound velocity, which obtained 1494 ms^{-1} for the $AgCr_{0.99}Mn_{0.01}Se_2$ sample. These synergistic effects resulted in a well- balanced thermoelectric performance, ultimately achieving a remarkable zT = 1 at 760K. This study highlights the effectiveness of Mn doping in fine-tuning the electronic and thermal properties of $AgCrSe_2$, paving the way for its potential application in next generation thermoelectric energy conversion.



Keywords: low lattice thermal conductivity; PLEC behavior; layered superionic conductor; zT enhancement; phonon scattering; energy conversion materials

References:

1. K. S. Rana et al., ACS Appl. Energy Mater., 7 (2024) 5621–5628.
2. F. Gascoin and A. Maignan, Chem. Mater., 23 (2011) 2510–2513.

EN-100

Interfacial Polysulfide-Rich Nickel Iron Vanadium-LDH/Cobalt Oxysulfide Heterostructures for Durable and Efficient Overall Water Electrolysis

R. Vengadesh, J. Archana, P Justin Jesuraj*

Center of Excellence in Materials and Advanced Technologies (CeMAT), Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Potheri, Chengalpattu – 603 203, India.

***Corresponding author e-mail:** justinp@srmist.edu.in

ABSTRACT

Developing efficient bifunctional electrocatalyst for overall water electrolyser application remains crucial. Among the Nickel Iron- layered double hydroxide (LDH) based electrocatalyst systems, third metal inclusion might induce electron redistribution which reinforces the catalytic activity of LDH systems. Herein, we report an insitu grown Nickel Iron Vanadium-LDH/cobalt oxysulfide (NFV-LDH/Co-O-S/NF) heterostructure on a nickel foam (NF) substrate. A three-pot hydrothermal synthetic process was carried out, followed by subsequent annealing treatment to fabricate the above mentioned heterostrucutre. X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) revealled that the polysulfide species of the cobalt oxysulfide substratum establish a highly conductive and redox-active sulfur network. Electrochemical (EC) data further demonstrated the active-site reconstruction of the heterostructure. The NFV-LDH/Co-O-S/NF catalyst achieved an exceptionally low oxygen evolution reaction (OER) overpotential of η_{10} = 218 mV and a Tafel slope of 51 mV dec^{-1} at 10 mA cm^{-2} current density. Alongside, same electrode exhbiits the hydrogen evolution reaction (HER) with η_{10} = 83 mV and a Tafel slope of 108 mV dec^{-1}. The membrane free two-cell electrolyzer operated at 1.58 V with 35 h with NFV-LDH/Co-O-S/NF electrodes. Morphological and elemental analysis were carried out on the catalyst after the chronoamperometry test to validate the robust nature of the proposed heterostrucutre electrode.

Keywords: NFV-LDH; hybrid architecture; substratum; Cobalt oxy sulfide; oxygen evolution reaction (OER); hydrogen evolution reaction (HER).

References:

1. A.M, P.M, K.S.R, T.T.T.N, Y.H, C.D, R.K.D, and T.H.O. Small 20, no. **26** (2024): 2310112.
2. B.L, S.Z, C.T, X.C, and Q.Z. Small 13, no. **25** (2017): 1700610.

EN-101

Synergistic Ni-MOF/MoS_2-based heterostructures for efficient bifunctional hydrogen electrocatalysis

G. Jose Agnel, J. Archana, P Justin Jesuraj*

Center of Excellence in Materials and Advanced Technologies (CeMAT), Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Potheri, Chengalpattu – 603 203, India.

***Corresponding author e-mail:** *justinp@srmist.edu.in*

ABSTRACT

The growing demand for sustainable energy technologies has positioned green hydrogen as a key component of future energy strategies, including national initiatives in India. Owing to its high energy density and carbon-free combustion, hydrogen is widely regarded as a promising energy carrier; however, its large-scale application is limited by sluggish reaction kinetics and dependence on costly noble-metal electrocatalysts. Nickel-based materials have emerged as attractive alternatives due to their abundance on Earth, rich redox chemistry, and activity toward water-splitting reactions. Nickel-based metal organic frameworks (Ni-2 Methyl Imidazole MOFs) are particularly attractive because they offer high surface areas, tunable coordination environments, and uniformly distributed active sites; however, their low electrical conductivity limits their practical performance. On the other hand, Two-dimensional 1T/2H heterophase MoS_2 combines the high electrical conductivity of the metallic 1T phase with the catalytically active edge sites of the 2H phase. This synergistic phase coexistence optimizes hydrogen adsorption energetics and facilitates charge transfer during HER, but the bifunctional water-splitting is hindered by its low affinity for OER intermediates (*OH, *O, *OOH) and structural instability under oxidative potentials. Incorporating Ni 2MIm-MOFs with MoS_2 into heterostructured frameworks offers a viable approach to tackle these difficulties via interfacial charge redistribution and synergistic catalytic capability. Ni 2MIm-MOF/MoS_2 heterostructures are developed to improve interfacial electronic interactions in bifunctional hydrogen electrocatalysis. Strong interface electronic coupling reduces charge transfer resistance, speeds reaction kinetics, and stabilizes catalysis. MOF-chalcogenide heterostructures are effective bifunctional water-splitting electrocatalysts due to cooperative proton-electron transfer between Ni-ligand coordination environments and Mo-S catalytic sites.

Keywords: Bifunctional electrocatalysis, metal-organic frameworks, interfacial engineering, proton-electron coupling

References:

1. John, G., Savariraj, A. D., Archana, J., Xie, W., & Jesuraj, P. J. (2025). *International Journal of Hydrogen Energy*, *167*, 150987.
2. Guo, Y., Tang, J., Qian, H., Wang, Z., & Yamauchi, Y. (2017). *Chemistry of Materials*, *29*(13), 5566-5573.

EN-102

Hybrid Fe_3O_4/PANI Nanocomposites for Advanced Electrochemical Energy Storage

K Calvin[1*], Hayato Nagasaka[1,2] Atsushi Nakamura[1,2*]

[1]*Graduate School of Science and Technology, Shizuoka University*

3-5-1 Johoku, Naka-ku, Hamamatsu, 432-8011 Japan

[2]*Research Institute of Electronics, Shizuoka University.*

***Corresponding author e-mail:** nakamura.atsushi@shizuoka.ac.jp

ABSTRACT

Supercapacitors serve as advanced electrochemical energy storage systems that bridge the performance gap between conventional capacitors and rechargeable batteries, offering superior power density, rapid charge–discharge capability, and outstanding cyclic stability. In this work, a nanocomposite of polyaniline (PANI) and magnetite (Fe_3O_4) was synthesized to exploit the synergistic pseudocapacitive behavior of both components. PANI, a conductive polymer with reversible doping–dedoping redox activity, provides a highly conductive network that promotes efficient electron transport, whereas Fe_3O_4 contributes faradaic charge storage through its redox-active sites and excellent chemical stability. The nanocomposite was prepared using a hydrothermal synthesis route, enabling uniform precursor dispersion, controlled morphology, and in-situ composite assembly under mild conditions. Structural and morphological characterizations performed by X-ray diffraction (XRD) and scanning electron microscopy (SEM) confirmed the formation of phase-pure crystalline Fe_3O_4 with a dominant (311) diffraction peak and spherical nanoparticle clusters forming dense, rough, and textured surfaces. These results demonstrate the potential of the PANI/Fe_3O_4 hybrid system as a promising electrode material for high-performance supercapacitor applications.

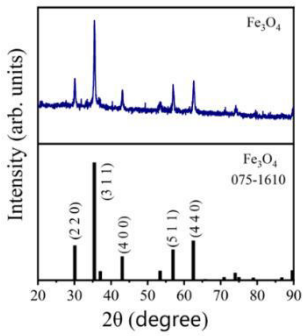


Fig. 1 XRD pattern of Fe_3O_4.

Keywords: Magnetite; super capacitor; PANI; energy storge system

References:

1. R. K. Singh et al., IJIREEICE, (2021).
2. P. Singh et al., J. Fluid Flow Heat Mass Transfer, (2024).

EN-103

Band Gap Engineered Cd-Pb Co-Doped SnS Nanoparticles via Microwave Solvothermal Route for DSSC Photoanodes

Kasthuri D and Sakthi Sudar Saravanan R*

PG & Research Department of Physics, Chikkanna Government Arts College, Tiruppur, Tamilnadu - 641 602, India

***Corresponding author e-mail:** rsakthiss@yahoo.com

ABSTRACT

Tin sulphide (SnS) is an emerging earth-abundant semiconductor with a suitable band gap for photovoltaic applications. In this work, pure SnS, Cd-doped SnS, Pb-doped SnS and Cd–Pb co-doped SnS nanoparticles (5 mol%) were synthesized through a rapid solvothermal microwave irradiation technique to obtain highly crystalline nanostructures. X-ray diffraction patterns of all the samples confirmed the formation of single-phase orthorhombic SnS, and the average crystallite size of the pure sample was found to be 12 nm, while the doped and co-doped samples exhibited a slight increase in crystallite size due to enhanced crystal growth and dopant-induced lattice strain. The absence of secondary phases suggests the successful incorporation of Cd and Pb ions into the SnS lattice. FESEM and HRTEM analyses revealed densely packed nanograins, and the doped samples showed relatively larger and more interconnected particles than the pure SnS, which is favorable for electron transport in photovoltaic devices. EDX spectra confirmed the presence and homogeneous distribution of the dopant elements. UV–Visible absorption studies indicated strong absorption in the visible region with a band gap of 1.81 eV for pure SnS, whereas the doped and co-doped samples exhibited a slightly reduced band gap, enabling broader light harvesting. When employed as photoanodes in dye-sensitized solar cells, the doped and co-doped SnS electrodes demonstrated enhanced charge transport and improved interfacial electron transfer compared to the pristine sample. The Cd–Pb co-doped SnS photoanode showed the best photovoltaic performance due to the synergistic effect of dual doping, which improved crystallinity, light absorption and carrier mobility. These results confirm that microwave-assisted dual doping is an effective strategy for tuning SnS nanomaterials for high-efficiency DSSC applications.

Keywords: SnS nanoparticles; doped and co-doped SnS nanoparticles; SMI technique; XRD analysis; EDX; HRTEM; UV-vis. Analysis; DSSC analysis

EN-104

Electronic Structure and Interface Modulation in Bi_2WO_6–Carbon Nitride Heterostructures Via Transition Metal Doping for Boosted Photocatalytic Nitrate-To-Ammonia Conversion

Lekshmi Priya SL[1], Hyoung-il Kim[2*] and Karthikeyan Sekar[1,2]*

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India*

[2] *Department of Civil & Environmental Engineering, Yonsei University, Seoul 03722, Republic of Korea*

***Corresponding author e-mail:** karthiks13@srmist.edu.in

ABSTRACT

Photocatalytic conversion of nitrate to ammonia has emerged as a promising approach for sustainable ammonia synthesis with potential applications as a fuel and storage medium for the transportation of hydrogen fuel. In this study, hydrothermally synthesized Cu doped Bi_2WO_6 / g-C_3N_4 is explored as the photocatalyst for nitrate-to-ammonia conversion. Bi_2WO_6, a well-explored photocatalyst, undergoes structural and electronic properties changes with the influence of Cu doping, while the incorporation of g-C_3N_4 enhances the light absorption and charge transfer efficiency. Spherical Bi_2WO_6 with spindle-like g-C_3N_4 nanosheets and varying percentages of copper were synthesized. The electronic structure and catalytic activity toward ammonia production are tuned by Cu doping, with the optimum doping level identified to maximize performance. The structural, morphological and chemical properties of the catalysts were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), photoluminescence spectroscopy (PL), time-resolved photoluminescence spectroscopy (TRPL), X-ray Photoelectron Spectroscopy (XPS) and UV-Visible spectroscopy (UV-Vis). The material demonstrates good catalytic activity towards nitrate reduction, and the optimal 2% Cu doping produces an exceptional ammonium yield of 289.3 μmol g^{-1} h^{-1}, which has been confirmed using the Indophenol method. Additionally, Nessler's reagent method and NMR were also employed to further confirm the production of ammonia. These findings not only deepen our comprehension of photocatalytic nitrate reduction processes but also highlight the potential of non-precious metal catalysts for sustainable ammonia production and environmental remediation applications.

References:

1. Chunran Zhao, Xiaojing Li, ACS Appl. Nano Mater. 2023, 6, 15709−15720
2. Xiaojing Li, Chunran Zhao, Front. Chem. Sci. Eng. 2023, 17(10): 1412−142

Synergistic Effect of Ni Doped in Zno Enhancing Charge Separation for Efficient Eco-Friendly Sun Light Driven Photodegradation

Saravanan Selvaraj[1]*, Simon Patrick[2], V. S. Manikandan[3], T. Govindaraj[2],

Arun Thirumurugan[3], M. Krishna Mohan[1], M. Navaneethan[2,]

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur- 6030203, India.*

[2]*Nanotechnology Research Centre (NRC), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur- 603 203, India.*

[3]*Sede Vallenar, Universidad de Atacama, Costanera 105, Vallenar-1612178, Chile*

***Corresponding author e-mail:** saravans3@srmist.edu.in

ABSTRACT

Herein, ZnO and Ni-doped ZnO nanoparticles were synthesized by co-precipitation method. The Structural, morphological, and optical characterization confirmed that Ni incorporation effectively modify the electronic structure of ZnO, reducing its band gap to 3.06 eV and suppressing electron-hole recombination. Notably, the optimized 3% Ni-ZnO showed the highest photocatalytic activity, achieving degradation efficiency of 94% for Methylene blue (MB) and 97% for Rhodamine (RhB) within 90 minutes, with corresponding kinetic rate constants of 0.02381 min^{-1} and 0.03489 min^{-1}, nearly fourfold greater than pure ZnO. The superior activity is attributed to the synergistic effect of Ni doping, which increases surface-active sites, efficient charge separation. The scavenger studies revealed that generation of hydroxyl radicals ($OH^{\bullet}$) and holes (h^{+}) reactive species, which are involved in the photodegradation process. The 3% Ni-ZnO photocatalyst maintained 85% efficiency, and XRD analysis confirmed its structural robustness after five consecutive cycles. These results highlight Ni-doped ZnO as a promising, durable, and sun light driven photocatalyst for sustainable waste water remediation.

Keywords: Ni-doped ZnO, Photocatalysis, Methylene blue (MB), Rhodamine B (RhB), dye degradation

EN-106

Mesoporous Silica Dispersed Polyethylene Glycol Nano-Phase Change Material Embedded Rooftop Tiles for Thermal Comfort and Energy Savings in Green Buildings

Naveen S. Lal, Aswin E. J, Dwija Nair, Minnu Elizabeth Sajan, Vishnuprasad Selvaraj*

Department of Chemical Engineering, Saintgits College of Engineering (Autonomous), Kottayam, Kerala – 686532

***Corresponding author e-mail:** *vishnuprasad.s@saintgits.org*

ABSTRACT

This research aims to develop mesoporous silica nanoparticle-enhanced polyethylene glycol (PEG) nano-phase change material (NPCM) with improved thermal energy storage characteristics for application in composite rooftop materials such as tiles and asbestos cement sheets. Mesoporous silica nanoparticles with average size of 100 nm and average pore size of 5.88 nm were successfully synthesized using a wet hydrothermal method. The surface area of the nanoparticles obtained using BET analysis was 842.50 m^2/g which contributes to achieve high latent heat capacity while maintaining low thermal conductivity to enhance thermal regulation and indoor thermal comfort in building applications. Mesoporous silica nanoparticles are incorporated into the PEG matrix to improve shape stability, prevent leakage during phase transition, and enhance thermal reliability through nanoscale confinement effects. Thermal analysis results showed that no significant changes in thermal conductivity and thermal diffusivity were observed for NPCM with the addition of mesoporous silica nanoparticles. The latent heat capacity of the nano-phase change material increased with nanoparticle concentration up to an optimal loading of 0.4 wt.% due to enhanced heterogeneous nucleation and improved crystallinity of PEG. A maximum enhancement of 4.41% in latent heat compared to PEG at 0.4 wt.% was obtained. The developed NPCM is integrated into rooftop composite tile, and its thermal performance is evaluated under a simulated experimental set-up. Results demonstrate significant improvement in latent heat storage capacity, enhanced thermal stability, and effective temperature regulation potential of the NPCM tile. The NPCM-integrated rooftop tile achieved an average indoor-side daytime temperature reduction of approximately 1–2°C, with peak-hour reductions of about 3–4°C during early afternoon conditions. This work contributes toward sustainable energy-efficient roofing solutions by combining nano-engineered phase change materials with practical construction materials.

Keywords: Mesoporous silica nanoparticles; Polyethylene glycol; Nano phase change material; Latent heat storage; Rooftop tile; Passive thermal management

References:

1. Khemlata Soni, Narayan Lal Panwar, Prog. Eng. Sci., 1 (2024) 100023.
2. Xiaowu Wang, Zhi Li, Min Hu, Qiong Liu, Ming Li, Xudong Cheng, Xiaoxu Wu, Appl. Clay Sci., 251 (2024) 107316.
3. Vishnuprasad Selvaraj, Haribabu Krishnan, J. Energy Storage, 45 (2022) 103774.

EN-107

Efficient and Stable Triple Cation Perovskite Precursor-Based Solar Cells Empowered by Interface with 2-2'-Dihydroxy-4-Methoxy Benzophenone Stabilizer

Peer Mydeen Mohammed Vajith Ali, Babu Poonguzhali, Nagarathinam Santhosh Kumar, Ramalingam Kishore, Ezhakudiyan Ravindran *

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Chengalpattu District, Tamil Nadu

***Corresponding author e-mail:** ravindre@srmist.edu.in

ABSTRACT

The current leading perovskite solar cells (PSCs) employ as a blend of formamidinium and methylammonium as their monovalent cations. Moreover, incorporating inorganic cesium into the mix, the resultant triple-cation perovskite compositions exhibit enhanced thermal stability, reduced phase impurities, and heightened resilience to variations in processing conditions. Moreover, effective trap-site passivation plays a dynamic role in weakening charge recombination and the subsequent energy loss within high-performance perovskite solar cells (PSCs). To effectively fulfill the role of a passivating agent, we have designed a molecular architecture named 2-2'-Dihydroxy-4-methoxy benzophenone (**DMP)**. The key solid-state analyses accomplish that they conceivably overwhelm the bottleneck of the surface defect. The obtained findings facilitate the attainment of more consistent device performances, ultimately achieving a stabilized power conversion efficiency (PCE) of 18.96%. These characteristics assume paramount significance for the industrialization of perovskite photovoltaics.

Keywords: Dual passivation, perovskite solar cells, grain boundaries, thin film device fabrications, surface coverage, and stability

References:

1. Y. Wang, X. Li, and H. Yu, Journal of Materials Chemistry *A*, 2021, *9*, 12345.
2. J. Chen, L. Zhang, and S. Liu, *Solar RRL*, 2020, *4*, 2000321.
3. N. J. Jeon, H. Na, and S. I. Seok, *Nature Energy*, 2018, *3*, 682.

EN-108

3D flower cobalt oxide nanoarchitectures for supercapacitor applications

Tamilmani Vairapperumal*

Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Tamilnadu, India, 603110

***Corresponding author e-mail:** tamilmaniv@ssn.edu.in

ABSTRACT

Ternary spinel $CuCo_2O_4$ nanoarchitectures have gained considerable attention as high-performance electrode materials for next-generation energy storage systems, owing to their remarkable electrical conductivity and superior electrochemical properties. In this study, we report the synthesis of a carbon-free, binder-free three-dimensional (3D) bottle-brush (BB) flower-like $CuCo_2O_4$ structure, which is directly grown on nickel foam (NF) via a simple hydrothermal method. This method ensures uniform growth and enhances structural integrity of the nanoarchitectures. Following the hydrothermal synthesis, the samples are annealed at a temperature of 420 °C for a duration of 2 hours. This annealing process is crucial for improving the crystallinity and electrochemical performance of the $CuCo_2O_4$ structures. The resulting $CuCo_2O_4$/NF composite, which exhibits varying ratios of Co^{2+} to Cu^{2+}, serves as the active electrode material in supercapacitor (SC) applications. The unique structural features of the flower-like architecture promote increased surface area and effective ion transport, significantly enhancing the charge-storage capacity and overall performance of the supercapacitor. Our findings indicate that the tailored $CuCo_2O_4$/NF composite demonstrates outstanding electrochemical properties, making it a promising candidate for high-performance energy storage devices. This work highlights the potential of 3D nanoarchitectures in advancing the field of sustainable energy storage technologies.

References:

1. Veeramani V, Madhu R, Chen S-M, Sivakumar M, ACS Sustainable Chemistry & Engineering, 4 (2016) 5013.
2. Jadhav H S, Pawar S M, Jadhav A H, Thorat G M, Seo J G, Scientific reports, 6 (2016) 31120.
3. Huang Y, Jiang Y, Zou L, Cheng J, Chi B, Pu J, Li J, Journal of The Electrochemical Society, 164 (2017) A3896

EN-109

Microwave-Assisted $Bi_{2-x}Sb_xS_3$ Alloy Nanoparticles for Enhanced Visible-Light Photocatalytic Dye Degradation

Sharon Sophia V, Sakthi Sudar Saravanan R*

PG & Research Department of Physics, Chikkanna Government Arts College, Tiruppur, Tamilnadu - 641 602, India.

***Corresponding author e-mail:** rsakthiss@yahoo.com

ABSTRACT

Narrow band gap bismuth sulphide (Bi_2S_3) is an efficient visible-light-responsive semiconductor; however, rapid charge carrier recombination limits its photocatalytic performance. In this work, pure Bi_2S_3 and Sb-alloyed $Bi_{2-x}Sb_xS_3$ (x = 0.1) nanoparticles were synthesized through a rapid solvothermal microwave irradiation technique to tailor the electronic structure and improve photocatalytic efficiency. X-ray diffraction analysis confirmed the formation of an orthorhombic phase for both samples, with an average crystallite size of 15 nm for pristine Bi_2S_3, while the alloyed $Bi_{1.9}Sb_{0.1}S_3$ exhibited a slightly larger crystallite size due to Sb^{3+}-induced lattice modulation that promotes crystal growth and enhances structural ordering. Energy dispersive X-ray spectroscopy verified the successful incorporation and homogeneous distribution of Sb in the Bi_2S_3 matrix. Optical absorption studies revealed a band gap of 1.53 eV for pure Bi_2S_3, whereas the alloyed sample showed a marginal band gap narrowing with enhanced absorption intensity in the visible region, facilitating improved photon utilization. The photocatalytic activity was evaluated through the degradation of methylene blue and rhodamine B under visible-light irradiation, and the alloyed $Bi_{1.9}Sb_{0.1}S_3$ exhibited significantly enhanced degradation efficiency compared to pristine Bi_2S_3. The superior performance of the alloyed sample is attributed to alloy-induced electronic structure modulation, which promotes efficient charge carrier separation, reduces recombination probability and accelerates interfacial charge transfer for the generation of reactive oxygen species. In addition, the increased crystallite size and improved crystallinity facilitate faster carrier transport, while the nanoscale dimensions provide a large surface area for dye adsorption and catalytic reaction. The microwave-assisted synthesis further ensures uniform nucleation and defect-assisted charge migration pathways. This study demonstrates that controlled Sb incorporation into the Bi_2S_3 lattice is an effective strategy for achieving synergistic enhancement in structural, optical and photocatalytic properties, making $Bi_{2-x}Sb_xS_3$ a promising visible-light-driven photocatalyst for wastewater remediation.

Keyword: $Bi_{2-x}Sb_xS_3$ alloy; Microwave solvothermal synthesis; Visible-light photocatalysis; Charge carrier separation; Dye degradation

EN-110

Band Structure Modulation in Co-Doped SnO_2 Nanoparticles for High-Performance UV Photocatalytic Dye Degradation

Sivaranjani T[1], Balan R[2], Sakthi Sudar Saravanan R[1,] *

[1]*PG & Research Department of Physics, Chikkanna Government Arts College, Tiruppur, Tamilnadu - 641 602, India.*

[2]*Department of Physics, Government Arts and Science College, Mettuppalayam, Tamilnadu - 641 104, India.*

***Corresponding author e-mail:** rsakthiss@yahoo.com

ABSTRACT

Nanocrystalline SnO_2 is an important wide band gap semiconductor widely explored for photocatalytic environmental remediation due to its high chemical stability and strong oxidation ability under ultraviolet irradiation. In the present study, pure SnO_2, Ce-doped SnO_2, Cu-doped SnO_2 and Ce–Cu co-doped SnO_2 nanoparticles with a dopant concentration of 5 mol% were synthesized using a rapid solvothermal microwave irradiation technique to obtain uniformly crystalline nanostructures. X-ray diffraction analysis confirmed the formation of a tetragonal rutile-type crystal structure for all the samples without the appearance of secondary phases, indicating successful incorporation of dopant ions into the host lattice. The average crystallite size of the pure SnO_2 was found to be 7 nm, while the doped and co-doped samples exhibited a slight increase in crystallite size due to dopant-induced lattice distortion and enhanced grain growth. Energy dispersive X-ray spectroscopy confirmed the elemental composition and uniform distribution of Ce and Cu in the SnO_2 matrix. UV–Visible absorption studies revealed an optical band gap of 3.68 eV for the pure SnO_2, whereas the doped and co-doped nanoparticles showed a marginal reduction in band gap with improved absorption in the near-UV region. The photocatalytic performance of the synthesized samples was evaluated through the degradation of Methylene Blue and Methyl Orange under UV light irradiation. The doped SnO_2 nanoparticles exhibited higher degradation efficiency than the pristine sample, while the Ce–Cu co-doped SnO_2 showed the fastest degradation rate for both dyes. The enhanced photocatalytic activity is attributed to dopant-induced defect states, improved charge carrier separation and increased availability of surface-active sites. The nanoscale crystallite size further facilitates higher dye adsorption and efficient generation of reactive oxygen species during irradiation. This study demonstrates that microwave-assisted dual doping is an effective strategy for tailoring the structural and optical properties of SnO_2 nanoparticles for efficient UV-driven photocatalytic wastewater treatment.

Keyword: SnO_2 nanoparticles; Ce and Cu doped and co-doped SnO_2 nanoparticles; SMI technique; XRD analysis; EDX; HRTEM; UV-vis. Analysis; Photocatalytic analysis

EN-111

Comparative Study of Reflux and Autoclave-Assisted Transesterification of Jatropha Oil Using Cao-Doped Mesoporous SBA-15

Thamizharasi Pugazhenthi, Ganesh Srinivasan, N.R. Sasirekha*

Catalysis Laboratory, CAS in Crystallography & Biophysics, University of Madras, Guindy Campus, Chennai 600025, Tamil Nadu, India

***Corresponding author e-mail:** nrsasirekha@gmail.com

ABSTRACT

An ever-increasing demand for fuel poses a significant challenge to researchers, as fossil fuel resources are dwindling. Biodiesel production from non-edible feedstocks has gained significant attention as a sustainable alternative to conventional fossil fuels. Low-cost Jatropha oil is considered as a potential non-edible feedstock for biodiesel production. In this study, a comparative investigation was conducted on both reflux and autoclave-assisted transesterification of Jatropha oil using CaO-doped SBA-15, a heterogeneous catalyst. The mesoporous SBA-15 support offers a high surface area and uniform pore structure, facilitating the effective dispersion of CaO and enhancing the availability of basic active sites required for transesterification. The catalyst was synthesized via the impregnation method and characterized to confirm its structural integrity and successful incorporation of active phase. Transesterification reactions were performed under optimized reaction parameters in both conventional reflux and autoclave systems. The reflux set-up provided continuous condensation and open-system heating, whereas the autoclave functioned as a closed static reactor without external pressure. The performance of both systems was evaluated in terms of biodiesel yield, reaction time, and catalytic efficiency. The results demonstrate notable differences in reaction kinetics and conversion efficiency between the two approaches. Autoclave-assisted transesterification showed improved conversion within shorter reaction time due to enhanced mass transfer and internal pressure effects, whereas the reflux system offered operational simplicity and low energy requirements. This comparative study highlights the influence of reaction environment on catalytic performance and provides valuable insights for selecting appropriate processing conditions for sustainable biodiesel production.

Keyword: Biodiesel, Jatropha oil, Transesterification, Wet impregnation, SBA-15

References:

1. D. Meloni et al., Appl. Catal. B, 184 (2016) 163–173.
2. R. Malhotra and A. Ali, Renew. Energy, 133 (2019) 606–619.
3. A. Z. Abdullah et al., Fuel Process. Technol., 90 (2009) 958–964.
4. A. Sarkar et al., Fuel, 348 (2023) 128537.
5. Y. Tan et al., Renew. Energy, 150 (2020) 370–381.

High-Performance Ru50/Pt50-MoS2/rGO Bifunctional Electrocatalyst for Sustainable Overall Water Splitting and Seawater Electrolysis

M. Arthick, G. Bharath*

Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu – 603203, India

***Corresponding author e-mail:** sribharath7@gmail.com and bharathg4@srmist.edu.in

ABSTRACT

Electrodes play a crucial role in bifunctional applications for alkaline environments, where they catalyze both hydrogen and oxygen evolution reactions. Advanced electrode materials like molybdenum disulfide (MoS_2) embedded in reduced graphene oxide (rGO) layers are pivotal for enhancing catalytic activity in these settings. Their design and material composition directly influence the efficiency and stability of energy conversion processes, making them key to addressing the supply-demand imbalance in renewable energy. In this work, we have synthesized MoS_2 nanoparticles embedded in rGO layers, enhancing their catalytic activity for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline environments. The development of such bifunctional electrodes is crucial for efficient water electrolysis, a key process in the sustainable production and utilization of renewable energy. The nanocomposite materials were characterized using various spectroscopic and microscopic techniques. A Tafel slope of approximately 40 mV/decade suggests that the Volmer-Heyrovsky mechanism predominates in the HER process with the MoS_2/GO composite acting as the catalyst, pinpointing electrochemical desorption of hydrogen as the rate-limiting step. The composite demonstrated superior catalytic behavior compared to the MoS_2/rGO composite, with lower activation energy values indicating faster HER kinetics. Importantly, the robust performance of these alkaline-based electrodes makes them particularly suitable for seawater electrolysis, where they can effectively handle the challenging conditions posed by high salinity and pH levels. This advancement is crucial for the OER as well, ensuring efficient and stable operation under such conditions. This work underlines the importance of developing stable, efficient electrodes for alkaline seawater electrolysis, contributing significantly to the field of energy conversion and storage in renewable energy systems.

Keyword: Bifunctional electrodes; Alkaline water electrolysis; MoS_2/graphene nanocomposites; Hydrogen evolution reaction (HER); Oxygen evolution reaction (OER).

Synergistic High-Entropy Oxide/Graphene Hybrids: Advancing Energy and Environmental Remediation

Arunaprabha A, Ravikirana*

High Temperature Materials Processing Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu 603 203, Tamil Nadu, India.

***Corresponding author e-mail:** ravikirs@srmist.edu.in

ABSTRACT

The quest for sustainable energy storage and environmental remediation has spurred the rise of advanced multifunctional materials. High entropy oxides (HEOs) have emerged as a groundbreaking class of materials, characterized by their unique structural stability, high configurational entropy, and exceptional physicochemical properties. Composed of multiple principal cations in near-equimolar ratios, HEOs exhibit entropy-stabilized single-phase crystal structures with remarkable mechanical strength, thermal stability, and tunable electronic characteristics, making them ideal for energy and environmental applications. When combined with reduced graphene oxide (rGO)—a 2D carbon material known for its conductivity and adsorption capabilities—a transformative composite emerges. This HEO/rGO hybrid exhibits remarkable electrochemical performance, enhancing supercapacitor efficiency with high specific capacitance, low resistance, and exceptional cycling stability. Simultaneously, it delivers unparalleled photocatalytic activity for degrading toxic dyes like methylene blue, addressing critical water pollution challenges. This study unveils the synthesis and multifunctional potential of HEO/rGO composites, demonstrating their prowess in bridging energy and environmental solutions. These materials not only promise breakthroughs in energy storage but also pave the way for cleaner, greener technologies.

Keyword: High entropy oxides, reduced graphene oxide, supercapacitors, photocatalysis, environmental remediation.

References:

1. P. Harika, G. G. Sravani, S. S. Rao, and A. L.-E. Kille, IEEE Trans. Nanobiosci., 24 (2025) 25–36.

EN-114

Exploring The Role of Interstitial Occupation of Cobalt on the Thermoelectric Properties of Co-Rich Te-Substituted Skutterudite.

Chaklathy Devassy Saagar[1], Tanu Choudhary[2], Raju K. Biswas[2], Ramesh Chandra Mallik[1,*]

[1]*Thermoelectric Materials and Devices Laboratory, Department of Physics, Indian Institute of Science, Bangalore 560012, India*

[2]*Department of Physics, Faculty of Natural Sciences, M S Ramaiah University of Applied Sciences, Bengaluru 560058, India*

***Corresponding author e-mail:** rcmallik@iisc.ac.in

ABSTRACT

Excess cobalt finding its niche at an interstitial position enables new modes of scattering in addition to scattering by mass fluctuations and rattlers. The positive Seebeck coefficient for the Co-rich sample indicates the p-type nature due to the excess cobalt occupying the energetically favourable interstitial site rather than its lattice site. The introduction of additional vibrational modes evidenced in Raman spectroscopy sanctions the interstitial occupation of the cobalt atom. These additional vibrational modes, concomitant with the mass fluctuations in Te substituted $CoSb_3$, maintain low thermal conductivity while optimizing the power factor due to increased carrier concentration. X-ray photoelectron spectroscopy studies revealed the rapid oxidation of the sample surface to form the native oxide Sb_2O_3 and $Co(OH)_2$. The electronic, structural and vibrational properties of pristine, Co-rich, and Te-substituted $CoSb_3$ were studied using density functional theory. The Co-rich system exhibits an enhanced Seebeck coefficient compared to pristine, driven by conventional and unconventional band convergence present in the valence band. Te substitution into Co-rich $CoSb_3$ induces n-type doping. This transformation is accompanied by the emergence of strong Co 3d and Te 5p orbital interactions, as revealed by Crystal Orbital Hamilton Population analysis, exhibiting a significant antibonding state just below the Fermi level. The resulting Co–Te bond weakening reduces lattice thermal conductivity.

EN-115

Tailoring the Electrochemical Performance of ZnO/NiS/MWCNT Ternary Composites for Supercapacitor Application

Poovitha Ganesan[1], B. Leena[1], S. Divyadharshini[1], D. Paul Joseph[2], Kovendhan Manavalan[1]*

[1]Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu - 603202, Tamilnadu, India.

[2]Department of Physics, National Institute of Technology-Warangal, Telangana state 506004, India.

***Corresponding author e-mail:** wchoi@kentech.ac.kr

ABSTRACT

Supercapacitors, also known as ultracapacitors have emerged as a promising energy storage device due to their high-power density, rapid charging-discharging and excellent cycle life. They effectively bridge the gap between conventional capacitors power density and batteries energy density. However, carbon-based materials provide high power density, excellent cyclic stability and fast charging-discharging rate and the disadvantages is low specific capacitance and energy density compared to batteries. Metal oxides and sulfides-based materials provide high specific capacitance and energy density due to faradaic reaction and the disadvantages are lower cyclic stability and power density. By combining carbon-based materials with metal oxides and sulfides have significantly increases their energy density and cyclic stability. The ZnO/NiS/MWCNT-x (x = 1, 5, 10%) nanocomposite synthesized via a hydrothermal method exhibits a higher specific capacitance, outstanding cyclic stability and excellent rate capability. A key differentiator of our system is the optimization of MWCNT incorporation, which has been carefully tuned to achieve an equilibrium between material conductivity, stability, and electrochemical activity. This work demonstrates the potential of integrating metal oxides, sulfides, and carbon-based nanocomposites to achieve high-efficiency supercapacitors. These advancements make the supercapacitors as a highly promising technology for the future energy storage system. The prepared samples will be characterized using XRD, SEM, FTIR, Raman spectroscopy, and electrochemical studies. The findings from these experimental analyses will be discussed in detail.

Keywords: Supercapacitors, metal oxides, sulfides, carbon-based materials, hydrothermal synthesis, energy storage.

References:

1. S. S. Rao, J. Energy Storage, 28 (2020) 101199.
2. F. Ahmad et al., J. Energy Storage, 81 (2024) 110430.

EN-116

Unlocking Synergy in MXene-Supported W-Cr-Ni_2P for Overall Water Splitting

Elveena Jose, Sellappan Senthilkumar*

Department of Chemistry, School of Advanced Sciences

Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India- 632014

***Corresponding author e-mail:** senthilkumar.s@vit.ac.in

ABSTRACT

Development of efficient and durable electrocatalysts for overall water splitting are essential for generating clean and sustainable hydrogen (H_2). In this work, we present the design of vanadium MXene-supported nickel-based trimetallic phosphides as advanced bifunctional electrocatalysts for H_2 and O_2 production. MXene nanosheets (NSs) are two-dimensional materials with unique metallic properties, including high surface area, tunable surface chemistry, moderate hydrophilicity and excellent electrical conductivity. The incorporation of vanadium MXene provides a conductive support to trimetallic phosphides (TMPs). In the nickel phosphide framework (Ni_2P), doping with multiple transition metals (such as Cr, W) plays a pivotal role in enhancing catalytic performance, increasing the density of active sites and fine-tuning the electronic structure, which leads to optimized adsorption energies for intermediates. Since phosphorus is more electronegative than transition metals, it facilitates electron transfer from metals, thereby enhancing their catalytic activity. Furthermore, the excellent corrosion resistance and metalloid character of phosphorus contribute to the durability of the catalyst under harsh environmental conditions. Various structural and electrochemical studies revealed that the hybrid catalyst exhibits low overpotentials for both hydrogen and oxygen evolution reactions. The synergistic interplay between the MXene NSs and TMPs, results in increased surface area, accelerated charge transfer and improved reaction kinetics. This study highlights the potential of MXene-supported nickel phosphides as a promising platform for scalable and sustainable water splitting technologies, offering new insights into catalyst design for clean energy applications.

References:

1. H. Pan, S. Perumal, M. Sakthivel, S.-N. Lin, M.-H. Yeh, W.-Y. Yu, and K.-C. Ho, Chem. Eng. J., 515 (2025) 163888.
2. S. Li, Y. Jiang, J. Liang, L. Zhang, F. Li, and X. Lv, J. Colloid Interface Sci., 704 (2025) 139476.
3. M. Jeong, S. Park, T. Kwon, M. Kwon, S. Yuk, S. Kim, C. Yeon, C.-W. Lee, and D. Lee, ACS Appl. Mater. Interfaces, 16 (2024) 34798–34808.
4. C.-H. Lin, S. Perumal, Y.-C. Lin, L.-Y. Hsiao, L.-Y. Lin, and K.-C. Ho, Int. J. Hydrog. Energy, 111 (2025) 40–51.
5. D. Guo, W. Tan, X. Guo, L. Wen, and X. Li, Appl. Surf. Sci., 721 (2025) 165481.

Electrodeposited Gadolinium-Doped Nickel Selenide: An Efficient Electrocatalyst for Hydrogen Evolution Reaction in Alkaline Media

K. Vaishnavi Chandran, Sellappan Senthilkumar*

Department of Chemistry, School of Advanced Sciences,

Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India-632014

***Corresponding author e-mail:** senthilkumar.s@vit.ac.in

ABSTRACT

Water electrolysis is an impressive and ecofriendly method of producing hydrogen (H_2) and oxygen (O_2) from aqueous medium. To date, noble metals (including Pt, Pd, Ru etc.) are considered as benchmark electrocatalysts, however, their scarcity and high cost limits their largescale industrial use. Hence, there is an urgent need of inexpensive and abundantly available materials, which can replace the noble metal based electrocatalysts. In this regard, nickel selenides (NiSe) have gained considerable attentions across the globe in energy conversion applications and can be synthesized by different approaches. The present work emphasizes on the synthesis of Gd doped NiSe on carbon cloth (CC) via simple electrodeposition technique. Further, the obtained material was characterized by various spectroscopic and microscopic techniques such as X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM) etc. In order to elucidate the catalytic efficiency towards hydrogen evolution reaction (HER), the fabricated materials are subjected to various electrochemical characterization studies. Notably, among the synthesized catalysts, NiSe-Gd-1.5 exhibited exceptional HER performance in 1 M KOH. The improved performance can be attributed to the engineered NiSe, which show synergistic interaction between the NiSe and Gd. NiSe-Gd-1.5 exhibited numerous active sites and high conductivity, thereby accelerating the HER performance. This strategy provides a viable platform to synthesize scalable quantities of Ni-based electrocatalyst.

References:

1. C.H. Mu, H.X. Qi, Y.Q. Song, Z.P. Liu, L.X. Ji, J.G. Deng, Y.B. Liao, F. Scarpa, RSC Adv. 6 (2015) 23–30.
2. C. Cannas, A. Musinu, A. Ardu, F. Orrù, D. Peddis, M. Casu, R. Sanna, F. Angius, G. Diaz, G. Piccaluga, Chem. Mater. 22 (2010) 3353–3361.
3. P. Salehan, A.A. Ensafi, Z. Andikaey, B. Rezaei, Sci. Rep. 13 (2023) 1–13.

EN-118

Structural, Optical, Magnetic, and Dielectric Properties of (1-x) NCFO + (x)BCZT Composites Synthesized via Solid-State Reaction

P. Naveen[1,2], N. Pavan Kumar[2], N. Kumar Swamy[1*]

[1]*Department of Physics, ISBM University, Nawapara (Kosmi), Gariaband, Chhattisgarh, 493 996, India*

[2]*Department of Physics, Matrusri Engineering College, Saidabad, Hyderabad – 500059, Telangana, India*

***Corresponding author e-mail:** nkumarswamy15@gmail.com*

ABSTRACT

In this study, novel multiferroic composites of (1-*x*) $Ni_{0.5}Co_{0.5}Fe_2O_4$+(*x*) $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (where *x* = 0.0,0.20, 0.40,0.60,0.80 and 1) were synthesized using the conventional solid-state reaction method. The structural characterization was carried out using X-ray diffraction (XRD), which provided crucial information about crystallite size, density, and lattice parameters through Rietveld refinement analysis. UV-vis spectra disclose the energy gap values, and for $Ni_{0.5}Co_{0.5}Fe_2O_{4,\ the}$ pure ferrite is 1.53 eV, the $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ pure ferroelectric phase is 2.99 eV, and energy gap values range from 1.46 eV to 2.17 eV across the composites. Surface morphology and grain size distribution were investigated using scanning electron microscopy (SEM), revealing the microstructural characteristics of the composites. Magnetic properties were analyzed using a vibrating sample magnetometer (VSM), which showed varying coercivity values across different compositions. The 60N40B composition demonstrated the highest coercivity at 491 O_e, while the 20N80B sample showed the lowest at 430 Oe. Other compositions showed intermediate values of 454 Oe for 80N20B and 474 Oe for 60N40B. The dielectric results demonstrate that (1-x) $Ni_{0.5}Co_{0.5}Fe_2O_4$ +(x) $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (where x = 0.0,0.20, 0.40, 0.60,0.80 and 100) composites exhibit promising characteristics for multifunctional applications. The dielectric constant $\varepsilon_{\circ}$ is high when the frequency range is between 100 and 1000 Hz. Moreover, the dielectric constant decreases and remains constant while increasing the frequency.

Keywords: Multiferroic composites, NCFO-BCZT, solid-state synthesis, Rietveld refinement, magnetic properties, lead-free materials, functional ceramics.

EN-119

Electrocatalytic Water Splitting Performance of $SrTiO_3$/rGO Composite for Hydrogen Evolution Reaction in Acidic Medium

B. Leena[1], S. Divyadharshini[1], D. Paul Joseph[2], Kovendhan Manavalan[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu – 603203, Tamilnadu, India.*

[2] *Department of Physics, National Institute of Technology, Warangal, Telangana – 506004, India*

***Corresponding author e-mail:** mkovendhan@gmail.com

ABSTRACT

The hydrogen evolution reaction (HER) is a pivotal process in sustainable energy technologies, particularly in water splitting for hydrogen production. This study investigates the electrocatalytic performance of $SrTiO_3$ (strontium titanate) and graphene oxide (GO) composites for HER. $SrTiO_3$ a perovskite oxide is known for its excellent photocatalytic properties, while rGO offers a high surface area and superior electronic conductivity. By combining $SrTiO_3$ with GO, we aim to enhance the HER activity through synergistic effects. $SrTiO_3$ holds immense potential for its application, offering unique properties and versatility. rGO because of its superior electrical conductivity, chemical stability, and large surface area, reduced graphene oxide (GO) has demonstrated considerable promise in energy storage applications. These properties can improve the efficiency of energy storage devices. This research aims to harness the unique properties of $SrTiO_3$-rGO composites for hydrogen evolution reaction, The $SrTiO_3$-rGO composites have electrical, mechanical, and electrochemical properties, making them ideal candidates for HER application. The characterizations (like XRD, SEM, TEM, XPS, UV, and Raman) confirm the presence of composite material, this study investigates the synthesis and optimization of $SrTiO_3$-rGO composites to achieve enhanced electrochemical performance for hydrogen evolution reaction (HER) application.

Keywords: Hydrogen evolution reaction, Strontium titanate, Graphene oxide, Heterostructure composite, Water splitting.

Reference

1. S. Fuentes, R. A. Zarate, E. Chavez, P. Muñoz, D. Díaz-Droguett, and P. Leyton, J. Mater. Sci., 45 (2010) 1448–1452.
2. H. Wang, W. Zhao, Y. Zhang, S. Zhang, Z. Wang, and D. Zhao, Solid State Commun., 236 (2016) 27–31.

EN-120

Structural and Magnetic Properties of Rare Earth-Doped $Ni_{0.8}Zn_{0.2}$ Ferrites Synthesized via Solid-State Reaction

Kante Mamatha[1], N. Pavan Kumar[2]
[1]*Department of physics, Government city college, Hyderabad,500003, Telangana, India*
[2]*Department of sciences and Humanities, matrusri Engineering Collage, Telangana, India*

ABSTRACT

A systematic series of cubic spinel ferrites were synthesized via solid-state ceramic reaction with progressive rare earth element (RE = Pr, Ho, Y) substitution to investigate structure-property relationships. Four compositions were prepared: the undoped reference $Ni_{0.8}Zn_{0.2}Fe_2O_4$, singly doped $Ni_{0.8}Zn_{0.2}Pr_{0.1}Fe_{1.9}O_4$, doubly doped $Ni_{0.8}Zn_{0.2}Pr_{0.05}Ho_{0.05}Fe_{1.9}O_4$, and triply doped $Ni_{0.8}Zn_{0.2}Pr_{0.03}Ho_{0.03}Y_{0.03}Fe_{1.9}O_4$. Powder X-ray diffraction (XRD) confirmed single-phase cubic spinel structures (space group *Fd*-3*m*) for all compositions with systematic lattice parameter modifications. Fourier transform infrared (FTIR) and Raman spectroscopy validated characteristic spinel metal-oxygen stretching modes. Scanning electron microscopy (SEM) revealed microstructural evolution and grain size refinement upon multi-dopant incorporation. Vibrating sample magnetometry (VSM) measurements demonstrated systematic variations in saturation magnetization, coercivity, and remanent magnetization with increasing rare earth dopant concentration. Elemental composition was confirmed via energy-dispersive X-ray spectroscopy (EDX). The multi-dopant system exhibited enhanced magnetic property tunability and refined grain morphology compared to single-dopant analogues, attributed to cooperative effects of Pr^{3+}, Ho^{3+}, and Y^{3+} substitution at iron sites. These findings demonstrate effective control of magnetic properties through strategic rare earth doping, with potential applications in high-frequency devices and tunable functional materials.

EN-121

Strategic Integration of Sns on Boronized Ni-ZIF for High-Performance Electrocatalysis and Energy Storage

G. John, J. Archana, P. Justin Jesuraj*
Center of Excellence in Materials and Advanced Technologies (CeMAT), Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Potheri, Chengalpattu 603203, India.
***Corresponding author e-mail:** justinp@srmist.edu.in

ABSTRACT

The escalating demand for sustainable energy conversion and storage technologies necessitates the development of high-performance, multifunctional electrocatalysts. Metal-Organic Frameworks (MOFs), particularly Nickel Zeolitic Imidazolate Frameworks (Ni-ZIF), are promising candidates; however, their practical application is often limited by poor intrinsic conductivity and a lack of accessible active sites. In this work, we report the strategic incorporation of tin sulfide (SnS) onto boronized Ni-ZIF (B:NiZIF) supported on nickel foam (NF) to create a robust bifunctional system for supercapacitors and alkaline water electrolysis. The resulting SnS/B:NiZIF/NF heterostructure demonstrates exceptional electrocatalytic activity in 1.0 M KOH, requiring low overpotentials of 290 mV for the oxygen evolution reaction (OER) and 72 mV for the hydrogen evolution reaction (HER) at 20 mA cm^{-2}. Furthermore, the integrated electrolyzer achieves a current density of 10 mA cm^{-2} at a cell voltage of only 1.54 V. For energy storage applications, the synergy between SnS and the B:NiZIF framework yields a superior specific capacitance of 2927.5 F g^{-1} (at 1 mA cm^{-2}). Characterization via X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) confirms that the enhanced performance originates from accelerated interfacial electron transfer and optimized sulfur exposure. The strong interfacial bonding within the SnS/B:NiZIF architecture ensures remarkable stability, highlighting its potential as a versatile electrode material for next-generation energy devices.

Study on the Thermoelectric Properties of BiCuOS-CuS Composites

Swathi D Warrier[1], Aryalakshmi Santhosh Kumar[2], Ramasubramanian Swaminathan *[1]

[1] *Department of Sciences, Amrita School of Physical Sciences Coimbatore, Amrita Vishwa Vidyapeetham, India*

[2] *Functional Materials Lab, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India*

***Corresponding author e-mail:** s_ramasubramanian@cb.amrita.edu

ABSTRACT

Reducing the global energy crisis requires efficient utilization of waste energy, and thermoelectric technologies offer a direct method to convert waste heat into electrical power. Bismuth copper oxy-chalcogenide (BiCuOCh) semiconductors have attracted attention as promising thermoelectric materials due to their low toxicity, environmental friendliness, and cost-effectiveness. While BiCuOSe has been widely studied and shows relatively good thermoelectric performance, its sulphur analogue BiCuOS exhibits intrinsically low electrical conductivity, leading to a low power factor and poor *z*T.

To address this limitation, this work enhances the thermoelectric properties of BiCuOS through composite engineering. A suitable secondary phase ensuring chemical compatibility, structural stability, and improved charge transport was selected. Copper sulphide ($Cu_{2-x}S$), a p-type conductor with high electrical conductivity, was chosen as the composite. $Cu_{2-x}S$ was synthesized via hydrothermal route, while BiCuOS was prepared by modified solid-state reaction method. BiCuOS– $Cu_{2-x}S$ composites with optimized ratios were then fabricated to tune the electrical transport properties. The incorporation of $Cu_{2-x}S$ improved electrical conductivity, enhancing the power factor and overall thermoelectric performance, providing a viable route toward efficient, stable, and environmentally friendly thermoelectric materials for waste heat recovery.

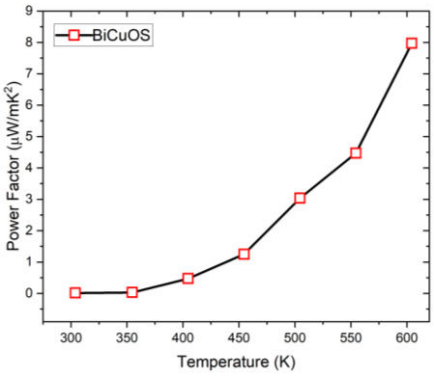


Fig 1: The power factor was achieved as 0.013 μW/mK² at room temperature and 7.98 μW/mK² at higher temperature range.

Keywords: Thermoelectrics, Oxy-chalcogenides, Composites.

References:

1. Labegorre J.-B., et al., *Chemistry of Materials*, **30** (2018) 1085–1094.
2. Tippireddy S., Kumar D. S. P., Das S., Mallik R. C., *ACS Appl. Energy Mater.*, **4** (2021). 2022–2040
3. Narjis A., et al., *J. Semicond.*, **39** (2018) 122001.

Optimizing $ZnCl_2$ Activation Temperature for Biomass-Derived Porous Carbons with Superior Energy and Power Density in Supercapacitors

Andem Sandeep[1], A.V. Ravindra[1*]

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai- 603 203, India.*

***Corresponding author e-mail:** venkatar1@srmist.edu.in

ABSTRACT

This study synthesizes a series of porous carbon materials (PS-Z-X, where X = 500, 600, 800, and 900 °C) through $ZnCl_2$-assisted chemical activation of biomass-derived precursors to assess their suitability as electrode materials for high-performance supercapacitors. HR-TEM and XRD analyses confirm the coexistence of amorphous carbon domains and residual ZnO, while BET analysis shows that surface area and pore volume increase with temperature. Among all samples, PS-Z-800 develops a hierarchical micro–mesoporous structure that enables efficient electrolyte ion transport and charge storage. Electrochemical tests in 1 M H_2SO_4 display ideal double-layer capacitive behavior, delivering a specific capacitance of 134 F g^{-1} at 1 A g^{-1} and excellent cycling stability with 98% retention after 5000 cycles. The symmetric device using PS-Z-800 achieves an energy density of 14.7 Wh kg^{-1} and a power density of 1176 W kg^{-1}, surpassing conventional activated carbon electrodes. Overall, this work demonstrates a simple, scalable, and economical approach to producing high-performance activated carbon from agricultural waste.

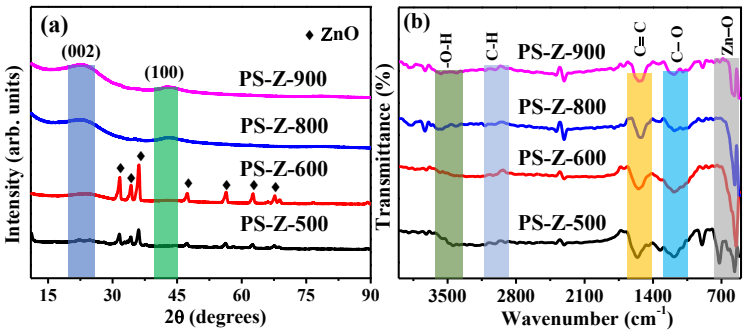


Fig. 1. (a) X-ray diffractograms and (b) FTIR spectra of all the prepared porous carbon samples.

Key Words: Supercapacitor; Hydrothermal; Activated Carbon; Carbonization.

EN-124

Sustainable Green Synthesis of CuO–ZnO Nanocomposite Heterostructures Using M. spicata L. for Catalytic Reduction of Various Dyes and Photocatalytic Degradation of Tetracycline

Kiruthika Murugesan[1], Siva Chidambaram[1], Maheswaran Rathinam[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603 203.*

***Corresponding author e-mail:** maheswar@srmist.edu.in

ABSTRACT

The extensive use and improper disposal of aromatic compounds, synthetic dyes, and antibiotics have caused their accumulation in water bodies, creating serious risks to human health and ecosystems. This necessitates the development of efficient, low-cost, and environmentally benign remediation technologies. In this study, a CuO-ZnO nanocomposite (NCs) was green-synthesised using *Mentha spicata* L. (mint) extract as a natural reducing and stabilising agent. FTIR analysis confirmed the presence of phytochemical functional groups from *M. spicata* L. on the CuO-ZnO NCs surface. The catalytic performance of the NCs was evaluated toward the reduction of 4-nitrophenol (4-NP), Rhodamine B (RhB), and Methyl Orange (MO), representing aromatic, cationic, and anionic pollutants, respectively. The CuO-ZnO NCs exhibited high reduction efficiencies of 94% (4-NP), 96.17% (RhB), and 94.38% (MO), with corresponding pseudo-first-order rate constants of 0.469, 0.03, and 0.247 min^{-1}. Furthermore, the NCs showed visible-light-driven photocatalytic activity toward tetracycline (TC), achieving 85.29% degradation within 25 min ($k = 0.1439\ min^{-1}$). The catalyst retained its activity after four consecutive cycles, indicating good stability and reusability. These results demonstrate that green-synthesised CuO-ZnO NCs are effective multifunctional catalysts for the removal of diverse organic pollutants from wastewater.

References:

1. A.G. Bekru, L.T. Tufa, O.A. Zelekew, M. Goddati, J. Lee, F.K. Sabir, ACS Omega 7 (2022) 30908–30919.
2. M. Bordbar, N. Negahdar, M. Nasrollahzadeh, Sep Purif Technol 191 (2018) 295–300.

EN-125

Structure–Function Modulation in Semiconductor Heterostructures for Efficient Solar Fuel Production

Srabanti Ghosh*, Dipendu Sarkar, Jishu Pramanik

[1]*Energy Materials & Devices Division (EMDD), CSIR - Central Glass and Ceramic Research Institute, Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, India*

[2]*Academy of Scientific & Innovative Research (AcSIR), 201 002, Ghaziabad, India*

***Corresponding author e-mail:** srabanti.cgcri@csir.res.in

ABSTRACT

Structure–Function modulation in semiconductor heterostructures, through the deliberate tuning of structural features at the atomic and nanoscales, enhances the photocatalytic efficiency of coupled semiconductor systems capable of driving multi-electron solar-to-chemical transformations, including water splitting for H_2 production, CO_2 reduction to value-added fuels, and N_2 fixation to NH_3 [1]. Engineering parameters, such as crystal phase, interface bonding, defect density, and heterostructures, enable precise control of electronic structure, band alignment, and interfacial charge dynamics. Strategic construction of type-II, Z-scheme, or S-scheme heterojunctions further allows selective retention of strong redox potentials while suppressing charge recombination. A wide range of representative systems, metal oxides, conducting polymers, bismuth oxyhalides (BiOX; X = Cl, Br, I), metal chalcogenides, oxide perovskites, and their heterostructures have been extensively investigated to clarify how these parameters influence light harvesting, charge carrier generation, and charge separation dynamics [2]. For example, layered BiOCl, owing to its intrinsic internal electric field derived from its unique crystal structure, exhibits markedly improved charge separation. When integrated into a heterostructure with Cu_2SnS_3, atomic-scale interfacial Bi–S bonds are formed, acting as effective charge-transfer channels between the two semiconductors and significantly boosting H_2 production efficiency [3]. More recently, atomic-level interface engineering and the establishment of built-in electric fields in S-scheme $Bi_2WO_6/ZnIn_2S_4$ heterojunctions have demonstrated pronounced improvements in water splitting [4]. A new class of $Sr_3FeCoO_{6.72}$ (SFC)-based composites have been introduced as catalysts for nitrogen reduction, where enhanced interfacial charge transfer and increased exposure of active sites improve the efficiency of NH_3 synthesis [5]. Parallel efforts toward practical implementation have led to the development of an indigenous prototype device for scalable applications. Collectively, structure–function modulation in semiconductor heterostructures establishes a powerful design paradigm for optimizing multifunctional performance in photocatalysis, enabling efficient solar energy conversion and stability, and selectivity for solar-driven fuel production.

References:

1. H. Song, S. Luo, H. Huang, B. Deng, and J. Ye, ACS Energy Lett., 7 (2022) 1043–1065.
2. S. Ghosh, K. A. Natalie, L. Ramos, S. Remita, A. Dazzi, A. D. Besseau, F. Goubard, P.-H. Aubert, and H. Remita, Nat. Mater., 14 (2015) 505–511.
3. D. Sarkar, M. Biswas, S. Ghosh, J. Chowdhury, B. Satpati, and S. Ghosh, ChemSusChem, 18 (2025) e202402655.
4. D. Sarkar, J. Pramanik, S. Ghosal, S. Paul, P.-K. Giri, A. Datta, S. S. Sinha, G. Roymahapatra, and S. Ghosh, Small, 21 (2025) 2505315.

EN-126

Engineering Next-Generation Photoelectrochemical Flow Reactors for Integrated Bio-oil Valorisation and CO_2 Reduction

Kajal Bist, Dr. G. Bharath

Sustainability Research Laboratory (SRL), Department of Physics & Nanotechnology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India.

***Corresponding author e-mail:** bharathg4@srmist.edu.in

ABSTRACT

The upgrading of biomass-derived bio-oil into renewable liquid fuels is constrained by its high oxygen content and the energy intensity of conventional thermocatalytic processes. Developing selective, low-energy routes that couple biomass valorisation with carbon management is therefore critical for sustainable fuel production. Here we report a solar-driven photoelectrochemical (PEC) flow reactor that integrates semiconductor photoelectrodes with electrocatalytic upgrading reactions to enable continuous bio-oil valorisation under mild conditions. The coupled photoelectrode–catalyst architecture directly utilises photogenerated charge carriers to drive redox transformations, reducing reliance on externally supplied hydrogen and high-temperature operation. Continuous-flow processing enhances mass transport, stabilises catalytic interfaces, and improves reaction selectivity while mitigating catalyst deactivation relative to batch systems. Under simulated solar illumination, the PEC flow reactor exhibits enhanced conversion of representative oxygenated bio-oil model compounds into value-added fuels and chemicals, with improved energy efficiency compared with purely thermocatalytic or electrochemical pathways. The modular reactor design further enables concurrent CO_2 reduction at the counter electrode, allowing simultaneous biomass upgrading and carbon utilisation within a single integrated platform. Sustained activity and selectivity are maintained during extended operation, highlighting the robustness of the photoelectrochemical catalytic interface. This work establishes photoelectrochemical flow catalysis as a scalable and energy-efficient strategy for coupling solar energy conversion with selective biomass upgrading and carbon recycling, providing a foundation for next-generation solar-driven biorefinery systems.

Keywords: Biomass valorisation; Bio-oil upgrading; Photoelectrochemical flow reactors; Green fuel production; Sustainable biorefineries

EN-127

The Impact of Catalyst Engineering, Solution Chemistry and Operational Conditions on the Photocatalytic Performance of SnS Thin Films

Aparna N*

College (Autonomous), Devagiri, Kozhikode, India, 673008

***Corresponding author e-mail:** aparnaraji81@gmail.com

ABSTRACT

Photocatalyst systems that perform well in laboratory studies often fail to deliver comparable performance under real-life conditions, where variations in water chemistry and operating conditions significantly reduce their effectiveness. Addressing the gap between laboratory evaluation and practical applicability, the present study provides an extensive investigation into the factors that govern the photocatalytic efficiency of SnS thin films, with a clear emphasis on conditions relevant to real-world wastewater management. SnS thin films were deposited at room temperature using a modified SILAR method, ensuring a simple, cost-effective, environmentally friendly, and energy-efficient deposition route suitable for large area applications [1]. Instead of relying on sophisticated or expensive modification strategies, the properties of the catalyst were intentionally tailored through post-deposition annealing a simple, popular, and cost-effective technique. Annealing-induced variations in crystallinity and optical bandgap were correlated with photocatalytic performance to elucidate the role of intrinsic catalyst properties alongside external reaction conditions. Photocatalytic efficiency was systematically evaluated by varying the reaction time, initial pollutant concentration, pH, and salinity of the solution, aeration, magnetic stirring, light intensity, etc. – parameters that closely mimic realistic wastewater environments. Both cationic and anionic dyes were employed as model pollutants to assess the versatility and robustness of the SnS thin films. The SnS thin film exhibiting maximum crystallinity and the lowest optical bandgap demonstrated the highest photocatalytic efficiency. Magnetic stirring and aeration improved degradation performance, whereas the influence of pH and salinity was governed primarily by their effect on initial dye adsorption at the catalyst surface. By combining room-temperature deposition, simple annealing-based property tuning, and the extensive analysis of real-life influencing factors, this work provides critical insights for translating SnS thin-film photocatalysts from laboratory studies to practical environmental remediation applications.

References:

1. N. Aparna, Reshma S. Philip, Meril Mathew, Appl. Surf. Sci. Adv., 18 (2023) 100510.

EN-128

Engineering Non-Centrosymmetric Bismuth-Based Photocatalyst and Investigation of Their Influence on Mixed Pollutant Degradation

Logamithrai D, Raveena P V, Anitha Christy Antonysamy, Debabrata Sarkar*

Applied NanoPhysics Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattangulathur – 603203, India.

***Corresponding author e-mail:** debabras@srmist.edu.in, ld0423@srmist.edu.in

ABSTRACT

The effective degradation of wastewater containing mixed organic pollutants is a significant challenge due to the persistence, structural diversity, and potential interactions between the pollutants themselves[1]. Layered bismuth-based nanomaterials have been extensively investigated as promising photocatalysts due to their tunable band gaps and large surface areas that provide abundant active sites for the effective degradation of pollutants [2-3]. Among them, the elimination of antibiotics is crucial, considering that even minimal quantities contribute to antimicrobial resistance, representing a significant threat to both environmental and human health. Herein, we have successfully synthesized layered centrosymmetric BiOBr and non-centrosymmetric $BiOBrO_3$ via a modified hydrothermal method, and they were validated through Rietveld refinement and TEM, revealing tetragonal and orthorhombic crystal structures as well as high purity. BiOBr exhibited lamellar structures (50–90 nm thick), while $BiOBrO_3$ formed unique cabbage-like morphology, both providing abundant active sites that promoted efficient surface reactions for simultaneous pollutant degradation of the ternary system. Raman, UV–vis , and XPS studies highlighted the contrasting coordination environments in BiOBr and $BiOBrO_3$, paving the way for material development for multifunctional photocatalytic applications. The photocatalytic activity of these layered bismuth-based semiconductors was investigated by comparing the structural contrast between non-centrosymmetric $BiOBrO_3$ and centrosymmetric BiOBr, classified according to inversion symmetry, with their efficiency evaluated in degrading a realistic mixed ternary pollutant system comprising dyes and antibiotics commonly found in Indian water bodies. The enhanced efficiency of $BiOBrO_3$ arises from its non-centrosymmetric lattice, where the stereochemically active Bi^{3+} lone pairs and the asymmetric BrO_3 unit generate internal electric fields that facilitate charge separation and suppress recombination. Kinetic analysis confirmed pseudo-first-order behavior, while radical trapping identified the multiple active species responsible for degrading each pollutant in the mixed system.

Keywords: BiOBr, $BioBrO_3$,Non-Centrosymmetric, Mixed Pollutant.

References:

1. X. Shi, Q. Chen, X. Qin, X. Rao, S. Li, G. Liu, J. Wang, X. Dong, D. Luo, F. Chen, ENERGY Environ. Mater. 2025, 8, e70006.
2. X.-D. Dong, Y.-M. Zhang, Z.-Y. Zhao, Inorg. Chem. 2021, 60, 8461.
3. F. Cao, J. Wang, Y. Wang, J. Zhou, S. Li, G. Qin, W. Fan, Nanoscale Adv. 2019, 1, 1124.

EN-129

Flexible Silver Chalcogenide Architectures on Carbon Fabric for Wearable Thermoelectric Energy Harvesting

Logaprabha G[1], K. P. Mohamed Jibri[2], Krishna Mohan M[1*], J. Archana[1], S. Harish[2], M. Navaneethan[2]

[1]*Center of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology, KTR Campus, Chennai 603203, Tamil Nadu, India*

[2]*Nanotechnology Research Centre, SRM Institute of Science and Technology, KTR Campus, Chennai 603203, Tamil Nadu, India*

***Corresponding author e-mail:** krishnam1@srmist.edu.in

ABSTRACT

The rise of IoT has driven the exploration of self-powered devices, leading to the emerging field of wearable thermoelectrics, which utilizes the temperature difference between the human body and the environment. Silver-based chalcogenides are promising materials for such applications due to their stable phase at room temperature. Ag_2Se, an efficient n-type material, exhibits high electrical conductivity, moderate Seebeck coefficient and low lattice thermal conductivity due to the high entropy as a result of intrinsic Se vacancies and Ag interstitials. while $AgSbSe_2$, a p-type material with a rock salt structure, offers a high Seebeck coefficient, moderate electrical conductivity, and extremely low thermal conductivity. The reduced thermal conductivity arises from local crystal distortions caused by Ag/Sb atomic positioning and Sb lone pair electrons. In situ growth of these chalcogenides on conductive carbon fabric enhances performance through energy filtering by scattering low-energy carriers while boosting Seebeck and electrical conductivity simultaneously along with achieving great flexibility. Further a good performing device can be built through the selected p and n type materials by optimizing the fill factor, minimizing contact resistance and maintaining a stable temperature gradient with an efficient heat sink.

Key Words: Wearable thermoelectrics, Chalcogenides, Energy filtering effect

References:

1. L. K. Allison and T. L. Andrew, Adv. Mater. Technol., 4 (2019).
2. C. V. Manzano, C. Llorente del Olmo, O. Caballero-Calero, and M. Martín-González, Sustain. Energy Fuels, 5 (2021) 4597–4605.
3. J. Vinodhini, V. Shalini, S. Harish, H. Ikeda, J. Archana, and M. Navaneethan, J. Colloid Interface Sci., 651 (2023) 436–447.

EN-130

Comparative Intercalation Behavior of Li, Na, and K Ions in Bilayer Graphene: An Experimental and DFT Study

Haneena Gathoon N P[1], Dr. Prashant S Alegaonkar*[1]

[1] *Department of Physics, Central University of Punjab, Bathinda, Punjab, India,151401*

***Corresponding author e-mail:** prashant.alegaonkar@cup.edu.in

ABSTRACT

Bilayer graphene (BLG) has gained substantial interest as an advanced electrode material for rechargeable batteries owing to its high electrical conductivity, large specific surface area, controllable interlayer spacing, and ability to facilitate fast ion and electron transport. Although lithium intercalation in bilayer graphene has been widely studied, a systematic and comparative understanding of how different alkali metal ions, particularly Na and K ions, interact with bilayer graphene and modify its structural and electronic properties remains limited. This study presents a combined experimental and density functional theory (DFT) investigation to unravel the distinct structural and electronic evolution of BLG upon Li^+, Na^+, and K^+ intercalation. A hydrothermal approach was employed to ensure identical processing conditions for all three systems. Structural and morphological changes were analyzed using XRD, Raman spectroscopy, and FESEM, while first-principles DFT calculations were performed to evaluate the adsorption energetics, charge-transfer characteristics, and relative stability of Li, Na, and K ions within the bilayer graphene framework. The results enable a direct comparison of the ion-dependent structural and electronic responses of bilayer graphene and provide insight into how ion size and interaction strength govern interlayer modulation and charge transfer. These findings clarify the fundamental limitations and advantages of Na and K storage in two-dimensional hosts and highlight bilayer graphene as a versatile platform for emerging energy storage systems.

References:

1. R. Raccichini, A. Varzi, S. Passerini et al., Nat. Mater., 14 (2015) 271–279.
2. K. S. Novoselov, V. I. Fal'ko, L. Colombo et al., Nature, 490 (2012) 192–200.
3. K. Sugawara, K. Kanetani, T. Sato et al., AIP Advances, 1 (2011) 022103.
4. K. Ji, J. Han, A. Hirata et al., Nat. Commun., 9 (2018) 5136.H. Shin, A. Benali, C. S. Johnson, ACS Phys. Chem. Au, 5 (2025) 478–489.

EN-131

Microwave-Assisted Synthesis of Gold-Graphene Quantum Dots Composite for Sensitization of TiO_2 in Dye-Sensitized Solar Cells

Athulya Jayakumar[1], Ambily Krishnan*[1]

[1]*Goverrntment Victoria College, Palakkad, Kerala, India, 678001*

***Corresponding author e-mail:** ambilykrishnan.gvc.ac.in

ABSTRACT

In this work, graphene quantum dots (GQDs) and gold-GQD composite (GGC) were synthesized using a simple, energy-efficient and rapid microwave-assisted method and used for enhancement of dye-sensitized solar cell (DSSC) performance. GQDs and GGC were characterized using UV–visible spectroscopy, X-ray diffraction (XRD) and transmission electron microscopy. For solar cell applications, titanium dioxide nanoparticles were synthesized and characterized using field emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDS), XRD and Raman spectroscopy. TiO_2 nanoparticle paste was applied over a compact TiO_2 layer grown on FTO coated glass by doctor-blade technique to fabricate the photoanode. The synthesized GQDs and GGC were used to sensitize the TiO_2 nanoparticles by immersing in the solutions for 24 hours each. Their morphological characteristics and composition were subsequently analysed using FESEM and EDS. The co-sensitized anode in combination with natural pomegranate dye gave enhanced light absorption. DSSCs were assembled using the sensitized TiO_2 photoanode, a platinum counter electrode and conventional iodide/triiodide redox electrolyte. Current–voltage measurements showed that while the natural dye resulted in relatively low photocurrents, introduction of GGC led to a significant enhancement in photocurrent demonstrating their potential as efficient co-sensitizers in DSSCs.

References:

1. X. Fang et al., Electrochim. Acta, 137 (2014) 634–638.
2. E. Muchuweni, B. S. Martincigh, and V. O. Nyamori, RSC Adv., 10 (2020) 44453–44469.
3. X. Fang et al., Electrochim. Acta, 137 (2014) 634–638.
4. L. S. Chougala et al., (2017). (Journal name not provided)
5. H. Ma et al., Sci. Rep., 9 (2019) 17065.

Upgrading Industrial Waste–Derived Carbon via Chemical Purification for Sustainable Environmental and Energy Applications

Muhammed Sinan CH[1], Prashant S Alegaonkar*[1]

[1] *Department of Physics, Central University of Punjab, Bathinda, Punjab, India,151401*

***Corresponding author e-mail:** prashant.alegaonkar@cup.edu.in

ABSTRACT

Carbon materials derived from industrial waste offer a sustainable and low-cost alternative to conventional carbon materials; however, the presence of residual inorganic impurities and trace metals can limit their performance in environmental remediation and energy storage applications. In this study, industrial waste–derived carbon was subjected to a systematic chemical purification process involving acid washing and chelation treatment to reduce metal impurities while preserving the structural integrity of the carbon framework. Raw and purified samples were comparatively characterized using FESEM–EDX for morphological and elemental analysis, FTIR for functional group evaluation, XRD for structural assessment, and quantitative metal analysis using AAS and ICP-MS. The results revealed a significant increase in carbon content and a marked reduction in inorganic elements such as aluminium and nickel following purification. FTIR confirmed the preservation of the carbon backbone with enhanced surface functional clarity, while FESEM images indicated a less compact and cleaner morphology in the purified sample. ICP-MS analysis quantitatively verified the reduction of trace metal concentrations. The findings demonstrate that the applied purification strategy effectively enhances the chemical purity of waste-derived carbon without compromising its structural framework, thereby improving its suitability for multifunctional applications in environmental remediation and energy storage systems.

References:

1. G. Pandolfo, A. F. Hollenkamp, J. Power Sources, 157 (2006) 11–27.
2. J. R. Miller, P. Simon, Science, 321 (2008) 651–652.
3. K. Fic, G. Lota, M. Meller et al., Energy Environ. Sci., 5 (2012) 5842–5850.
4. J. R. Dahn, Science, 270 (1995) 590–593.

Doping-Induced Carrier and Phonon Transport Modulation in $Bi_2Sn_2O_7$ Pyrochlore Oxide for Flexible Wearable Thermoelectric Energy Harvesting

Rohidsuriyakanth S R [1], Sivakami Mohandos[1]*

[1] *Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603 203*

***Corresponding author e-mail:** sivakamm@srmist.edu.in

ABSTRACT

The growing demand for sustainable, self-powered electronic devices has intensified interest in thermoelectric materials capable of directly converting low-grade heat into electricity. In particular, wearable electronics require thermoelectric systems that operate efficiently under small temperature gradients, are mechanically robust, and exhibit long-term chemical stability. Bismuth stannate ($Bi_2Sn_2O_7$) is an emerging oxide thermoelectric material for wearable energy harvesting owing to its chemical stability, oxidation resistance, and environmental compatibility. In this study, the thermoelectric performance of $Bi_2Sn_2O_7$ is enhanced through controlled doping and defect modulation to enable efficient operation under body-heat-driven temperature gradients ($\Delta T \approx 25^{o}C$). Substitution at the Bi or Sn lattice sites effectively tunes carrier concentration and mobility via charge compensation mechanisms, including oxygen vacancy formation, thereby improving electrical conductivity while preserving a favorable Seebeck coefficient. Concurrently, enhanced point-defect scattering and grain boundary effects suppress lattice thermal conductivity. This synergistic regulation of electronic and phonon transport improves thermoelectric response at near-ambient temperatures. Flexible thin-film fabrication further ensures mechanical robustness and stable power output under bending conditions, highlighting doped $Bi_2Sn_2O_7$ as a scalable oxide platform for wearable thermoelectric generators and sustainable low-grade heat recovery.

Keywords: $Bi_2Sn_2O_7$; wearable thermoelectric; oxide thermoelectric materials; flexible energy harvesting; defect-modulated transport.

EN-134

Phase-Engineered NiTi Shape Memory Alloy for Enhanced Alkaline Hydrogen Evolution

Sreetama Ghosh[1,2*]

[1]*Dutch Institute for Fundamental Energy Research (DIFFER), De Zaale 20, 5612 AJ Eindhoven, Netherlands*

[2]*CO2 Research and Green Technologies Centre, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India.* [3]*Department of Chemistry, Indian Institute of Science Education and Research (IISER) Tirupati, India*

***Corresponding author e-mail:** sreetama.ghosh@vit.ac.in

ABSTRACT

The hydrogen evolution reaction (HER) in alkaline media is kinetically slower than in acidic systems, limiting the efficiency of alkaline and anion exchange membrane water electrolysis.[1,2] Although nickel-based materials are attractive due to their earth abundance, their strong hydrogen binding and surface hydride formation restrict catalytic performance.[3] Strategies that simultaneously optimize adsorption energetics and catalyst stability remain essential for advancing cost-effective hydrogen production. In this work[4], we investigate a commercially available near-equiatomic NiTi shape memory alloy (SMA) as an electrocatalyst for alkaline HER. NiTi undergoes a thermally induced phase transformation from monoclinic martensite at room temperature to cubic austenite at elevated temperatures. Electrochemical measurements were conducted in 1 M KOH between 20–80 ºC to correlate phase evolution with catalytic activity. Structural characterization confirmed progressive transformation to the austenite phase above 60 ºC. The electrocatalytic performance exhibits a strong temperature dependence. While the room-temperature activity is moderate, the fully transformed austenitic phase at 80 ºC delivers exceptional HER performance. At industrially relevant current densities, NiTi outperforms monometallic Ni, Ti, and benchmark Pt electrodes. At 10 mA cm^{-2}, the overpotential decreases dramatically with increasing temperature, reaching values lower than Pt at 80 ºC. Current densities as high as 445 mA cm^{-2} at −0.4 V vs RHE were achieved at 80 ºC. Electrochemical impedance and surface area analyses confirm that the enhancement arises primarily from intrinsic catalytic improvements rather than surface area changes. Chronopotentiometry demonstrates stable operation with Faradaic efficiencies exceeding 90 %. Overall, this study demonstrates that thermally activated phase transformation in a shape memory alloy provides a simple and scalable route to enhance alkaline HER performance without complex nanostructuring or precious metals. The findings highlight phase-engineered bulk alloys as promising candidates for next-generation alkaline and AEM water electrolyzers.

References:

1. Y. Zhu, L. Li, H. Cheng and J. Ma, *JACS Au*, 2024, **4**, 4639–4654.
2. Y. Hao, Q. Zhang, Y. Yang, F. Li and A. Xu, *Curr. Opin. Electrochem.*, 2026, **55**, 101781.
3. L. Huo, C. Jin, K. Jiang, Q. Bao, Z. Hu and J. Chu, *Adv. Energy Sustain. Res.*, 2022, **3**, 2100189.
4. S. Ghosh, D.Haycock, N. Mehra, S. Bera, H. Johnson, I.-L. Roiban, M. Aouine et al., *J. Phys. Chem. Lett.*, 2024, **15**, 933–939.

EN-135

Ni-rich with reduced Ni-content $LiNi_{0.7}Mn_{0.15}Co_{0.15}O_2$ cathode delivered enhanced rate and cycle life in Li-ion batteries

Yuvashri Jayamkondan[1], Prasant Kumar Nayak[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** prasantn1@gmail.com

ABSTRACT

Ni-rich layered oxide cathodes ($LiNi_xMn_\gamma Co_zO_2$, NMC) are widely investigated for next-generation lithium-ion batteries owing to their high energy density. However, increasing nickel content often compromises structural stability during prolonged electrochemical cycling. In this work, a systematic comparison between Ni-rich NMC85 and NMC70 cathodes was carried out to elucidate the influence of nickel concentration on electrochemical performance and structural evolution. Both materials were synthesized via a sol–gel method and evaluated through electrochemical testing and post-cycling structural analysis. NMC85 exhibited a high initial discharge capacity of approximately 220 mAh g^{-1}, but suffered notable degradation, retaining only about 65% of its capacity after 100 cycles at 0.1 C. In contrast, NMC70 delivered an initial capacity of 165 mAh g^{-1}, which gradually increased to ~180 mAh g^{-1} during cycling, accompanied by superior capacity retention of 86%. Average discharge voltage analysis indicated more severe voltage decay in NMC85 compared to NMC70, reflecting reduced structural reversibility in the higher nickel composition. Rate capability measurements further confirmed improved stability of NMC70 at elevated current densities. Morphological examination of cycled electrodes revealed pronounced particle cracking in NMC85, whereas NMC70 largely preserved its structural integrity. Overall, the study demonstrates that while higher nickel content enhances initial capacity, an optimized composition such as NMC70 offers improved durability and electrochemical stability for long-term high-energy lithium-ion battery applications.

Keywords: Ni-rich layered oxides, Microcracks, Capacity fade, NMC85

References

1. G. L. Xu, X. Liu, A. Daali, R. Amine, Z. Chen, K. Amine, *Adv. Funct. Mater.* **2020**, *30*, 1–45.
2. Y. Su, G. Chen, L. Chen, Y. Lu, Q. Zhang, Z. Lv, C. Li, L. Li, N. Liu, G. Tan, L. Bao, S Chen, F. Wu, *ACS Appl. Mater. Interfaces* **2019**, *11*, 36697–36704.
3. B. Song, W. Li, P. Yan, S. M. Oh, C. M. Wang, A. Manthiram, *J. Power Sources* **2016**, *325*, 620–629.

EN-136

Nanoclusters of Metal–Organic Frameworks on NiO Nanosheets for Water Splitting

Ramar Gunaseelan[1], Sundaramoorthy Marimuthu[1] and Govindhan Maduraiveeran[1]*

[1]*SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** mgovindhan@aus.edu, pgmadura@yahoo.co.in

ABSTRACT

We demonstrate a metal–organic framework (MOF)-assisted electrochemical approach to engineer iron nanoclusters anchored on nickel oxide nanosheets (MOF-Fe NC|NiO NS), creating well-defined heterointerfaces that enable precise electronic modulation and highly active tri-junction catalytic sites. The as-developed MOF-Fe NC|NiO NS electrode exhibits exceptional bifunctional activity, requiring overpotentials (η) of only ~280 mV for the oxygen evolution reaction (OER) and ~202 mV for the hydrogen evolution reaction (HER) to attain 10 mA cm^{-2} in 1.0 M KOH, along with favorable electrochemical intrinsic characteristics and remarkable operational durability (250 h). The MOF-Fe NC|NiO NS||MOF-Fe NC|NiO NS delivers a low cell voltage of 1.67 V at 10 mA cm^{-2}, surpassing benchmark RuO_2||Pt/C systems. The superior performance originates from strong Fe–NiO interfacial coupling, which modulates the adsorption energies of H* and OH* intermediates, increases accessible active-site density, accelerates charge-transfer kinetics, and enhances adsorption–desorption processes.

References:

1. Marimuthu, S.; Maduraiveeran, G. Langmuir, *40* (43), 2024,22549-22560.
2. Shankar, A.; Marimuthu, S.; Maduraiveeran, G. J.Mater. Chem. A, *12* (1), 2023, 121-127.

EN-137

Synergistic Charge Separation in $ZnMn_2O_4$/Cu_3P Composites for Photocatalytic Hydrogen Evolution

Neelamegan J [1], Jayapandi S [1], Bernaurdshaw Neppolian [1]*

[1] *Energy and Environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu - 603 203, Tamil Nadu, India*

***Corresponding author e-mail:** neppolib@srmist.edu.in

ABSTRACT

Copper phosphides have been found to be highly efficient cocatalysts for photocatalytic splitting of water for the production of hydrogen gas. In the course of this study, the synthesis of a nanoparticle-based Cu_3P cocatalyst was successfully achieved and then successfully deposited on the surface of the ZMO nanoparticles via the wet impregnation method, which facilitated the formation of an internal electric field effect. When the photocatalyst Cu_3P/ZMO composite was exposed to light, it was able to split the water into hydrogen and oxygen gas efficiently. This is because the Cu_3P/ZMO composite was able to split the water into hydrogen gas very efficiently due to the high electrical conductivity of Cu_3P. In comparison with the pure ZMO sample, the Cu_3P/ZMO composite sample was much better at splitting the water into hydrogen gas. The Cu_3P/ZMO composite sample has shown high photocatalytic efficiency for the generation of hydrogen gas, with the efficiency rate being 660 μmol g^{-1} h^{-1}, compared with the pure ZMO sample, which confirmed the high photocatalytic efficiency for the splitting of water into hydrogen gas by the Cu_3P/ZMO composite sample. This highly efficient photocatalytic splitting of the water molecule by the Cu_3P/ZMO composite sample can be attributed to the high efficiency

EN-138

UV Light Induced Structural Transformation Enhances Electrocatalytic and Photoelectrocatalytic Efficiencies of Novel Metal-Organic-Materials

Amrutha V. Madhusudhanan and Goutam Kumar Kole*

Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203, India.

***Corresponding author e-mail:** goutamks@srmist.edu.in

ABSTRACT

Metal–organic materials have become revolutionary platforms in material science, offering creative solutions to global problems, such as in environmental remediation and sustainable energy due to their remarkable tunability and multifunctionality. Their structures can undergo dynamic transformations induced by external stimuli, such as light-induced [2+2] cycloaddition, converting zero-dimensional complexes into higher-dimensional networks that significantly influence electronic, optical, and catalytic properties. In this study, we designed and synthesized two discrete complexes incorporating novel organic ligand, *E*-1-(4'-pyridyl)-2-(4"-quinolinyl) ethylene (PQE) and 2-chlorobenzoic acid (2-ClBz). The synthesized metal complexes $[Co(PQE)_2(2\text{-}ClBz)_2(H_2O)_2]$ (1) and $[Ni(PQE)_2(2\text{-}ClBz)_2(H_2O)_2]$ (2), satisfying the topochemical criterion ($d < 4.2$ Å), undergo [2+2] photocycloaddition reaction in the solid state under exposure to UV light. This led to a structural transformation of the zero-dimensional complexes into one-dimensional coordination polymers. Further, these two discrete complexes, as well as the dimerized one-dimensional coordination polymers were employed for electrocatalytic water splitting reactions. This study aims to study the effect of structural transformation in the catalytic efficiencies of discrete complexes and one-dimensional coordination polymers for both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). Further, their photocatalytic properties have also been attempted.

Keywords: Multifunctional materials; Metal-organic-materials; Electrocatalysis; Water splitting reactions

References:

1. K. M. Y. Baig, S. Marimuthu, E. Zangrando, G. Maduraiveeran, and G. K. Kole, *Mater. Today Chem*., 43(**2025**) 102464.
2. K. M. Y. Baig, S. Marimuthu, G. Maduraiveeran and G. K. Kole, *Dalton Trans.*, 54 (**2025**) 11025-11035.
3. R. F. Li, H. Zhang, M. Z. Hong, J. G. Shi, X. F. Liu, and X. Feng, *Dalton Trans.*, 51 (**2022**) 3970–3976.

EN-139

Fabrication of Zinc Oxide Nanocomposites with carbon paste as a modified Platinum Electrode for Electrocatalytic conversion of substituted alcohols

Nandhakumar Duraisamy [a], Susila Saviriraj [b], Joseph Selvaraj [b] and Aruljothy John Bosco [a*]

[a] *Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu -603 203, India.*

b PG and Research Department of Chemistry, St. Joseph's College (Autonomous), Tiruchirappalli, Tamil Nadu -620 002, India.

***Corresponding author e-mail:** johnbosa@srmist.edu.in, sjc_selvaraj@yahoo.com

ABSTRACT

The electrochemical oxidation of alcohols provides sustainable and efficient pathways for chemical transformations. Electro organic synthesis has also paved a new way to green chemical process by introducing environmentally benign reagents compared to conventional redox reactions. Through a combination of experimental and theoretical approaches, the mechanistic pathways governing the electrochemical oxidation can be elucidated and selective oxidation protocols developed. Herein, we introduced a biphasic electrolysis methodology as a sustainable route for the conversion of substituted alcohols using potassium iodate as a redox catalytic mediator at an ambident temperature. The present electrolysis was conducted in an undivided cell with platinum as anode modified carbon paste as a cathode. The In-situ generated potassium iodate dealt in the upper aqueous phase and substrate alcohols dissolved with the chloroform performed in the bottom organic phase. The optimized parameters were conducted with the high selectivity of the alcohol's conversion to aldehydes from moderate to good yield. Moreover, this methodology has paved a greener way for the sustainable solutions in the organic chemistry.

Keywords: Biphasic Electrolysis, galvanostatic, potassium Iodate and Carbon paste electrode.

References:

1. Savari Susila, G., Joseph Selvaraj, S., Novel electrocatalytic oxidation of benzyl alcohol on various electrode in biphasic medium using potassium periodate as a mediator, IJCBS, 22(2022):244-256.
2. John Bosco, A., Lawrence, S., Christopher, C., Radhakrishnan, S., Arul Joseph Rosario, A., Raja, S., and Vasudevan, D., Redox-mediated oxidation of alcohols using Cl- /OCl redox couple in biphasic media, J. Phys. Org. Chem. 2015, 28 591-595.
3. Paliakkara Lona Deena & Savariraj Joseph Selvaraj, Electrochemical conversion of benzene sulphonyl azide into sulphoamide assisted by sodium ascorbate, Indian Journal of Chemistry, 2023, Volume 62, Page No.980-985.

EN-140

Enhanced Rate Performance of $Na_xLi_{1/5}Ni_{1/5}Mn_{2/3}O_2$ Hybrid Supercapacitor in Monovalent and divalent Aqueous Electrolytes

Preethi R[1], Prasant Kumar Nayak[1*]

[1] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Chengalpattu District, Tamil Nadu*

***Corresponding author e-mail:** prasantn1@srmist.edu.in

ABSTRACT

Supercapacitors (SC) are evolving as promising electrochemical energy storage devices because of their high power density, light weight, and long lifecycle. Supercapacitors are increasingly used in flexible and wearable electronics and in electric vehicles because of their high power density. Supercapacitors bridge the gap between conventional capacitors and batteries by withstanding many charge-discharge cycles, but they lack the energy density of batteries. Thus, this study aims to improve the energy density of SC without compromising their power performance by optimizing the electrode materials and selecting the appropriate electrolyte. In this study, the electrochemical capacitance properties of hydrothermally synthesized mixed metal ions of NLNMO were investigated in aqueous electrolytes of 1 M $NaNO_3$, 0.5 M $Mg(NO_3)_2$ and 0.5 M $Ca(NO_3)_2$. Although 0.5 M $Mg(NO_3)_2$ enables a higher specific capacitance than 1M $NaNO_3$ and 0.5 M $Ca(NO_3)_2$ electrolyte, it exhibits limited rate capability. On the other hand, the prepared NLNMO shows great rate capability and cycling stability in 0.5 M $Ca(NO_3)_2$ electrolyte which corresponds to the charge density and hydrated ion size of Mg^{2+} and Ca^{2+}. Later, an aqueous hybrid supercapacitor of AC||LNMNO is assembled. This results in significant enhancement in specific capacitance, rate capability and cycling stability of the device.

Keywords

Specific capacitance, Rate capability, Cycling stability, Mixed dual-ion electrolyte

References:

1. Nechikott, A. A.; Yoo, H. D.; Nayak, P. K. *A Mixed Dual-Ion Electrolyte for High-Rate Performance and Remarkable Cycling Stability of $NaMnO_2$ in Hybrid Supercapacitors.* **J. Power Sources 2024**, *591*, 233825.
2. Chen, P.-Y.; Adomkevicius, A.; Lu, Y.-T.; Lin, S.-C.; Tu, Y.-H.; Hu, C.-C. *The Ultrahigh-Rate Performance of Alkali Ion-Pre-Intercalated Manganese Oxides in Aqueous Li_2SO_4, Na_2SO_4, K_2SO_4, and $MgSO_4$ Electrolytes.* **J. Electrochem. Soc. 2019**, *166* (A1875–A1883)

Synergistic Ni_3Se_2/CoFeLDH Heterostructure Electrocatalyst as an Efficient Bifunctional Electrocatalyst for Overall Water Splitting

G. Shamini, Sarath Pevin and T. Maiyalagan*

Electrochemical Energy Laboratory, Department of Chemistry,

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India

***Corresponding author e-mail**: maiyalat@srmist.edu.in & maiyalagan@gmail.com

ABSTRACT

Creating effective and widely available electrocatalysts is essential for sustainable hydrogen generation through water electrolysis. This study presents a thoughtfully engineered heterostructured electrocatalyst consisting of cobalt–iron layered double hydroxide (CoFeLDH) consistently developed on Ni_3Se_2 supported on nickel foam for effective alkaline water splitting. The Ni_3Se_2 substrate offers outstanding electrical conductivity and enables swift charge transport, thus enhancing the kinetics of the hydrogen evolution reaction (HER). Simultaneously, the CoFeLDH layer provides a wealth of redox-active Co and Fe sites that promote the adsorption and transformation of oxygen-containing intermediates, improving oxygen evolution reaction (OER) efficiency. The effectively connected heterointerface of Ni_3Se_2 and CoFeLDH facilitates synergistic electronic interactions, enhanced adsorption energetics, and sped-up reaction kinetics. Moreover, the three-dimensional nickel foam structure provides a significant electrochemically active surface area and strong structural integrity, guaranteeing durability in catalytic performance. This study presents a logical approach to developing transition-metal-based heterostructured electrocatalysts for effective and long-lasting overall water splitting in alkaline environments.

EN-142

Tuning Oxygen Evolution via Dual-Mode Fe Incorporation in CaO and $KCaPO_4$ Catalysts

Prabhakar Sujita [1], Sethumathavan Vadivel [1]* and Manabu Fujii [2]

[1] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu 603203, India.*

[2] *Department of Civil and Environmental Engineering, Institute of Science Tokyo Meguro-Ku, Tokyo 152-8552, Japan*

***Corresponding author e-mail**: vlvelu7@gmail.com.

ABSTRACT

Developing cost-effective electrocatalysts for the oxygen evolution reaction (OER) is crucial for scalable water electrolysis. Herein, calcium oxide (CaO) and phosphate frameworks are engineered with iron sourced from rust to fabricate two catalysts: CaOFe and CPFe ($KCaPO_4$-Fe) derived from marine biowaste. While CaOFe features surface-dispersed Fe species, CPFe integrates Fe into the phosphate matrix ($KCaPO_4$). Comprehensive structural,morphological, and surface analyses confirm distinct environments for Fe incorporation. Extensive electrochemical studies reveal a unique performance crossover: CPFe exhibits superior activity at low overpotential (η_{10}=297mV) with a Tafel slope of (147mV dec^{-1}), whereas CaOFe outperforms at higher current densities (η_{100}=424mV) with a lower Tafel slope (107mV dec^{-1}), attributed to enhanced kinetics via surface Fe. Impedance and Bode plot analyses further confirm distinct charge-transfer dynamics between the two catalysts. Overall, this work demonstrates how the local environment of iron governs electrocatalytic behavior, by providing mechanistic insights into tuning OER performance through waste-derived bimetallic systems.

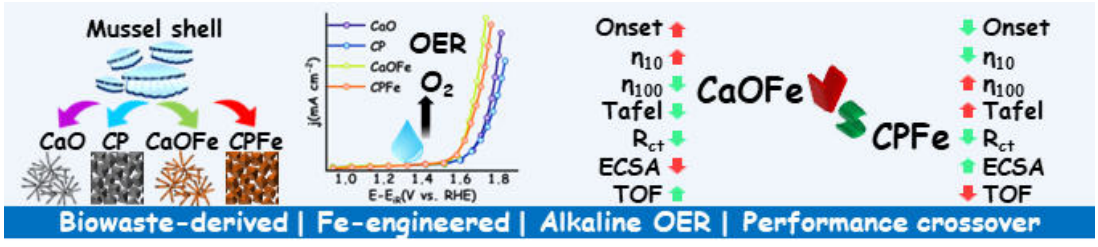


Figure 1. Graphical Abstract

EN-143

Temperature-induced Antisite Defects in Dopamine-based Carbon-$LiFePO_4$ Cathodes for Lithium-ion Batteries

Rekha Kumari[1,2] and Aninda Jiban Bhattacharyya[1,2*]

[1]*Solid State and Structural Chemistry Unit*

[2]*Interdisciplinary Centre for Energy Research Institute of Science, Bangalore, Karnataka-560012*

***Corresponding author e-mail**: anindajb@iisc.ac.in

ABSTRACT

Atomic-scale defects have a significant influence on the electrochemical behaviour of olivine-type $LiFePO_4$ cathodes. In this work, antisite defects and structural changes in carbon-coated $LiFePO_4$ are systematically investigated using Rietveld refinement of X-ray diffraction data. Carbon-coated $LiFePO_4$ samples were synthesised using dopamine as a carbon source in $LiFePO_4$ by varying calcination temperature at 500°C, 700°C and 800°C. Synthesised products were characterised by various spectroscopic analyses such as FTIR, Raman, PXRD, SEM, TEM etc. Rietveld refinement confirms the presence of Fe–Li antisite defects. Notably, antisite disorder is observed in dopamine-based carbon-coated $LiFePO_4$ calcined at a relatively high temperature of 700 °C. Three representative samples, designated as LFP/C-500, LFP/C-700 and LFP/C-800, were further examined using cyclic voltammetry, galvanostatic charge–discharge measurements and electrochemical impedance spectroscopy to evaluate the impact of antisite defects on electrochemical perOformance. At a 0.1 C rate, LFP/C-700, containing antisite defects, delivers a lower discharge capacity of 158 mAh g^{-1} compared to 162 mAh g^{-1} for LFP/C-500. Additionally, LFP/C-700 exhibits inferior rate capability and reduced cycle stability across all investigated C-rates. The results clearly demonstrate that even a small amount of antisite defects significantly hinders the electrochemical performance of $LiFePO_4$, highlighting the importance of precise defect control during synthesis.

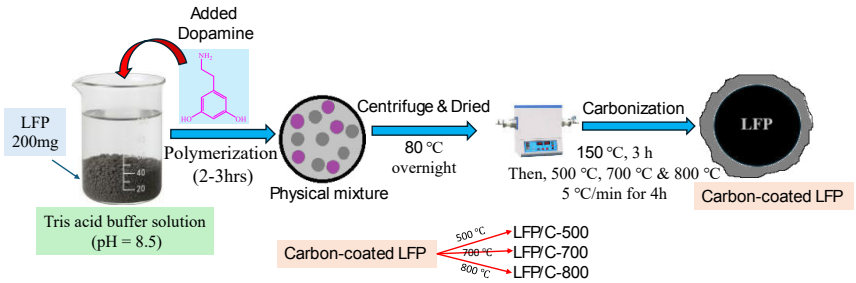


Figure 1. Schematic representation of the coating mechanism of polydopamine on the surface of LFP

Keywords: Carbon coated $LiFePO_4$; Antisite defects; Rietveld refinement

References:

1. R. Malik, A. Abdellahi, and G. Ceder, *J. Electrochem. Soc.*, **160** (2013) A3179–A3197.
2. S.Y. Chung, J. T. Bloking, and Y.M. Chiang, *Nat. Mater.*, **1** (2002) 123–128.
3. J. Ma, B. Kang, and G. Ceder, *J. Electrochem. Soc.*, **157** (2010) A925–A931.

EN-144

A Cyber-Physical Automation Framework for Intelligent Energy Management and Safety in Hydrogen Fuel Cell Autonomous Vehicles

Marthala Vag Vikas Reddy[1], Inkollu Nithish Babu[1], Sourodeep saha[1], Yerra Keerthan Sri Harsha[1], Sunkara Geeta Gokul Sai Koushik[1], Dontabakhtuni Gowtham Sai Teja[1], Seemakurthi Lakshmi Narasimha Sukeerthi[1], Naveen Viganesh[1], Irukulla Sai Sathwik[1], Kirubhakaran[1], Joy Nehamiah[1], Vishok[2], G.Y.Rajaa Vikhram[3], Phani Teja Bankupalli[4], Rajesh[4]

[1]*Dept of Electronics and Communication Engineering, SRMIST, Kattankulathur*

[2]*Dept of Computing Technologies, SRMIST, Kattankulathur*

[3]*Dept of Electronics and Instrumentation Engineering, SRMIST, Kattankulathur*

[4]*Dept of Electrical and Electronics Engineering, SRMIST, Kattankulathur*

ABSTRACT

Hydrogen proton exchange membrane (PEM) fuel cell systems are emerging as a promising zero-emission energy solution for next-generation autonomous mobility platforms. However, large-scale deployment requires integrated optimisation of electrochemical energy conversion, dynamic power management, and material-level safety assurance. This research work presents a comprehensive cyber-physical automation framework for intelligent energy management and safety supervision in hydrogen fuel cell autonomous vehicles (HFCAVs), with explicit consideration of fuel cell electrochemical behaviour and hydrogen sensing materials. A detailed PEM fuel cell stack model is developed in a Simulink environment incorporating polarization characteristics, dynamic voltage response, hydrogen consumption kinetics, and thermal effects. An intelligent energy management strategy is designed to regulate fuel cell power output in accordance with real-time vehicle load demand, thereby enhancing stack efficiency, reducing material degradation, and improving operational longevity. To address safety challenges associated with hydrogen storage and transport, a multi-modal leak detection architecture is proposed. The framework integrates electrochemical hydrogen sensors and ultrasonic sensing modules, leveraging material-specific sensitivity, selectivity, and response dynamics. An AI-assisted decision layer performs real-time anomaly detection, risk evaluation, and autonomous intervention, including electrical isolation and controlled system shutdown. The proposed architecture further incorporates electrical, thermal, pressure, flow, and impact sensing integrated through a central vehicle control unit, forming a tightly coupled cyber-physical safety network. Virtual implementation results demonstrate improved energy efficiency, reliable hydrogen leak detection performance, and rapid fault response under dynamic operating conditions. The presented framework establishes a materials-aware, device-centric cyber-physical platform for safe and efficient hydrogen fuel cell autonomous vehicles, contributing toward the advancement of intelligent functional energy devices for sustainable mobility.

Keywords: Proton Exchange Membrane Fuel Cell, Hydrogen Energy Materials, Electrochemical Devices, Intelligent Energy Management, Hydrogen Sensing Materials, Cyber-Physical Systems, Autonomous Vehicles.

Synthesis of Surface-Modified ZrO_2 via Non-Thermal Plasma for Enhanced Photocatalytic Degradation of Ciprofloxacin and Crystal Violet

Harshini Mohan[1], Subash Mohandoss[1], Sivachandiran Loganathan[2], Natarajan Balasubramaniyan[1]*

[1]*Laboratory of Plasma Chemistry and Physics (LPCP), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603203, Chennai, India.*

[2]*Department of Civil and Environmental Engineering, University of Nevada, Reno, NV, 89557-0258, USA.*

***Corresponding author e-mail:** natarajb@srmist.edu.in

ABSTRACT

This study investigates the efficacy of non-thermal plasma (NTP) as a rapid alternative to high-temperature thermal treatment for synthesizing zirconium dioxide (ZrO_2) photocatalysts. ZrO_2 was treated under an air plasma at 16 kV for 30 min and compared with a sample conventionally calcined at 800°C. Characterization via XRD and SEM revealed that NTP treatment preserves smaller crystallite sizes and prevents the heavy grain agglomeration typical of high-temperature calcination. UV-Vis spectroscopy showed a narrowed bandgap, while XPS confirmed a higher density of surface oxygen vacancies and reactive species in the plasma-treated samples. The photocatalytic activity was evaluated through the degradation of Ciprofloxacin (CIP) and Crystal Violet (CV). The NTP-treated ZrO_2 exhibited significantly higher degradation efficiency compared to the 800°C calcined sample. This improvement is attributed to the plasma-induced surface defects which act as electron traps, effectively reducing charge carrier recombination. These results highlight NTP as an energy-efficient, high-speed method for engineering high-performance photocatalysts for environmental remediation.

Keywords: Non-Thermal Plasma (NTP), Photocatalysis, Surface Modification, Degradation, Oxygen Vacancies

EN-146

Synthesis of Activated Carbon from Biowaste Materials for Energy Storage Applications

Poonam Saini, Sonia Bansal

Department of Physics, JC Bose University of Science & Technology, YMCA Faridabad, Haryana-121006, India

*Corresponding author: poonam05dahiya@gmail.com

ABSTRACT

The growing demand for sustainable energy storage has intensified the search for cost-effective, environmentally friendly electrode materials. This study reports the synthesis of activated carbon from renewable biowaste precursors for advanced energy storage applications. Biowaste materials with high carbon content were carbonized and activated under optimized conditions to develop a porous carbon framework. Key synthesis parameters, including activation temperature, activating agents, and processing duration, were tuned to enhance surface area and pore distribution. Physicochemical characterization confirmed activated carbon with a well-developed pore structure, high specific surface area, and suitable pore size, enabling efficient ion transport and charge storage. Electrochemical evaluation using cyclic voltammetry, galvanostatic charge–discharge, and impedance spectroscopy revealed high specific capacitance, good rate capability, and excellent cyclic stability, demonstrating potential for supercapacitors and hybrid energy storage devices. This work highlights a sustainable approach to convert waste biomass into functional carbon materials, offering scalability, low cost, and environmental compatibility, making biowaste-derived activated carbon a promising alternative for next-generation energy storage.

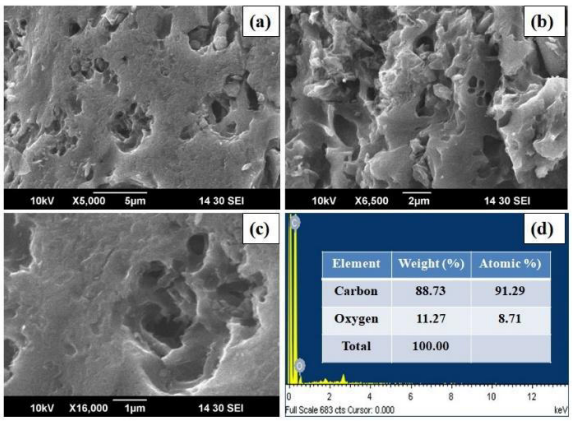


Fig. 1 (a) SEM and EDX analysis of activated carbon from walnut-shell biowaste.

Keywords: Activated carbon; Biowaste; Energy storage; Supercapacitor; Porous carbon; Sustainable materials; Electrochemical performance.

References:

1. S. Zhang et al., Nanomaterials 13 (2023) 456.
2. Y. Zhao et al., Carbon Trends 8 (2024) 100285.
3. R. Bose, T.K. Mandal, J. Energy Storage 93 (2024) 112134.

EN-147

Vanadium Oxide–Sulfide Nanocomposites as Efficient Electrocatalysts for Overall Water Splitting in Alkaline Media

Sophia Jacquline L and Elangovan Elamurugu*

DARE Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur - 603 203, Tamilnadu, India.

***Corresponding author e-mail:** elongove@srmist.edu.in

ABSTRACT

The main goal of developing the hydrogen economy is to design an efficient and low-cost catalyst that can use earth-abundant materials for hydrogen production from water, preferably with minimal external energy input[1,2]. However, single-species electrocatalysts often show limited efficiency in improving the hydrogen evolution reaction (HER)[3]. Therefore, in this work, to overcome this limitation a composite material was prepared by combining vanadium oxide (V_2O_5) with layered VS_2 to utilize their synergistic effect for enhancing HER activity. The V_2O_5/VS_2 hybrid catalyst shows improved HER kinetics with a low overpotential of 252 mV at a current density of 100 mA cm^{-2} and a Tafel slope of 86 mV dec^{-1}. The incorporation of VS_2 into the metal oxide reduces the band gap of the composite, which helps in better charge transfer and ion movement. As a result, a high hydrogen evolution rate of 1.66 mmol h^{-1} cm^{-2} is achieved at −0.5 V versus RHE. The enhanced performance of the VS_2 enriched catalyst is due to the presence of more active sites and better proton adsorption, which improves HER activity. Moreover, the V_2O_5/VS_2 composite demonstrates an overall water splitting potential of 1.67 V to attain 10 mA cm^{-2}, highlighting its potential as a practical and economical alternative to noble metal-based electrocatalysts.

References:

1. Tackie-Otoo, B.N., Mahmoud, M. and Raza, A., *Energy Fuels,* 39(37), (2025), pp.17730–17762.
2. Sohail, M., Rauf, S., Irfan, M., Hayat, A., Alghamdi, M.M., El-Zahhar, A.A., Ghernaout, D., Al-Hadeethi, Y. and Lv, W., *Nanoscale advances*, *6*(5), (2024), pp.1286-1330.
3. Bhatia, Shally, Atul Khanna, and Ravish Kumar Jain., Materials Research Express, 8, (2019), pp.086409.

EN-148

Investigations of the Charge Storage Behaviour in the rGO-$CuWO_4$ Encapsulated PANI Nanocomposite based Symmetric Supercapattery Device

V. Gajraj[1*], N. Sundriyal[2], N. Kumar[3], A. Sen[4*]

[1]*Department of Electronics and Communication Engineering, Manipal University Jaipur, Jaipur, Rajasthan-303007, India*

[2]*Department of Physics, Indian Institute of Technology Delhi, New Delhi-110016, India*

[3]*Department of Electronics and Communication Engineering, Graphic Era (Deemed to be University), Dehradun, Uttrarakhand-248002, India*

[4]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Katttankulathur 603203, India*

*** Corresponding author: e-mail:** vikash.gajraj@jaipur.manipal.edu

ABSTRACT

In this article, we are presenting the facile synthesis of the rGO-$CuWO_4$ encapsulated PANI nanocomposite by the in-situ polymerization approach and investigated its charge storage properties. X-ray diffraction reflection confirms the formation of the composite. Further morphological studies based on scanning electron microscopy (SEM) reveal the adsorptions of the copper tungstate nanoparticles over reduced graphene oxide which are homogenously distributed into the matrix of polyaniline. The energy dispersive X-ray (EDX) further confirms the homogenous distribution of the constituent elements. Electrode kinetics and the deconvolution of the charge storage process such as capacitive and diffusion-controlled process have been evaluated by using the Dunn's and Trassati's approach. For the practical utilizations, a symmetric device has been fabricated utilizing two identical electrode face to face configuration. The assembled device exhibits excellent performance in terms of the high specific capacity, good rate capability, long term cycling stability and impressive specific energy and specific power. Based on these outcomes it is believed to this nanocomposite could be the alternative electrode material for the next generation charge storage device.

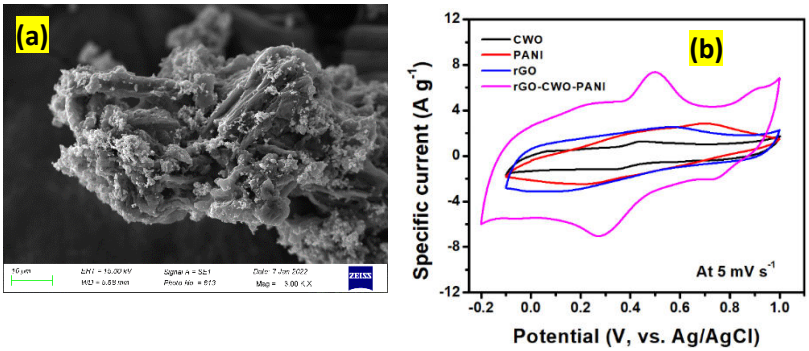


Fig. (a) SEM image of the rGO-$CuWO_4$ encapculated nanocomposite, (b) Cyclic voltammetry plots of $CuWO_4$, PANI, rGO, and the rGO-$CuWO_4$-PANI nanocomposite

Keywords: transition metal oxides; supercapacitors; polymer composite; renewable energy materials.

EN-149

Development of Biomass-derived Activated Carbon/Impregnated with NMC111 composites for Supercapacitor Applications

Jayapriya. J[1], Kalaivani. T[1*]

[1*]Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India

[*]**Corresponding author e-mail:** kalaivat@srmist.edu.in

ABSTRACT

This study investigates the performance of 5% Activated Carbon-based Carbon Dots (ACCD) integrated into a The (Li ($Ni_{1/3}Mn_{1/3}Co_{1/3}$) O_2) (NMC111) matrix synthesized via a one-step hydrothermal method. Electrochemical analysis demonstrates that the 5%ACCD@NMC111 composite achieves a superior specific capacitance of 400.0 F/g at 1 A/g, a substantial enhancement over the 136.0 F/g recorded for pristine NMC111. The integration of 5%ACCD facilitates accelerated ion diffusion and improves electronic conductivity, resulting in a three-fold increase in charge storage capacity. These results suggest that 5%ACCD is a highly effective additive for optimizing the electrochemical properties of NMC-based materials for advanced energy storage applications.

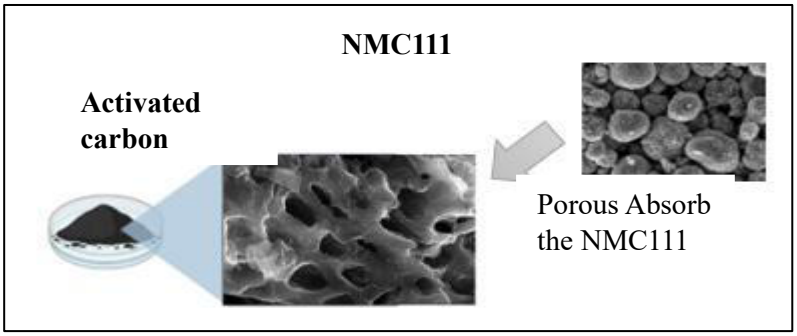


Fig: 1 activated carbon porous impregnated with nmc111.

Keywords: 5%ACCD; NMC111 Composite; Hydrothermal Method; Specific Capacitance; Energy Storage; Carbon Dots.

References:

1. Shrestha, Rajesh, and Narendra Phulara. "Review on Activated Carbon for Supercapacitors." *Semiconductor Science and Information Devices* 5.2 (2023): 11-18.
2. 2.Deng, Dingfei, et al. "A novel layered activated carbon with rapid ion transport through chemical activation of chestnut inner shell for capacitive deionization." *Desalination* 531 (2022): 115685.
3. Sevilla, Marta, and Robert Mokaya. "Energy storage applications of activated carbons: supercapacitors and hydrogen storage." *Energy & Environmental Science* 7.4 (2014): 1250-1280.

EN-150

Optimizing Thermoelectric Properties of Mixed Metal Oxide/Metal Molybdate Material by Doping

Premkumar Venkatesalu[1], Sivakami Mohandos[1]*

[1] *Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603 203*

***Corresponding author e-mail:** sivakamm@srmist.edu.in

ABSTRACT

Cobalt-based mixed metal oxides and metal molybdates are emerging as promising thermoelectric materials for wearable electronics and mid-temperature waste heat recovery due to their intrinsic thermal stability, chemical robustness, and environmental compatibility. However, their thermoelectric efficiency is often limited by relatively high lattice thermal conductivity and insufficient charge carrier concentration. Doping engineering provides an effective strategy to overcome these limitations by tailoring the electronic band structure and enhancing phonon scattering within the crystal lattice. The incorporation of transition metal or rare-earth dopants enables controlled modulation of carrier concentration and mobility, improving electrical conductivity while simultaneously suppressing lattice thermal conductivity. This synergistic optimization enhances the Seebeck coefficient–electrical conductivity balance, leading to improved dimensionless figure of merit (ZT) values. Such dopant-induced transport modulation is particularly advantageous for oxide-based thermoelectric operating under harsh or oxidative environments, where long-term stability is essential. These advances highlight the potential of doped cobalt-based oxides and molybdates as cost-effective, mechanically robust, and scalable materials for flexible wearable power sources and sustainable mid-temperature energy harvesting systems.

Keywords: Mixed metal oxides, Metal Molybdates, Doping, Thermoelectric application.

EN-151

Solar Hydrogen Production by $Cu_2ZnTi(S,Se)_4$, $Cu_2ZnTi(S,Se)_4$, and $Cu_2ZnTi(S,Se)_4$ Quaternary Chalcogenide Nanocrystals as Visible-Light Photocatalysts

Ragul R[1], Saravanan K[1], Natarajan B[2*]

[1] *Research Scholar, Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattangulathur, Tamil Nadu, India, 603203*

[2] *Professor, Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattangulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** natarajb@srmist.edu.in.

ABSTRACT

To develop highly efficient solar hydrogen production systems, one of the major challenges that must still be addressed is enhancing the separation of photogenerated charge carriers in semiconductor photocatalysts. For the first time, a novel ternary photocatalytic system based on $Cu_2ZnTi(S,Se)_4$, $Cu_2NiTi(S, Se)_4$, and $Cu_2CoTi(S, Se)_4$ quaternary chalcogenide nanocrystals were successfully synthesized using a simple hydrothermal method. As expected, under visible light irradiation, the $Cu_2ZnTi(S,Se)_4$, $Cu_2NiTi(S,Se)_4$, and $Cu_2CoTi(S,Se)_4$ heterostructure photocatalyst exhibits a significantly enhanced photocatalytic activity for hydrogen evolution during water splitting. According to recycling experiments, the $Cu_2ZnTi(S,Se)_4$, $Cu_2NiTi(S,Se)_4$, and $Cu_2CoTi(S,Se)_4$ composites exhibit excellent photocatalytic stability and can be efficiently reused up to four consecutive cycles. The present work not only introduces new, low-cost, and highly efficient photocatalysts for visible-light-driven hydrogen production but also proposes a novel strategy for designing and fabricating high-performance heterostructure photocatalysts for solar hydrogen generation.

References:

1. Jia, Xuguang, et al. "Theoretical and experimental study on the optical and electrical properties of Cu2ZnTiS4 and its photovoltaic applications." *Applied Physics Letters* 111.2 (2017).
2. Wang, Congcong, et al. "Design of I2–II–IV–VI4 semiconductors through element substitution: the thermodynamic stability limit and chemical trend." *Chemistry of Materials* 26.11 (2014): 3411-3417.

EN-152

Green-Derived Ni–Co–Ti Ternary Oxide Nanocomposites: A Comparative Electrochemical Insights for High-Performance Supercapacitors

Anushiya S[1], Arun Kumar D[1], Satish Kumar R.C.[1], Maiyalagan T[2], Kesavan M[1]*

[1]*Interdisciplinary Institute of Indian System of Medicine, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India,603 203.*

[2]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India,603 203.*

***Corresponding author e-mail:** kesavanm@srmist.edu.in

ABSTRACT

The development of sustainable and high-performance electrode materials is crucial for advancing next-generation supercapacitor technologies. In this study, a green synthesis approach was employed to fabricate nickel–cobalt–titanium oxide (Ni–Co–Ti oxide) nanocomposites using *Andrographis paniculata* leaf extract as a biogenic agent. The phytochemical constituents present in the extract contribute to environmentally benign material processing while enhancing surface functionality and electrochemical activity. Comprehensive physicochemical characterizations were performed using X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR) and Brunauer–Emmett–Teller (BET) surface area analysis. The results confirmed the formation of well-defined crystalline phases, homogeneous morphology, and a nanostructure with increased surface area, which are favourable for efficient electrolyte ion diffusion and rapid redox reactions. Electrochemical performance was evaluated in a three-electrode configuration with aqueous KOH electrolyte through Cyclic Voltammetry (CV), Galvanostatic Charge–Discharge (GCD), and Electrochemical Impedance Spectroscopy (EIS). A comparative analysis of the oxide materials and the ternary nanocomposite revealed that the Ni–Co–Ti oxide electrode exhibits superior specific capacitance, enhanced rate capability, and excellent cycling stability. The improved efficiency is attributed to synergistic redox interactions among Ni, Co, and Ti species and improved charge transfer characteristics. This work highlights the potential of plant-assisted ternary oxide nanocomposites as sustainable and high-efficiency electrode materials for advanced energy storage applications.

References:

1. Navaneethan, M., Nithiananth, S., Abinaya, R., Harish, S., Archana, J., Sudha, L., ... & Hayakawa, Y. (2017). Hydrothermal growth of highly monodispersed TiO_2 nanoparticles: functional properties and dye-sensitized solar cell performance. *Applied Surface Science*, *418*, 186-193.
2. Singh, J., Choudhury, A., Syed, A., Khan, S., AL-Shwaiman, H. A., Wong, L. S., & Yang, D. J. (2025). Preparation of nickel oxide nanoparticles/biomass-derived activated carbon composites for high-performance aqueous asymmetric supercapacitor electrode. *Surfaces and Interfaces*, *56*, 105736.

EN-153

In-situ Hydrothermally Prepared Honeycomb-Like Structured NiO Electrode for Acetaminophen Drug Detection and Supercapacitor Applications

Naresh Koppula[1], Joel K Joseph[1], S. Suneetha[1], S. Murali Mohan[2], Thangaraju Kuppusamy[1*]

[1]Organic Optoelectronics Devices Lab, Department of Physics, National Institute of Technology, Warangal-506004, India

[2]Department of Chemical Engineering, National Institute of Technology, Warangal-506004, India.

***Corresponding author e-mail:** ktr@nitw.ac.in

ABSTRACT

The development of a multifunctional electrode for energy storage and drug detection is an extremely important technology for the next generation. In this study, Nickel oxide (NiO) was synthesised via an in situ hydrothermal method and used in a symmetric supercapacitor device for efficient energy storage. The Field Emission Scanning Electron Microscope images reveal the honeycomb-like nanostructures. The XRD studies exhibit the average crystalline size of 4.6 nm and the purity of the Nickel Oxide/nickel foam (NiO/nf) electrode. The electrochemical studies [Cyclic voltammetry (CV), Galvanic charge-discharge (GCD) and Electrochemical impedance spectroscopy (EIS)] reveal the battery-type nature, showing the diffusion-controlled charge-storage behavior (60 %) of the prepared NiO/nf electrode. It exhibits the high specific capacity of 769 Cg^{-1} at 1 Ag^{-1} from the GCD study. The NiO/nf electrode detects acetaminophen at various concentrations, even at low temperatures. The fabricated symmetric coin-cell supercapacitor exhibits a high specific capacity of 198 C/g with battery-like behavior. The excellent electrochemical storage and sensing capabilities of the NiO/nf make it a promising multifunctional electrode for energy storage and drug detection applications.

References:

1. Lanting Qian, Reem Elmahdy, Antony Raj Thiruppathi and Aicheng Chen, Analyst, 2021, 146, 4525-4534, DOI: 10.1039/d1an00755f.
2. Thierry Brousse, z Daniel B´elanger and Jeffrey W. Longd, Journal of The Electrochemical Society, 2015, 162 (5) A5185-A5189, DOI: 10.1149/2.0201505jes

EN-154

Bi-MOF@$NiCo_2O_4$ Composite Electrodes: A Synergistic Approach Toward Superior Electrochemical Performance

Bhavani Sankaran[1], Swetha T[1], T. Kalaivani[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603203, Chengalpattu District, Tamil Nadu, India.*

*Corresponding author e-mail: kalaivat@srmist.edu.in

ABSTRACT

Energy storage systems (ESS) play a vital role in addressing the intermittent nature of renewable energy sources and enhancing grid reliability. Among various energy storage technologies, supercapacitors have attracted significant attention due to their high power density, rapid charge–discharge capability, and long cycling stability, bridging the gap between conventional capacitors and batteries. The development of advanced electrode materials is essential to further improve their energy storage performance. In this study, a metallic metal–organic framework (Bi-MOF) integrated with $NiCo_2O_4$ (Bi-MOF@$NiCo_2O_4$) was designed and synthesized as a high-performance electrode material for supercapacitor applications. The synergistic combination of the tunable porosity and high surface area of Bi-MOF with the excellent electrical conductivity and rich redox activity of $NiCo_2O_4$ enhances charge storage behavior. The composite structure facilitates rapid ion diffusion, provides abundant electroactive sites, and improves overall electrochemical kinetics. Structural and morphological characterizations confirm the successful formation of the heterostructured composite. Electrochemical investigations demonstrate that Bi-MOF@$NiCo_2O_4$ exhibits enhanced specific capacitance, good rate capability, and superior cycling stability compared to the individual components.

Keywords: Supercapacitors, Metal organic frameworks, MOF, High Surface area

References:

1. Simon, P.; Gogotsi, Y., *Materials for electrochemical capacitors,*Nature Materials, 2008, 7, 845–854. (Fundamental review on supercapacitor materials.)
2. Conway, B. E, *Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications,* Springer, 1999,(Classic book on supercapacitor theory.)
3. Wang, H.; Zhu, Q.-L.; Zou, R.; Xu, Q, *Metal–Organic Frameworks for Energy Applications.* Chemical, 2017, 2, 52–80,(MOFs in energy storage and conversion.)

EN-155

Enhanced Electrochemical Performance of Nickel Phosphide/CeO_2 Nanocomposite for Supercapacitor Applications

Kavibharathi Murugesan[1], T. Kalaivani[1*]

[1]*Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Tamil Nadu 603203, India*

***Corresponding author e-mail:** kalaivat@srmist.edu.in

ABSTRACT

The development of high-performance electrode materials is crucial for next-generation supercapacitors with enhanced energy and power density. Traditional carbon-based materials exhibit poor electrochemical activity and low energy density. Transition metal phosphides have emerged as an excellent electrode materials for supercapacitors due to their metal-like properties and offering superior performance in energy storage and conversion. This work has Nickel Phosphide (Ni_2P) successfully synthesized via a two-step approach involving precursor formation followed by Phosphorization. Nickel phosphide has high electrical conductivity, multiple redox states and good electrochemical activity. But it has poor structural stability and limited ion diffusion. Then Nickel phosphide was integrated with CeO_2, a rare-earth oxide has excellent structural stability, oxygen storage capacity and reversible Ce^{3+}/Ce^{4+} redox behavior. The Ni_2P/CeO_2 composite demonstrate improved electrochemical performances when compared to individual components due to synergistic interactions at the interface, enhanced electron transport and increased active sites for Faradaic reactions. The electrochemical properties and behavior of the material were evaluated through CV, GCD, EIS. The composite electrode exhibited high specific capacitance, excellent rate capability, and superior cycling stability in alkaline electrolyte. The enhanced performance is attributed to the combined pseudocapacitive behavior of the Ni^{2+}/Ni^{3+} and Ce^{3+}/Ce^{4+} redox couples. This study highlights the potential of transition metal phosphide–rare earth oxide composites as promising electrode materials for advanced energy storage systems.

Keywords: Ni_2P, CeO_2, Energy storage, Electrochemical performance, Cycling stability.

EN-156

Synergistic Effect and Thermal Performance of Poly-Hydroxyethyl Methacrylate Encapsulated Graphene Quantum Dot-Paraffin Hybrid Nanofluid

Mariya Binoy[1], Aswin E. J[1], Minnu Elizabeth Sajan[1], Vishnuprasad Selvaraj*[1]

[1]*Department of Chemical Engineering, Saintgits College of Engineering (Autonomous), Kottayam, Kerala – 686532*

***Corresponding author e-mail:** vishnuprasad.s@saintgits.org

ABSTRACT

A novel water-based hybrid nanofluid was developed using poly-hydroxyethyl methacrylate-encased graphene quantum dot-paraffin nanocomposite (HEMA GQD-P) in this work. Graphene quantum dots (GQD) with an average size of 10 to 15 nm were synthesized by citric acid nucleation and the HEMA GQD-P nanocomposites were synthesized by an emulsion polymerization reaction. The emission spectra of GQD obtained using photo-luminescent spectroscopy confirm the occurrence of quantum confinement effect. The synthesis of HEMA GQD-P was carefully carried out to ensure its optimal properties. The synergistic effect due to high thermal conductivity of GQD and high latent heat capacity of paraffin were recognized in the enhanced properties of nanocomposite and hybrid nanofluid. The latent heat capacity of the synthesized nanocomposite was found to be 21.8% higher than the pure paraffin. The prepared hybrid nanofluid possesses high dispersion stability at pH 7 and the thermal conductivity of the hybrid nanofluid enhances with an increase in nanoparticle concentration. A maximum thermal conductivity enhancement of 53% (±2) was obtained for the hybrid nanofluid (0.3 vol.%) at 30 ºC. The viscosity and surface tension of the hybrid nanofluid also increase with an increase in nanoparticle concentration. The present work reveals that the encapsulation of GQD-paraffin in a poly-hydroxyethyl methacrylate shell creates nanocomposites with high heat transfer properties. The synergistic effect of the HEMA GQD-P enhances their potential in the preparation of hybrid nanofluids with enhanced properties for desired thermal management applications.

Keywords: Graphene quantum dots; Paraffin; Hybrid Nanofluid; Thermal conductivity; Latent heat capacity; Emulsion polymerization..

References

1. O. Kazaz, N. Karimi, S. Kumar, G. Falcone, M.C. Paul, J. Mol. Liq. 385 (2023) 122385.
2. Vishnuprasad Selvaraj, Haribabu Krishnan, Appl. Therm. Eng. 187 (2021) 116580.
3. C.J. Ho, K.Y. Liu, T.F. Yang, S. Rashidi, W.M. Yan, Case Stud. Therm. Eng. 33 (2022) 101939.

EN-157

Time dependent synthesis of a Cu_9S_5/CuS@Ni Foam Heterostructure for Visible-Light-Driven Photocatalytic Degradation and Supercapacitor Applications

Akashdeep Dey, M.S. Gaikwad, S. Noyel Victoria*

Department of Chemical Engineering, National Institute of Technology Raipur, Raipur-492010, Chhattisgarh, India

***Corresponding author e-mail:** snvictoria.che@nitrr.ac.in

ABSTRACT

A Cu_9S_5/CuS heterostructure supported on nickel foam (Cu_9S_5/CuS@NF) was rationally engineered via a time-dependent hydrothermal route to function as a floatable and electroactive photocatalyst for efficient visible-light-driven degradation of organic pollutants and supercapacitor application. The in-situ formation of the Cu_9S_5/CuS heterointerface enables rapid photoinduced charge separation and directional electron transfer, while the conductive Ni foam provides a three-dimensional porous scaffold that ensures maximum light exposure, effective mass transport, and facile recovery without filtration. FESEM analysis revealed a uniform nanosheet network of Cu_9S_5 and CuS intimately anchored onto the Ni foam skeleton, offering a large surface area and abundant active sites. Cyclic voltammetry (CV) exhibited distinct and reversible Cu^{2+}/Cu^{+} redox transitions, confirming high electroactive surface area and charge storage capacity, while electrochemical impedance spectroscopy (EIS) demonstrated significantly reduced charge-transfer resistance, validating improved interfacial conductivity and faster electron transport across the heterojunction. The material showed promising specific capacitance value of >1500 F/g. Under visible-light irradiation, Cu_9S_5/CuS@NF achieved >90% degradation of malachite green within 75 minutes, following pseudo-first-order kinetics. The photocatalyst retained its morphology, floating ability, and photocurrent stability over multiple cycles, indicating excellent durability and recyclability. The superior photocatalytic performance stems from the synergistic coupling of Cu_9S_5/CuS phases and the conductive, floatable Ni foam support, which collectively enhance charge separation, light utilization, and structural stability. This study presents a rational and scalable approach for developing floatable, electrochemically active heterostructure photocatalysts for sustainable solar-assisted environmental remediation and energy storage applications.

References:

1. Dey, A.; Gaikwad, M. S.; Victoria, S. N. Assembly of Two-Dimensional Nanosheets of Copper Sulfide on Nickel Foam for High-Efficiency Energy Storage Applications: Exploring the Effect of pH. *Resources Chemicals and Materials.* **2025**, *4* (3), 100119.
2. Cao, S.; Feng, W.; Tang, Y.; Ding, Y.; Pang, H. Fabrication of CoTi-ZIF-9-derived carbon/MXene heterostructures for enhanced capacitive deionization in simulated seawater desalination. *Desalination* **2025,** *613*, 119059.

EN-158

Impact of Ag and Mn Co-Doping on Carrier Enhancement and Thermoelectric Performance of Cu_2SnSe_3 at Intermediate Temperatures

S. Karunakaran [a,b], V. Vijay [c], M. Navaneethan [c], J. Archana [a]*

[a] *Centre of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India.*

[b] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India.*

[c] *Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur- 603203, India.*

***Corresponding author e-mail:** jayaram.archana@gmail.com

ABSTRACT

Copper tin selenide has emerged as a promising thermoelectric material, particularly suited for operation in the intermediate temperature range of 500–700 K [1,2]. However, its inherently low electrical conductivity remains a significant limitation that restricts further enhancement of its thermoelectric efficiency. In this study, a series of Mn-substituted solid solutions, ($Cu_{1.85}Ag_{1.5}Sn_{1-x}Mn_xSe_3$), were successfully synthesized via mechanical alloying followed by spark plasma sintering, enabling precise compositional control and dense microstructures. X-ray diffraction analysis confirmed the formation of a single-phase structure without detectable secondary phases, indicating that Mn was effectively incorporated into the host lattice. Hall measurements revealed that Mn substitution significantly increases the carrier concentration, reaching 6.2 × 10^{19} cm^{-3}, which directly contributes to improved charge transport. Notably, partial replacement of Sn by Mn simultaneously enhances the electrical conductivity to 1254.08 S cm^{-1} and maintains a relatively high Seebeck coefficient of 80.47 µV K^{-1}, demonstrating a favorable balance between transport parameters. Consequently, the optimized MN20 composition exhibits a maximum power factor of 616 µW m^{-1} K^{-2}, corresponding to an enhancement of approximately 85% compared with the undoped sample. These findings highlight Mn substitution as an effective strategy for tuning carrier concentration and optimizing the electronic transport properties of Cu-based chalcogenide thermoelectric, providing valuable insight for the rational design of high-performance materials in this class.

Keywords: Copper tin Selenide, Phonon Scattering, Weighted mobility, Activation energy.

References:

1. C. Raju, M. Falmbigl, P. Rogl, P. Heinrich, E. Royanian, E. Bauer, R.C. Mallik, Thermoelectric properties of Zn doped Cu2SnSe3, Mater Chem Phys 147 (2014) 1022–1028.

EN-159

Understanding the Green Hydrogen Production Capability in Copper (Cu) and Vanadium (V) based Materials

Isaac Emmanuel J[1] and Bhaskar Chandra Behera[1*]

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu – 603 203, India*

***Corresponding author e-mail:** bhaskarb@srmist.edu.in

ABSTRACT

Complex metal oxides have emerged as an interesting class of electrocatalysts for water splitting applications, owing to their highly tunable electronic structures and exceptional stability in aqueous electrolytes[1,2]. Copper (Cu) and Vanadium (V) based materials are two such independent systems recently being widely explored for their electrocatalytic activity[3–5]. Here, we summarise recent advances in isolated Cu- and V-based electrocatalysts for the Hydrogen Evolution Reaction (HER)[4–7]. We try to understand how high electrical conductivity and morphological flexibility of Cu and accessible oxidation states and flexible redox chemistry of V can independently boost intrinsic catalytic activity[6,7]. This analysis also summarises various engineering techniques to minimise overpotentials and discusses reasonable design options for transition metal systems for sustainable hydrogen production.

References:

1. Zhu, Y. et al. Metal oxide-based materials as an emerging family of hydrogen evolution electrocatalysts. Energy Environ. Sci. 13, 3361–3392 (2020).
2. Zhu, Y. et al. Beyond conventional structures: emerging complex metal oxides for efficient oxygen and hydrogen electrocatalysis. Chem. Soc. Rev. 54, 1027–1092 (2025).
3. Zou, X. & Zhang, Y. Noble metal-free hydrogen evolution catalysts for water splitting. Chem. Soc. Rev. 44, 5148–5180 (2015).
4. Meena, A. et al. Pt-like hydrogen evolution on a V2O5/Ni(OH)2 electrocatalyst. J. Mater. Chem. A Mater. 7, 15794–15800 (2019).
5. Muthukumar, P., Pannipara, M., Al-Sehemi, A. G. & Anthony, S. P. Highly enhanced bifunctional electrocatalytic activity of mixed copper-copper oxides on nickel foam: Via composition control. New Journal of Chemistry 44, 11993–12001 (2020).
6. Alhawa, D. A. et al. Theoretical and experimental investigations of vanadium pentoxide–based electrocatalysts for the hydrogen evolution reaction in alkaline media. Emergent Mater. 7, 1359–1374 (2024).
7. Zhang, J. et al. Cobalt-stabilized oxygen vacancy of V2O5 nanosheet arrays with delocalized valence electron for alkaline water splitting. Chem. Eng. Sci. 227, (2020).

Dual Z-Scheme $BiVO_4$/CuO/g-C_3N_4 Ternary Heterojunction for Enhanced Visible-Light-Driven Ciprofloxacin Degradation

Vijayalakshmi C[1], Bakiyaraj G[1*]

[1, 1*]*Department of Physics & Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603 203*

***Corresponding author e-mail:** bakiyarg@srmist.edu.in

ABSTRACT

Water pollution caused by organic pollutants demands efficient remediation techniques. However, limited visible-light absorption and high charge recombination rates limit photocatalytic efficiency. In this work, a $BiVO_4$/CuO/g-C_3N_4 ternary heterojunction was fabricated to enhance visible-light-driven photocatalytic performance. $BiVO_4$ was synthesized using *Tabernaemontana divaricata* leaf extract as a natural reducing and stabilizing agent, followed by the integration with CuO and g-C_3N_4 by ultrasonication to construct a heterostructure. Structural, morphological, optical, and surface analyses (XRD, FTIR, UV–vis DRS, PL, SEM, TEM, XPS, and BET) confirmed successful heterojunction formation with enhanced light absorption and reduced charge recombination. The synthesized $BiVO_4$/CuO/g-C_3N_4 composite attained 85% degradation of ciprofloxacin within 60 minutes under visible light irradiation, with a rate constant of 0.0211 min^{-1}, approximately eight times higher than pristine $BiVO_4$. In addition, the composite exhibits broad-spectrum activity toward tetracycline (94%), rhodamine B (84%), and methylene blue (60%) within one hour. The $BiVO_4$/CuO/g-C_3N_4 heterojunction provides enhanced photocatalytic degradation efficiency compared to pristine photocatalysts, which highlights its potential for sustainable wastewater treatment.

References:

1. Liu, Yang-Cheng, et al. *Journal of Environmental Chemical Engineering* 12.5 (2024): 113668.
2. Yaghoot-Nezhad, Ali, et al. *Energy & Fuels* 34.11 (2020): 13588-13605.
3. Li, Jing, et al. *Water Environment Research* 93.10 (2021): 2010-2024.

Development of Biomass-Derived Electrode Material for Supercapacitor Applications

T. Gajalakshmi [1], G.Murali[2], T. Kalaivani [1*],

[1] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai – 603203, Tamil Nadu, India*

[2]*Directorate of Research, SRM Institute of Science and Technology, Kattankulathur, Chennai – 603203, Tamil Nadu, India.*

***Corresponding author e-mail:** kalaivat@srmist.edu.in.

ABSTRACT

In recent years, porous carbon-based material has been one of the most promising materials for environmentally safe and sustainable electrochemical energy storage and conversion. Excitingly, the synthesis of highly absorbent carbon compounds from biomass has gained popularity as a research area among scientists. Here, we report on highly porous carbon achieved from food waste is carbonized by sulfuric acid (H_2SO_4) and activated with various potassium hydroxide concentrations (1:1, 1:3, and 1:5) on a simple and direct microwave pyrolysis. The derived carbon's surface area and pore size are modified. As the KOH concentration increases, the surface area substantially increases, achieving an excellent specific surface area of 1500 m2 g-1 (1:3 mass ratio). The highly porous carbon indicates a charge storage capacitance of 300 F/g at 1 A/g. The highly porous structured carbon structure's electrochemical storage behavior is mainly due to the optimal combination of micro- and mesopore existence with more edge defects sites, which permits a larger surface area and improved conductivity.

Keywords: Porous carbon, food waste carbon, high surface area, specific capacitance.

EN-162

Real-Time Experimental Validation of Thermally Enhanced Nano Composite Phase Change Materials for Photovoltaic Module Cooling.

S.Indirani

Department of Electronics and Instrumentation Engg.

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** indirans@srmist.edu.in

ABSTRACT

Thermal regulation of photovoltaic (PV) modules is critical for maintaining electrical efficiency and ensuring long-term reliability of electronic components. In this study, a nano-composite phase change material (PCM) was developed and characterized for passive thermal management of solar PV systems. The composite PCM was synthesized by incorporating thermally conductive nanofillers into a base PCM to enhance thermal conductivity while preserving latent heat storage capacity. The thermophysical properties of the developed nano-composite were systematically evaluated using Differential Scanning Calorimetry (DSC), thermal conductivity measurements, and morphological analysis to establish structure–property relationships. Results revealed enhanced thermal conductivity, stable phase transition behavior, and negligible degradation in latent heat capacity, along with good thermal cycling stability. The nano-composite PCM was integrated into a photovoltaic module and assessed under real-time outdoor operating conditions. Experimental findings demonstrated a reduction in peak module temperature, resulting in improved power conversion efficiency and enhanced electronic reliability. The analysis further confirmed that uniform nanoparticle dispersion within the PCM matrix plays a key role in improving heat transfer performance. Overall, the study demonstrates that nano-composite PCMs provide a promising materials-based solution for advanced thermal management of photovoltaic electronics and other temperature-sensitive electronic systems.

Keywords: Nano-composite phase change materials; thermophysical characterization; photovoltaic modules; electronic thermal management; Differential Scanning Calorimetry (DSC); real-time experimental evaluation.

EN-163

In-Situ Synthesized Gel Polymer Electrolyte for Long-Life Sodium-Ion Batteries

Debalina Deb,[1] Aninda J. Bhattacharyya[1, 2*]

[1]*Interdisciplinary Centre for Energy Research, Indian Institute of Science, Bengaluru, Karnataka, 560012 India*

[2]*Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru, Karnataka, 560012*

***Corresponding author e-mail:** anindajb@iisc.ac.in

ABSTRACT

We present a solid-state sodium-ion conducting gel polymer electrolyte (GPE), in-situ synthesized directly on sodium metal or electrode surfaces, as a promising alternative to conventional liquid and ceramic electrolytes for high-performance sodium-ion batteries (SIBs). The GPE is fabricated through a straightforward protocol involving in-situ polymerization of a liquid electrolyte (LE) and polymer precursor (PP) mixture within a highly porous electrospun polyacrylonitrile (PAN) membrane pre-mounted on either Na metal or suitable electrodes. The membrane's high porosity enables significant LE entrapment (~60 vol%), which upon polymerization forms a robust, thermally and mechanically stable amorphous gel. The resulting GPE exhibits high ionic conductivity (~1 mS cm^{-1}, comparable to LE), a high Na^+ transference number (0.63), a wide electrochemical stability window (up to 5.2 V vs. Na^+/Na), and excellent interfacial compatibility. Importantly, the chemically stable GPE effectively suppresses dendrite growth, enabling sustained Na plating/stripping for hundreds of cycles at various current densities with low overpotentials. Electrochemical impedance spectroscopy (EIS) studies reveal that, unlike LE which shows unstable solid–electrolyte interphase (SEI) evolution over ~1 month, the GPE supports long-term stable SEI growth lasting over ~2 months. In half cells (Na||$Na_3V_2(PO_4)_3$) and symmetric NVP||NVP configurations, the GPE delivers outstanding cycling stability with consistent performance at 1C for 500–1000 cycles at room temperature. Furthermore, its compatibility with emerging Sn-based alloy anodes—considered viable alternatives to hard carbons—demonstrates the versatility and broad applicability of the GPE for future SIB technologies.

Keywords: Sodium-ion batteries (SIBs), Gel polymer electrolyte (GPE), Electrospun PAN membrane, Stable SEI formation, Sn-based alloy anode

References

1. Deb, D.; Pal, S.; Kravets, Y.; Adelhelm, P.; Bhattacharyya, A.J.; In-Situ Polymerized Gel Electrolytes on Na Metal/Electrodes for High Performance Sodium-Ion Batteries; Small, Willey, 2025, Volume 21, Issue 46, Pages e06134
2. Choe, G.; Kim, H.; Kwon, J.; Jung, W.; Park, K.-Y.; Kim, Y.-T. Re-Evaluation of Battery-Grade Lithium Purity toward Sustainable Batteries. Nature communications 2024, 15 (1). https://doi.org/10.1038/s41467-024-44812-3.

EN-164

Carbon Nanotube-Integrated Co-phthalocyanine/NiFe-LDH Hybrid with Superior Bifunctional Activity for Water Splitting

Tanisha Mavjekar and T. Maiyalagan*

Electrochemical Energy Laboratory, Department of Chemistry,

SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India.

***Corresponding author e-mail** :maiyalat@srmist.edu.in & maiyalagan@gmail.com

ABSTRACT

The worldwide transition to a less carbon-intensive energy infrastructure goes hand in hand with the need for efficient, scalable and stable electrolyzers that run on earth-abundant materials. Here, we demonstrate the synergy between molecular and inorganic hybrid electrocatalyst by coupling electron-rich and tuneable Co phthalocyanine (CoPc) molecules with NiFe layered double hydroxide (NiFe-LDH) nanosheets and conductive multi-walled carbon nanotubes (MWCNTs). The NiFe-LDH/CoPc/MWCNT ternary composite (80:10:10) obtained via a one-step hydrothermal route results in a hierarchically interconnected architecture where the π–d electronic coupling between Co–N_4 and Ni–Fe oxyhydroxide enhances the intrinsic catalytic activity, while the MWCNT network offers a continuous electron-transport pathway, prevents nanosheet restacking and thereby remarkably improves the hybrid's mechanical and electrochemical stability.

The synergistically engineered interface facilitates the optimized adsorption and conversion of key intermediates for OER and HER, the overpotentials are thus extraordinarily low and measured to be 270 mV for the OER and 142 mV for the HER at 10 mA cm^{-2} and can maintain stable operation for more than 70 h in alkaline media. The key to the success of the presented strategy lies in the combination of molecular CoPc units, LDH nanosheets and carbon nanotube scaffolds to fabricate the next-generation bifunctional catalysts that match noble-metal systems yet allow for practical and scalable water-splitting technologies.

Keywords: Co-phthalocyanine, NiFe-LDH, Carbon Nanotubes, Water Splitting, Bifunctional Catalyst, HER, OER, Hydrothermal Synthesis

EN-165

Electrochemical Fabrication of Self-Supported Pt-Nanoporous Gold for Efficient Hydrogen Evolution Reaction

Suriya Thomas, Veni SoundaraKrishnan, and Anandhakumar Sukeri*

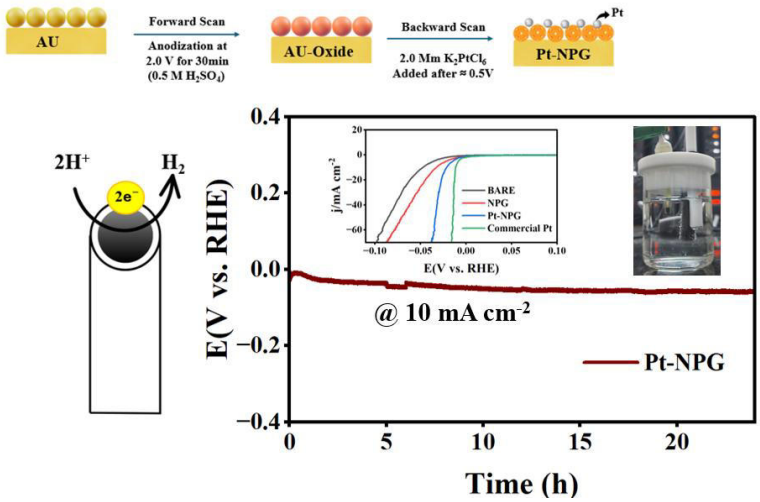
Nanoscale Materials Electrochemistry Laboratory, Department of Chemistry

SRM institute of Science and Technology, Kattankulathur – 603203, Tamil Nadu, India.

***Corresponding author e-mail:** anandhas2@srmist.edu.in

ABSTRACT

Developing highly active electrocatalysts for the hydrogen evolution reaction (HER) is essential for improving the overall efficiency of the water splitting reaction. In this contest, we prepared a self-supported ultra-low platinum (Pt) loaded nanoporous gold (Pt-NPG/Au) electrocatalyst, which significantly enhances HER activity with excellent stability. The Pt-NPG was fabricated through "anodization followed by an electrochemical reduction" approach on an Au substrate in sulfuric acid solution, where in-situ generated oxygen bubbles during the anodization can act as a dynamic template in the formation of a 3D nanoporous framework. A controlled incorporation of Pt precursor during the reverse scan enabled uniform deposition of Pt nanostructures onto the NPG surface. The as-synthesized Pt-NPG catalyst was characterized using TEM, EDX, and cyclic voltammetry. Electrochemical studies revealed excellent electrocatalytic activity by achieving the benchmark current density of 10 mA cm^{-2} at 23 mV with long-term stability. This work introduces a simple, scalable, and cost-effective strategy for developing Pt-minimized HER electrocatalysts comparable to commercial Pt, offering promising potential for clean energy applications.



Reference:

1. Sukeri, A., de Carvalho Junior, E. J., and Bertotti, M, Electrochemistry Communications, 2019, 100, 96-99.

EN-166

Environmentally benign synthesis of phase-pure Ni3V2O8 Nanoparticles with Enhanced Pseudocapacitance for Electrochemical Energy Storage Applications

D. Christy, Aruljothy John Bosco*

Department of Chemistry, Faculty of Engineering and Technology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

Corresponding author e-mail: johnbosa@srmist.edu.in ,

ABSTRACT

Energy storage devices are a wide range of technologies that stores energy for later use. These are essential for enhancing power system stability, improving power quality and enabling integration of renewable energy sources. Transition metal oxide nanoparticles have gained significant attention in various fields due its promising electrochemical, catalytic and optical properties. This work presents a sustainable and environmentally benign strategy for synthesizing nickel vanadate (Ni3V2O8) nanoparticles through a green synthesis pathway, utilizing vitis vinifera (grape) fruit extract as a natural stabilizing agent. Characterization techniques such as X-ray diffraction for crystallinity, Fourier-transform IR spectroscopy for functional group analysis, and field-emission SEM for surface morphology were employed to characterize the material thereby confirming the formation of phase-pure Ni3V2O8 with uniform nanoscale morphology. Surface parameters were obtained from Brunauer–Emmett–Teller analysis indicating surface area value of 20.176 m2g-1. The optical characteristics were examined using UV–Visible diffuse reflectance spectroscopy (UV-DRS) showing a band gap of 2.65 eV. Electrochemical characteristics were assessed through cyclic voltammetry, galvanostatic charge–discharge analysis and electrochemical impedance measurements, all of which confirmed remarkable capacitive performance. The Ni3V2O8 electrode possessed a high specific capacitance of 122.1 F/g and remarkable cycling stability up to 2000 cycles thereby making it a favourable material to be utilized in energy storage devices. The findings emphasize the usefulness of green-synthesized nanomaterials for efficient and sustainable supercapacitor applications.

Keywords: BET, EIS, UV-DRS, vitis vinifera

References:

1. Christy D., Gifta J, Jerold Antony A, Hirachand Patil R., Basavegowda N, Ashraf I.M., Ibrahim A, and Shkir M. Environmentally benign synthesis of phase-pure Ni3V2O8 nanoparticles with enhanced pseudocapacitance for electrochemical energy storage applications. J. Phys. Chem. Solids, 209, 113333.
2. K. Thiagarajan, J. Theerthagiri, R.A. Senthil, P. Arunachalam, J. Madhavan, M.A. Ghanem, Synthesis of Ni3V2O8@graphene oxide nanocomposite as an efficient electrode material for supercapacitor applications, J. Solid State Electrochem. 22 (2018) 527–536.

EN-167

Synergistic CdTe@ Sulfur Doped g-C_3N_4 Nanocomposite as a High-Performance Electrode for Advanced supercapacitor Application

Navathitha Dharshini M, Raji Sekar, Sundaravadivel Elumalai*

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603203, India

***Corresponding author e-mail:** sundaravadivelchem@gmail.com

ABSTRACT

The development of efficient electrode materials is essential for advancing high performance supercapacitors with superior energy storage capability and long cycling stability. In this work, a synergistic CdTe@ Sulfur Doped g-C_3N_4 Nanocomposite was designed and synthesized to enhance electrochemical performance. The incorporation of CdTe nanoparticles into the layered S-g-C_3N_4 framework creates a hetrostructured architecture with abundant electroactive site, improved electrical conductivity, and accelerated charge transport pathways. Sulfur doping induces defect states and enhance electronmobility, while the CdTe component contributes pseudocapacitive behavior and facilitates rapid redox reactions. Structural and morphological analyses condirms the successful formation of the composite and uniform dispersion of CdTe nanoparticles over the doped carbon nitride matrix.The electrochemical inverstigations reveal that the CdTe@ Sulfur Doped g-C_3N_4 electrode exhibits significantly enhanced specific capacitance, superior rate capability and excellent cycling stability compared to pristine g-C_3N_4. The improved performance is atributed to the synergistic interaction between CdTe and S-g-C_3N_4, which promotes efficient ion diffusion, reduces internal resistance, and suppresses charge recombination. The hetrostructured nanocomposite demonstrates strong potential as a high-performance electrode material for next-generation energy storage devices. These findings highlight a promising strategy for engineering doped carbon nitride-based hetrostructures to achieve enhanced electrochemical energy storage performance.

Keywords:

Cadmium telluride, Sulfur-doped graphitic carbon nitride, Supercapacitor, energy storage.

Reference:

1. Abdelmohsen, S. A., Alanazi, M. M., Sulayem, L. M., Aman, S., Farid, H. M. T., & Waheed, M. S. (2025). Synthesis of graphitic carbon nitride (g-C3N4)-doped metal sulfide nanocomposite for supercapacitor applications. *Chemical Papers*, *79*(12), 8829-8842

EN-168

CoAl-N Nanostructures Derived from Spent $LiCoO_2$ Cathodes for High-performance Bifunctional Oxygen Electrocatalysis

Nesan R. K. Yabesh [1], and Govindhan Maduraiveeran*[1,2]

[1] *Materials Electrochemistry Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu-603 203, India*

[2] *Materials Research Center, American University of Sharjah, PO Box 26666, Sharjah, United Arab Emirates*

***Corresponding Author E-mail:** maduraig@srmist.edu.in and mgovindhan@aus.edu

ABSTRACT

The rapid global expansion of lithium-ion battery (LIB) usage has accelerated the depletion of critical transition metals while simultaneously generating large volumes of hazardous waste, highlighting the urgent need for sustainable recycling approaches [1]. In this work, we present a facile and efficient strategy to convert spent $LiCoO_2$ (LCO) cathodes into three-dimensional heterostructured CoAl-N|B nanosheets that function as bifunctional electrocatalysts for both the oxygen evolution reaction (OER) and oxygen reduction reaction (ORR). Cobalt-based heterostructures were directly recovered from LCO leachates through a single-step electrochemical deposition onto a carbon-fibre substrate, enabling controlled composition and nanoscale structural tuning. Among the synthesized materials, the 3D CoAl-N|B nanosheets displayed outstanding bifunctional performance, delivering an ORR onset potential of ~0.88 V vs. RHE with a catalytic current density of -0.51 mA cm^{-2}, along with an OER overpotential of ~330 mV at 10 mA cm^{-2} in 1.0 M KOH [2]. This enhanced activity arises from the synergistic electronic coupling between Co, Al, and N functionalities, which optimizes the local electronic structure, increases the exposure of active sites, and facilitates interfacial charge transport. Additionally, the engineered heterostructures exhibit strong methanol tolerance and excellent long-term durability. Overall, this study introduces a circular economy driven approach for upcycling battery waste into high-performance oxygen electrocatalysts, offering a scalable and environmentally sustainable route for future energy conversion and storage technologies.

Keywords: Spent $LiCoO_2$ Cathode; Transition-Metal Oxides; Bifunctional Catalyst; Oxygen Electrocatalysis; Oxygen Evolution Reaction; Oxygen Reduction Reaction.

References:

1. N.R.K. Yabesh, M.V. Inbaraj, G. Maduraiveeran, Recycling spent Li-ion batteries into functional nanomaterials for energy systems, Mater. Today Chem. 52 (2026) 103432. https://doi.org/10.1016/j.mtchem.2026.103432.
2. N.R.K. Yabesh, K.K.R. Datta, G. Maduraiveeran, CoAl-N Nanosheets Derived from Spent LiCoO2 Cathodes for High-Performance Bifunctional Oxygen Electrocatalysis, ACS Appl. Nano Mater. (2026). https://doi.org/10.1021/acsanm.6c00258.

EN-169

Metal-Organic Framework–Based Architectures for High-Efficiency Supercapacitive Energy Storage

Kavipriya Baskar, Aruljothy John Bosco

Department of Chemistry, Faculty of Engineering and Technology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

Corresponding author email*: johnbosa@srmist.edu.in

ABSTRACT

Metal–organic frameworks (MOFs) represent a promising class of materials for high-performance supercapacitors; however, their practical implementation remains constrained by intrinsic low electronic conductivity and structural instability during faradaic processes. In this study, a novel Cu–Ce bimetallic MOF hybridized with graphene oxide (GO) was synthesized via a facile co-precipitation route. The integration of heterometallic centers (Cu^{2+}/Ce^{3+}) within the benzene-1,3,5-tricarboxylate (BTC) framework facilitates synergistic redox transitions and provides a high density of electroactive sites. Concurrently, the incorporation of a GO-based conductive network serves as a structural scaffold, enhancing long-range charge transport and mitigating mechanical strain during ion intercalation.

Keywords: Bimettalic MOF, GO, Co-precipitation, Supercapacitor.

References:

1. Ramachandran, R., Xuan, W., Zhao, C., Leng, X., Sun, D., Luo, D., & Wang, F. RSC Adv., 2018, 8, 3462-3469
2. Aashi, Rekha Rani, Srinivasan Alagar, Jatin Sharma, Arun k, and Vivek Bagchi ACS Materials Lett. 2024, 6, 1769−1778

EN-170

Design and Fabrication of Flexible Solid-State Interdigitated Micro-Supercapacitors Using Activated Carbon Microfibers

Mariyarathinam Vinoth Inbaraj[1], and Govindhan Maduraiveeran*[1,2]

[1] *Materials Electrochemistry Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India*

[2] *Materials Research Center, American University of Sharjah, Sharjah - 26666, UAE*

***Corresponding author e-mail:** mgovindhan@aus.edu & pgmadura@yahoo.co.in

ABSTRACT

Micro-supercapacitors stand out as promising candidates for compact energy storage solutions in wearable and portable electronic systems. The growing demand in this field emphasizes the need for low-cost, highly active electrode materials that can be fabricated through simple and scalable methods. In this work, we introduce activated carbon microfiber electrodes prepared via an electrochemical activation route. This process effectively increases the specific surface area while simultaneously enriching the surface with oxygen-containing functional groups, thereby improving electrochemical performance. The optimized carbon microelectrode delivers an areal capacitance of ~30.5 mF cm^{-2}, maintaining excellent cycling stability with 142.8% capacitance retention after 50,000 cycles. Furthermore, a symmetric solid-state interdigitated micro supercapacitor assembled with these electrodes exhibits an energy density of 0.015 μWh cm^{-2} at 0.3 mA cm^{-2} and a power density of 11.24 μW cm^{-2}, along with outstanding durability over 20,000 cycles, retaining 125% of its initial capacitance.

References

1. M. V. Inbaraj, G. Maduraiveeran, Chem. Commun. 2025, 61, 5459.
2. Z.-S. Wu, Y.-Z. Tan, S. Zheng, S. Wang, K. Parvez, J. Qin, X. Shi, C. Sun, X. Bao, X. Feng and K. Müllen, J. Am. Chem. Soc., 2017, 139, 4506–4512.
3. Y. Bräuniger, S. Lochmann, J. Grothe, M. Hantusch and S. Kaskel, ACS Appl. Energy Mater., 2021, 4, 1560–1567.

EN-171

In-Situ Sulfidation-Derived Selenium-Doped β-Bi_2O_3/Bi_2S_3 Heterostructure as an Effective Electrode for Supercapacitor Applications

Rajapandeeswari.G , Nirmal Nathan. A and Sundaravadivel Elumalai*

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203, India,

Department of Chemistry, Faculty of Engineering and Technology.

***Corresponding author e-mail:** sundaravadivelchem@gmail.com

ABSTRACT

Selenium-doped β-Bi_2O_3/Bi_2S_3 heterostructured electrode materials were produced using a simple hydrothermal process, followed by in-situ sulfidation, for enhanced supercapacitor performance. The integration of selenium into the β-Bi_2O_3 lattice generates many oxygen vacancies and markedly enhances electrical conductivity. Following controlled in-situ sulfidation, a thin, conductive Bi_2S_3 layer forms on the oxide surface, creating a distinct oxide–sulfide heterointerface. This heterostructure facilitates rapid electron transport and efficient ion diffusion through the inherent interfacial electric field and cooperative redox activity. The Se-β-Bi_2O_3/Bi_2S_3 electrode has improved pseudocapacitive behavior, elevated specific capacitance, superior rate capability, and prolonged cycling stability. Additionally, an asymmetric supercapacitor device constructed with the optimised composite exhibits enhanced energy and power densities, underscoring the efficacy of the hydrothermal in-situ sulfidation method for advanced energy storage applications.

Keywords: Selenium-doped the β-Bi_2O_3, Bi_2S_3; In-situ sulfidation; Hydrothermal method; Oxide–sulfide heterostructure; Supercapacitors application.

EN-172

Accelerated Discovery of Cu-Based Lead-Free Hybrid Halide Perovskitoids Using Machine Learning for Solar Water Splitting Application

Mahalaxmi M C, Meenal Deo*

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** meenald@srmist.edu.in

ABSTRACT

Lead-free hybrid halide perovskites have emerged as promising materials for optoelectronic applications because of their compositional versatility and tunable electronic structures. Despite these advantages, their intrinsic instability in aqueous environments has restricted their integration into solar water splitting systems, where prolonged exposure to water degrades the material rapidly. In response to the toxicity of Pb and the instability of Sn-based analogues, substitution with Cu has recently attracted significant attention as a viable alternative. The presence of Cu^{2+} introduces strong Jahn–Teller distortion, disrupting the ideal BX_6 octahedral connectivity and transforming the conventional three-dimensional perovskite lattice into low-dimensional architectures commonly termed 'perovskitoids'. While this structural distortion modifies the electronic landscape, it simultaneously enhances chemical robustness, leading to markedly improved air and water stability. These characteristics position Cu-based perovskitoids as compelling candidates for solar water splitting, provided that their optoelectronic properties can be appropriately tuned. In regard to this, to navigate the vast compositional space efficiently, machine learning regression models are employed to predict application specific target properties, particularly band gaps, across diverse Cu-based hybrid halide compositions with the help of key descriptors. The predicted and estimated outputs are then incorporated into a hierarchical screening strategy that systematically narrows down to the pool of potential candidates. By integrating data-driven prediction with physics-informed screening, this framework enables accelerated identification of stable, lead-free Cu-based perovskitoids with electronic properties tailored for solar water splitting applications, thereby advancing rational materials discovery in this emerging class of compounds.

EN-173

Electrospun ZnX_2O_4 (X=Co, Mn, Fe) Nanofibers as Efficient Electrocatalysts for Electrochemical Water Splitting

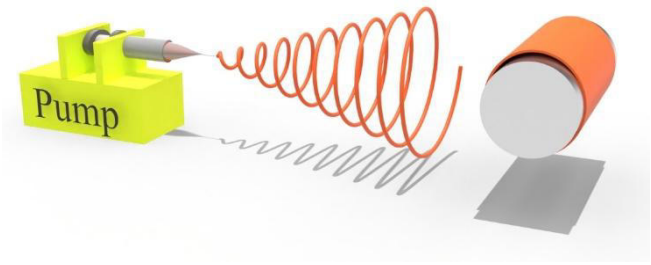
P. Chinnappan Santhosh[1], Suresh Jayakumar[1], Vasudev KJ[1], A. V. Radhamani*[1]

[1]*Energy and Innovative Materials Laboratory (EIML), Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST), Kattankulathur, Chengalpattu, 603203, Tamilnadu, India.*

***Corresponding author e-mail:** radhamaa@srmist.edu.in

ABSTRACT

Electrochemical water splitting is regarded as a promising and sustainable strategy for large-scale hydrogen production; however, its practical implementation is hindered by the sluggish kinetics of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Developing efficient, earth-abundant, and durable electrocatalysts is therefore essential to reduce overpotentials and enhance catalytic efficiency. In this work, we report the rational design and fabrication of one-dimensional spinel oxide nanofibers based on $ZnCo_2O_4$, $ZnMn_2O_4$, and $ZnFe_2O_4$ as cost-effective bifunctional electrocatalysts for overall water splitting. The fibrous architecture, prepared via a controllable electrospinning strategy followed by thermal treatment, provides a continuous conductive pathway, high aspect ratio, and abundant exposed active sites. The incorporation of Co, Mn, and Fe into the spinel lattice effectively modulates the electronic structure, enhances charge transfer kinetics, and optimizes adsorption/desorption behavior of reaction intermediates. Among the investigated catalysts, $ZnCo_2O_4$ nanofibers exhibit superior OER activity due to the favorable redox couple of Co^{2+}/Co^{3+}, while $ZnFe_2O_4$ and $ZnMn_2O_4$ contribute to enhanced HER performance through improved electrical conductivity and synergistic metal-oxygen interactions. The interconnected porous nanofiber network facilitates electrolyte penetration and rapid electron transport, resulting in reduced charge-transfer resistance and improved catalytic stability. Consequently, the optimized spinel nanofiber electrodes demonstrate low overpotentials, small Tafel slopes, and excellent long-term durability in alkaline media. This study highlights the significance of structural engineering and transition-metal synergy in spinel oxide nanofibers, providing a scalable and economically viable pathway toward high-performance bifunctional electrocatalysts for sustainable hydrogen generation.



References:

1. Cao, X., Wang, T. & Jiao, L. Adv. Fiber Mater. 3, (2021) 210–228.
2. X. Lyu, Y. Hu, Y. Han, X. Li, Q. Yu, B. Wen, X. Zhao, Q. Dong and A. Du, J. Colloid Interface Sci., 675, (2024) 326–335.

Water Treatment and Microplastic Degradation by Carbon Nitride-Supported Single-Atom Catalyst

Akshaya Radhakrishnan[1], Noufal Kandoth[2], Arthanareeswari Maruthapillai[1]*

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India.*

[2]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India*

***Corresponding author e-mail:** arthanam@srmist.edu.in

ABSTRACT

Microplastic pollution has become a major environmental issue in aquatic systems, posing significant risks to ecosystems and human health due to its persistence and ability to adsorb toxic pollutants. Conventional water treatment treatments are typically unsuccessful at eliminating microplastics, particularly nano-sized fractions, necessitating more advanced remediation strategies. We demonstrate the design and implementation of a carbon nitride-supported single-atom catalyst (SAC) tailored for effective water treatment and oxidative degradation of microplastic particles. The catalyst was developed by scattering transition metal centers (e.g., Fe, Co, or Ni) into a graphitic carbon nitride (g-C_3N_4) structure. This resulted catalyst that shows a high surface area, plentiful active sites, and improved charge separation under visible light irradiation. Photocatalytic studies revealed that the SAC system removed and degraded polystyrene and polyethylene microplastics more efficiently than bulk g-C_3N_4 and traditional catalysts. Visible light increased the formation of reactive oxygen species (ROS), such as •OH and $O_2^{\bullet-}$. This accelerated the chain scission and oxidation of microplastic polymers, resulting in low-molecular-weight fragments and mineralised products. Mechanistic studies revealed that the single-atom sites functioned as active electron transfer centers, supporting efficient ROS generation while inhibiting charge recombination. The modified catalyst was extremely stable and reusable over numerous cycles, with low metal species leaching. This study demonstrates a viable technique for incorporating single-atom catalytic systems into sophisticated water treatment technologies, providing an effective pathway for reducing microplastic contamination in environmental waters.

Keywords: g-C_3N_4, SAC, Microplastics, Water treatment

EN 175

Boron-Doped MOF-Derived NiO as an Enhanced Electrocatalyst for Alkaline Water Splitting: A Comparative Study with Pristine Ni-ZIF

Adhwaith Narayan K. N, Jose Agnel G, J Archana[1], P. Justin Jesuraj[1]*.

[1] *Center of Excellence in Materials for Advanced Technologies (CeMAT), SRM Institute of Science and Technology, Kattankulathur, Potheri, Chengalpattu, 603 203, India.*

***Corresponding author e-mail:** justinp@srmist.edu.in

ABSTRACT

Nickel-based metal-organic frameworks (Ni-MOFs) have emerged as versatile precursors for designing efficient, earth-abundant electrocatalysts for alkaline water splitting. In this study, pristine Ni-ZIF was synthesized via a solvothermal route and thermally transformed into porous NiO while preserving its template-derived architecture. To further tailor the electronic structure, boron doping was introduced during the derivation process to engineer defect density and modulate charge distribution. Structural analysis confirmed the complete phase conversion of Ni-ZIF to crystalline NiO after calcination. This MOF-templated strategy enables the retention of hierarchical porosity, providing an enlarged electrochemically active surface area and improved electrolyte diffusion. Boron incorporation is expected to induce lattice distortion and generate additional defect sites, thereby enhancing electrical conductivity and promoting faster interfacial charge transfer compared to pristine Ni-ZIF and undoped NiO. The combined effect of MOF-derived structural porosity and heteroatom-induced electronic modulation is anticipated to strengthen intrinsic catalytic activity and accelerate reaction kinetics for both oxygen evolution and hydrogen evolution processes in alkaline media. Furthermore, the optimized NiO and B-NiO systems will be strategically heterostructured with transition metal sulfides to enhance hydrogen evolution reaction (HER) performance. The formation of oxide-sulfide interfaces is expected to promote synergistic charge transfer, improve hydrogen adsorption energetics, and facilitate faster reaction kinetics, thereby strengthening overall bifunctional water-splitting efficiency.

Keywords: Metal organic framework, MOF-derived metal oxide, Bifunctional catalyst.

References:

1. A. Raveendran et al., RSC Adv., 2023, 13, 3843–3875.
2. J. George et al., Chem. Rec., 2025, 25, e202400254.

EN-176

Integration of Metal Selenide with Rare Earth Element for Oxygen Evolution Reaction

Rajalakshmi Pandian[1] and Arulmozhi Rajaram*[1]

[1] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur Tamil Nadu, India 603203.*

***Corresponding author e-mail:** arulmozr@srmist.edu.in

ABSTRACT

The development of efficient and cost-effective electrocatalysts for the oxygen evolution reaction (OER) is crucial for advancing sustainable hydrogen production through water splitting. In this work, rare earth element doped metal selenide electrocatalysts were synthesized directly on nickel foam via a facile electrodeposition method. The influence of deposition duration on the structural, morphological, and electrochemical properties of the catalysts was systematically investigated. Structural and surface analyses confirmed the successful incorporation of rare earth element doped metal selenide framework, leading to modified electronic structure and enhanced active sites. Electrochemical measurements reveal that the optimized electrode exhibits significantly improved OER performance compared to pristine metal selenide delivering a lower overpotential along with favourable reaction kinetics and good electrochemical stability. This study demonstrates that rare-earth element doping is an effective strategy to tune the electronic structure of transition metal selenides and enhance their catalytic efficiency for water oxidation.

References:

1. T. Huang, Y. L. Wu, Z. P. Sun, Y. Y. Chen, S. Lei, Y. Pan, L. W. Zhu, D. Liu, X. Cao and Z. Yan, *Inorg. Chem.*, 2024, **63**, 23450–23458.
2. Z. Qiu, C. W. Tai, G. A. Niklasson and T. Edvinsson, *Energy Environ. Sci.*, 2019, **12**, 572–581.
3. X. Ji, Y. Lin, J. Zeng, Z. Ren, Z. Lin, Y. Mu, Y. Qiu and J. Yu, .
4. K. C. Majhi and M. Yadav, *ACS Eng. Au*, 2023, **3**, 278–284.
5. H. Xiang, Q. Dong, M. Yang and S. Liu, *Mater. Chem. Front.*, 2024, **8**, 1888–1926.

EN-177

Investigation on Structural and Optical Properties of Quaternary Oxides for Energy Conversion and Storage Applications

Sugi Sundaramoorthi[1], Devika Rajan Sajitha[1] & Shyju Thankaraj Salammal[1]*

[1] *Centre of Excellence for Energy Research, Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India.*

***Corresponding author e-mail:** ssugi9701@gmail.com

ABSTRACT

Bismuth copper vanadium oxide (BCVO) was synthesized as a quaternary oxide system comprising Cu, Bi, and V elements, designed to form a single-phase crystalline structure. The structural features of BCVO were thoroughly analysed using X-ray diffraction (XRD), micro-Raman spectroscopy, and UV-Visible spectroscopy. The XRD analysis confirmed a Monoclinic phase with $P2_1/n$ m symmetry typical compound the of $BiCu_2VO_6$. Raman spectral analysis further supported the structural integrity, revealing distinct vibrational modes, confirming strong lattice coupling among the constituent metal–oxygen units. The optical properties of BCVO were examined using UV–Visible diffuse reflectance spectroscopy (DRS). The absorption spectrum exhibited a broad and intense absorption band in the visible region, confirming its strong light-harvesting ability. The optical band gap energy, calculated from the Tauc plot, was found to be in the range of 1.8–2.1 eV, which is lower than that of pure $BiVO_4$, indicating enhanced visible-light absorption due to Cu and Bi incorporation. The reduced band gap is attributed to the hybridization between Cu 3d and O 2p orbitals, as well as the structural distortions introduced by the quaternary cationic lattice. These optical and structural characteristics collectively indicate that BCVO possesses favourable electronic transitions and charge carrier mobility, making it a potential material for visible-light-driven photocatalytic and energy conversion applications. The incorporation of Cu and Bi within the vanadate structure leads to slight lattice distortions and structural strain, attributed to the difference in ionic radii and coordination environments of the cations. These structural modifications play a crucial role in tailoring the electronic structure and defect states, which directly influence the material's functional performance in energy-related applications.

Keywords: Quaternary Oxide, Co-precipitation Synthesis, Band gap energy, Photocatalytic, Energy Storage.

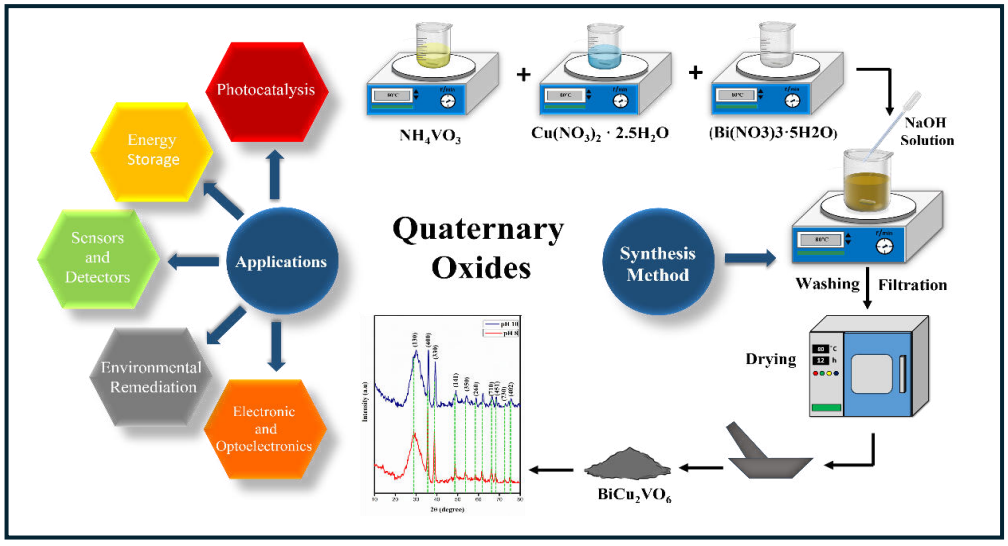


Figure 1: Schematic diagram for metal oxides classification, Synthesis and Applications.

Reference:

1. L. Zhou, E. Bainglass, M. Masroor, B. Giri, G. Li, A. Carl, R. L. Grimm, M. N. Huda, L. V. Titova, and P. M. Rao, J. Mater. Chem. A 9, 1643 (2021).
2. U. P. M. Ashik, S. Kudo, and J. Hayashi, in Synth. Inorg. Nanomater. (Elsevier, 2018), pp. 19–57.
3. C. Wang, Y. Zhang, L. Zhao, C. Wang, F. Liu, X. Sun, X. Hu, and G. Lu, J. Colloid Interface Sci. 592, 186 (2021).

MnO_2 Cathodes for High Performance Aqueous Zinc-Ion Battery Applications

Jasmine Beulah Salome S[1], Ajay Rakkesh R[1*]

[1]*SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** ajayr1@srmist.edu.in ajayrakkesh@gmail.com

ABSTRACT

MnO_2 has emerged as a promising cathode material for aqueous zinc-ion batteries (AZIBs) due to its high theoretical capacity and low cost. The electrochemical performance of MnO_2 is strongly governed by the synthesis route. MnO_2 is synthesized by the hydrothermal method, which is tailored for AZIB applications. This method enables controlled formation of various MnO_2 polymorphs (α-, β-, γ-, δ-MnO_2) and nanostructures such as nanorods, nanosheets, nanoflowers, and porous frameworks. Optimized synthesis route enhances Zn^{2+} diffusion kinetics, improves structural stability during repeated Zn^{2+} insertion/extraction, and mitigates Mn dissolution in aqueous electrolytes. Overall, rational design and scalable synthesis of MnO_2 cathodes are crucial for advancing high-performance, durable, and low-cost aqueous zinc-ion batteries for large-scale energy storage applications.

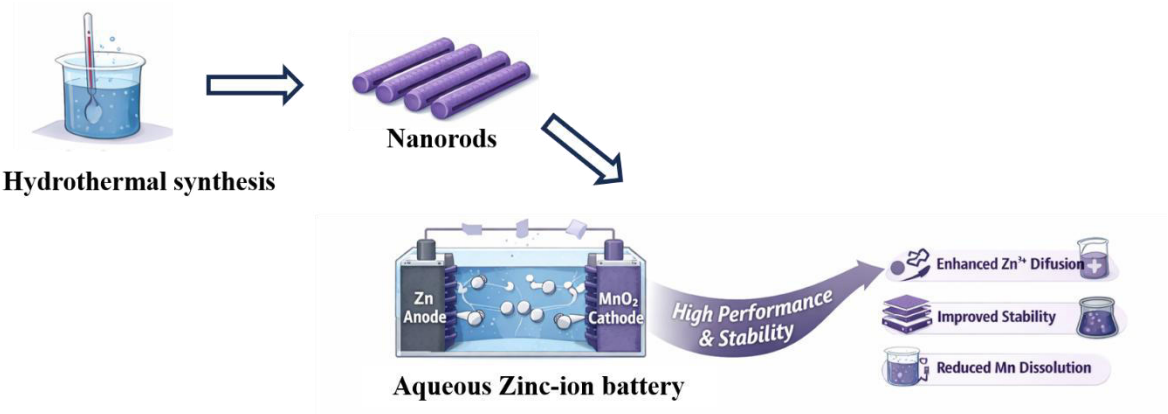


Fig. 1 MnO_2 for aqueous zinc-ion battery

Keywords: Cathode, Aqueous Zinc-ion battery

References:

1. Fang, G., Zhou, J., Pan, A., & Liang, S. (2018). Recent advances in aqueous zinc-ion batteries. ACS Energy Letters, 3(10), 2480-2501.
2. Liao, Y., Chen, H. C., Yang, C., Liu, R., Peng, Z., Cao, H., & Wang, K. (2022). Unveiling performance evolution mechanisms of MnO2 polymorphs for durable aqueous zinc-ion batteries. Energy Storage Materials, 44, 508-516.

EN-179

Crystal Structure and Short-Range Order of Lithium Cobaltate by High Energy X-ray Diffraction and Neutron Diffraction Studies

Kriti[1], Sourabh Wajhal[2], Margit Fabian[3], Hirdesh[4], and Atul Khanna[1]*

[1]*Glass & Sensors Lab, Department of Physics, Guru Nanak Dev University, Amritsar, Punjab, India*

[2]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India*

[3]*HUN-REN Centre for Energy Research, Konkoly Thege Miklos st. 29-33, 1121 Budapest, Hungary*

[4]*Neutron Spectroscopy Department, Centre for Energy Research, Konkoly Thege Miklos st. 29-33, 1121 Budapest, Hungary*

***Corresponding author e-mail:** atul.phy@gndu.ac.in

ABSTRACT

Lithium cobalt was prepared using solid state sintering method in the temperature range of 700-800° C. The crystal structure and short-range structural properties of the lithium cobaltate was characterized using high energy x-ray diffraction (HEXRD, λ=0.165202 Å) and neutron diffraction studies. Reitveld refinement of both HEXRD and neutron diffraction data was carried out. HEXRD studies confirms the formation of hexagonal $LiCoO_2$ phase with the unit cell dimensions of $a = b = 2.81$ Å and $c = 14.05$ Å, $\alpha = \beta = 90°$ and $\gamma = 120°$. Similarly, the Rietveld analysis of neutron diffraction datasets gave the unit cell dimensions of $a = b = 2.82$ Å and $c = 14.14$ Å, $\alpha = \beta = 90°$ and $\gamma = 120°$. The HEXRD pair distribution function shows the first two peaks at 1.91 Å and 2.83 Å due to Co-O and Co-Co bonds respectively.

Keywords: Lithium cobaltate; high energy x-ray diffraction; neutron diffraction; reitveld refinement.

EN-180

Valorization of pyrolysis-derived bio-oil into high-performance biodegradable polymers

Crossline Ajona[1, 2], Ayyadurai Saravanakumar[2, *]

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603 203, Chengalpattu District, Tamil Nadu, India*

[2]*Centre for Research in Environment, Sustainability Advocacy and Climate Change (REACH), Directorate of Research and Virtual Education, SRM Institute of Science and Technology, Kattankulathur – 603 203, Chengalpattu District, Tamil Nadu, India*

[*]**Corresponding author e-mail**: sara_mnes@yahoo.co.in & saravana7@srmist.edu.in

ABSTRACT

The growing accumulation of plastic waste has increased interest in bio-derived polymer systems made from renewable feedstocks. Among emerging routes, pyrolysis-derived bio-oil from biomass and waste streams presents a promising but underexplored platform for producing biodegradable polymers. This review analyses the complex chemical composition of bio-oil, which includes phenolic compounds, furans, organic acids, and various oxygenated intermediates. It also assesses catalytic upgrading methods aimed at transforming these components into polymerizable monomers. The discussion focuses on the feasibility of synthesizing high-performance biodegradable polymers, including polylactic acid (PLA), polyhydroxyalkanoates (PHA), and systems based on lignin, starch, and protein, with respect to monomer purity, oxygen removal efficiency, and process scalability. A comparative analysis of structure–property relationships that influence mechanical performance, thermal behaviour, and degradation characteristics is conducted to pinpoint essential material limitations. This review evaluates upgrading pathways and polymerization routes, highlighting technical challenges and innovative strategies for utilizing pyrolysis bio-oil as a sustainable feedstock for next-generation biodegradable materials.

Keywords: Pyrolysis-derived bio-oil, Catalytic upgrading, Biodegradable polymers, Polymerization mechanisms, Biomass valorization

Metal Organic Framework Assisted Optical and Interfacial Engineering of TiO_2 Photoanodes For Efficient Quantum Dot Sensitized Solar Cells

Arshiya Wadhwa[1], Aman Mahajan[1]*

[1]*Department of Physics, Guru Nanak Dev University, Amritsar, Punjab, India 143005*

***Corresponding author e-mail:** aman.phy@gndu.ac.in

ABSTRACT

The dependence on fossil fuels for global energy raises serious concerns, leading to a shift towards renewable sources such as solar energy harvesting, however, enhancing the efficiency of solar cells continues to be a significant hurdle. To this, quantum dot-sensitized solar cells (QDSSCs) have garnered considerable attention due to the unique properties of semiconductor quantum dots (QDs) such as tunable band gap and high absorption coefficient[1]. However, the performance of QDSSCs is often limited by inefficient light harvesting and rapid charge recombination at the photoanode-electrolyte interface[2]. In this regard, the present study focuses on the integration of ZIF-67, a cobalt-based metal organic framework (MOF), into the electron transport layer of the QDSSC device to increase its light harvesting and charge transport properties. ZIF-67 was synthesized via a room temperature solution method and subsequently incorporated into the TiO_2 matrix, followed by deposition of quantum dots via successive ionic layer adsorption and reaction (SILAR) method. The resulting QDSSC device exhibited improved short circuit current density (J_{sc}) and overall power conversion efficiency compared to the reference TiO_2-based QDSSC, showing an enhancement of more than 50%, attributed to the increased surface area and porous structure of ZIF-67, which provides more active sites for quantum dot loading and light absorption. Additionally, MOF particles act as light scatterers in the TiO_2 matrix due to the relatively greater particle size of ZIF-67 that facilitates enhanced absorption of incident photons resulting in increased exciton generation while also suppressing back recombinations at the photoanode-electrolyte interface, highlighting the potential of MOFs as effective additives for high performance QDSSCs.

References:

1. P. V Kamat, J. Phys. Chem. Lett. 4, 908 (2013).
2. I. Singh, V. Bhullar, and A. Mahajan, Energy & Fuels 37, 15054 (2023).

EN-182

Synergistic Effects of $Ti_3C_2T_X$ MXene/Sm_2O_3 Electrode and PVA/H_2SO_4/KNN Gel Electrolyte for Flexible All-Solid-State Supercapacitor

Parika Mahajan[1], Aman Mahajan[1]*

[1]*Department of Physics, Guru Nanak Dev University, Amritsar, India, 143005*

***Corresponding author e-mail:** aman.phy@gndu.ac.in

ABSTRACT

In recent years, $Ti_3C_2T_X$ MXene has attracted considerable attention as an electrode material for supercapacitor applications owing to its excellent electrical conductivity, high surface area, abundant redox-active sites, and tunable surface functional groups; however, its practical application is often hindered by restacking of nanosheets which limits accessible surface area and ion diffusion (1). To overcome this limitation, herein, $Ti_3C_2T_X$ MXene was composited with Sm_2O_3, which acted as an effective spacer to prevent sheet restacking while also providing additional electroactive sites, thereby enhancing overall redox activity. The electrochemical performance of both pristine MXene and MXene/Sm_2O_3 composite was systematically evaluated in different aqueous electrolytes, including KOH, H_2SO_4, and Na_2SO_4 and among these, both electrodes exhibited highest specific capacitance in H_2SO_4 electrolyte, making it the most suitable liquid electrolyte for further optimization (2). However, the use of liquid electrolytes is often associated with leakage issues that limit their applicability in flexible and solid-state devices. Therefore, a PVA/H_2SO_4 gel electrolyte was developed to improve device stability and prevent leakage; nevertheless, a slight reduction in capacitance from 107.36 F/g to 92.03 F/g for MXene and from 430.66 F/g to 385.13 F/g for MXene/Sm_2O_3 electrode was observed at 10 mV/s scan rate due to restricted ion mobility caused by gelation effect. Thus, to maintain device stability without sacrificing electrochemical performance, potassium sodium niobate (KNN) was incorporated into PVA/H_2SO_4 gel matrix, enabling improved ionic transport and minimizing capacitance loss while preserving structural integrity. The optimized MXene/Sm_2O_3 electrode integrated with PVA/H_2SO_4/KNN gel electrolyte exhibited an enhanced specific capacitance of 548.24 F/g at 10 mV/s, and superior cycling stability, thereby demonstrating its strong potential for high-efficiency, stable, and flexible supercapacitor applications.

References:

1. Sarycheva and Y. Gogotsi, Chem. Mater. 32 (2020), 3480.
2. P. Mahajan, S. Sardana and A. Mahajan, Appl. Phys. Lett. 124 (2024) 111602

EN-183

Solvent-Assisted Morphological Control and Structural Evolution of Nickel-Based Metal–Organic Frameworks (Ni-BTC)

Venkateswaran Krishnamoorthy[1], Elangovan Elamurugu[1*]

[1]*iDARE Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603 203.*

***Corresponding author e-mail:** elangove@srmist.edu.in, eevan2003@yahoo.co.in

ABSTRACT

For Metal–Organic Frameworks (MOFs) to be as effective as possible in catalysis, sensing, and energy storage applications, precise control over their morphology and structural development is essential [1]. Nickel-trimesate (Ni-BTC) frameworks were synthesized in this work using a simple solvothermal method, with an emphasis on the effects of coordination environments and solvent dielectric properties on the resulting structural features [2]. X-ray diffraction (XRD) analysis confirmed the targeted Ni-BTC phase. A thorough examination using a variety of solvents, including methanol (MeOH), ethanol (EtOH), N, N-dimethylformamide (DMF), and a DMF/EtOH mixed solvent, revealed notable changes in the material structure. Scanning Electron Microscopy (SEM) results show that methanol promotes the formation of extremely smooth and well-defined microspheres [Fig 1 (a)]. On the other hand, the ethanol-based synthesis yields spherical particles with notable surface agglomerations, suggesting altered growth dynamics [Fig 1 (b)]. A strong, uneven rock-like formation with prominent macro-crystalline characteristics is the result of the substantial morphological change brought about by the application of DMF [Fig 1 (c)]. Moreover, the DMF/EtOH binary solvent system promotes the formation of hierarchical structures, demonstrating that polar aprotic and protic solvents work in concert to effectively regulate particle size and surface morphology [Fig 1 (d)][3]. The wide range of structures seen, from uniform spheres to macro-crystalline rock-like forms, emphasizes how important solvent templating is for the bottom-up synthesis of Ni-MOFs. A methodical approach to improving the morphology and pore accessibility of functional materials designed for specific industrial applications is presented in this work.

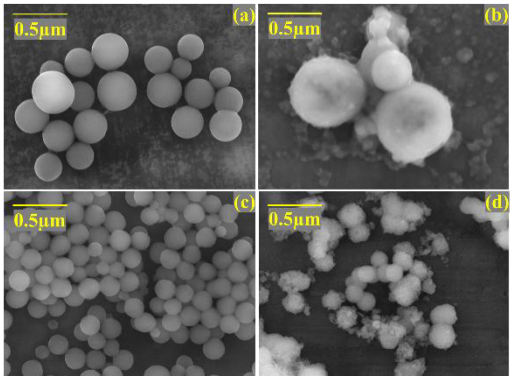


Fig 1 SEM images of Ni-BTC synthesized in different solvents: (a) Methanol (smooth microspheres), (b) Ethanol (agglomerated spheres), (c) DMF (rock-like morphology), and (d) DMF+Ethanol (hierarchical clusters).

References:

1. H. Furukawa, K. E. Cordova, M. O'Keeffe, O. M. Yaghi, *Science*, 341 (2013) 1230444.
2. S. S. Y. Chui, S. M. F. Lo, J. P. H. Charmant, A. G. Orpen, I. D. Williams, *Science*, 283 (1999) 1148.
3. J. W. Sun, J. F. Chen, G. W. Wang, *Chem. Eng. J.*, 313 (2017) 1218-1226.

EN-184

Titanium-induced Modulation of Phonon and Charge Transport Enables Enhanced Thermoelectric Performance in WS_2

Murugadass T[1,2], K. D. Nisha[1,2]*, M. Navaneethan[3], J Archana[1], S. Harish[3]

[1]*Centre of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur – 603203, India.*

[2]*Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur – 603203, India.*

[3]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur – 603203, India.*

***Corresponding author e-mail:** nishad@srmist.edu.in

ABSTRACT

Layered WS_2 is a promising thermoelectric material due to its intrinsically low lattice thermal conductivity and anisotropic transport, yet its performance is limited by low carrier concentration. In this work, the effects of substitutional and excess Ti incorporation on the thermoelectric properties of WS_2 were systematically investigated. $W_{1-x}Ti_xS_2$ and Ti_xWS_2 (x = 0.005–0.05) were synthesised by solid-state reaction and hot pressing. Structural analysis confirmed retention of the hexagonal 2H-WS_2 phase, with lattice contraction in substitutional samples indicating successful Ti-for-W incorporation, while excess Ti was accommodated at interstitial or defect sites. Substitutional Ti moderately increased carrier concentration and preserved mobility at low doping levels, whereas excess Ti significantly increased carrier density but reduced thermopower. Thermal conductivity decreased with Ti incorporation due to enhanced phonon scattering from mass fluctuation and lattice distortion. An optimized balance between electrical conductivity, Seebeck coefficient, and thermal conductivity yielded a maximum zT of ~0.11, over five times higher than pristine WS_2. These results demonstrate that site-selective Ti incorporation is an effective route to tune coupled charge and heat transport in WS_2-based thermoelectrics.

Keywords: Layered semiconductors, Carrier concentration tuning, Thermoelectric performance, WS_2, Mass fluctuation

EN-185

Bi_2O_3-Incorporated V_2O_5 Nanoparticles: Enhanced Structural, Optical, and Electrochemical Properties for Supercapacitor Applications

Jency Sebatine P [a], Sherin Celshia S[b], Muthamizh S*[b], K. Arul varman[c] Mohan Kumar R*[a].

[a]*Department of Physics, Presidency College Chennai 600005, Tamil Nadu, India.*

[b]*Department of Physiology, Saveetha Dental College & Hospitals, Saveetha Institute of Medical & Technical Sciences, Saveetha University, Chennai - 600077, Tamil Nadu, India.*

[c]*Department of Physics & Nanotechnology, SRM Institute of Science & Technology, Kattankulathur-603203, Tamil Nadu, India.*

***Corresponding author e-mail:** muthamizh23@ymail.com, mohan66@hotmail.com.

ABSTRACT

Vanadium pentoxide (V_2O_5) is one of metal oxides that is most widely considered for supercapacitor devices because of its fast and reversible redox reactions, the layered nature of its crystal structure, and the high theoretical capacitance. The present work is an attempt to explore the impact of bismuth oxide (Bi_2O_3) at different concentrations (5%, 10%, and 15%) on the structural, optical, and electrochemical features of hydrothermally synthesized V_2O_5 nanoparticles. Structure characterization via X-ray diffraction (XRD) confirmed that the orthorhombic phase of V_2O_5 remains in all doping samples, with slight changes caused by Bi_2O_3 doping. The study of optical properties involved absorption Ultraviolet–Visible Diffuse Reflectance Spectroscopy (DRS-UV), and the results pointed to the band-gap narrowing, notably for highly Bi_2O_3-doped samples. The shape changes as well as the particle distribution changes due to the composite formation were confirmed by Field Emission Scanning Electron Microscopy (FE-SEM) and High-Resolution Transmission Electron Microscopy (HR-TEM). X-ray Photoelectron Spectroscopy (XPS) study showed that the pure V_2O_5 chemical environment had been changed after the addition of Bi_2O_3. Electrochemical evaluations, achieved by cyclic voltammetry and charge-discharge cycling, revealed considerable improvements in capacitance as well as stability the 15% Bi_2O_3/V_2O_5 electrode demonstrated exceptional cycling durability with the largest specific capacitance (487 F g^{-1} at 1 A g^{-1}), higher rate capability, and outstanding retention of 89% after 5000 cycles among the investigated concentrations. The built asymmetric device with 15% Bi_2O_3/V_2O_5 and activated carbon attained an exceptional energy density of 38.4 Wh kg^{-1} and a power density of 16,000 W kg^{-1}.

Keywords: Vanadium Pentoxide (V_2O_5); Bismuth oxide; Nanocomposite; Structural Properties; Optical Properties; Supercapacitors; Energy Storage.

EN-186

PVA-Assisted Fabrication of $PrCoO_3$ Cubic Perovskites for Advanced Hybrid Energy Storage

Sabareeswaran Meyyanathan[1], Devikala Sundaramurthy*

[1]*Department of Chemistry, College of Engineering and Technology SRM Institute of Science and Technology, Kattankulathur-603203*

Tamil Nadu, India.

***Corresponding author e-mail** : sdevikala@gmail.com

ABSTRACT

Rare-earth binary oxides are emerging as versatile functional materials, where compositional tuning and structural tailoring strongly govern their electrochemical energy storage behavior. In this work, praseodymium cobaltite ($PrCoO_3$) perovskites were synthesized through a PVA-assisted route followed by controlled thermal treatment. The Pr/Co ratio played a decisive role in directing the formation of ultrathin nanosheets, crystallinity, and perovskite phase stability. Subtle lattice contraction/expansion induced by stoichiometric variation altered sheet dimensions and aspect ratios, while calcination conditions further modulated the morphology. These synergistic structural evolutions translated into distinct improvements in electrochemical performance. The pseudocapacitive behavior of $PrCoO_3$-based electrodes (PC-1, PC-2, and PC-3) was systematically evaluated. Pr/Co composites synthesized at varying molar ratios (PC-1, PC-2, and PC-3) were comprehensively characterized using XRD, FTIR, RAMAN, XPS, UV–Vis, SEM, AFM, TEM, VSM, WCA analysis, BET surface area measurements, and TGA to investigate their structural, optical, morphological, surface wettability, and thermal properties. The binary metal oxide with an optimized Pr:Co molar ratio of 0.5:1.5 (PC-3) exhibited a maximum specific capacitance of 398.7 F g^{-1}/ 199.45 C g^{-1} at 1 A g^{-1}, with a remarkable 99.3 % retention after prolonged cycling. Furthermore, molar fraction adjustments and surface modifications resulted in varying crystallite sizes, electrochemical kinetics, and charge storage properties across PC-1, PC-2, and PC-3 electrodes. The assembled hybrid supercapacitor device exhibited an impressive energy density of 47.47 Wh kg^{-1} at a power density of 4612 W kg^{-1}, maintaining 99.6% of its initial capacitance with 100% of coulombic efficiency after 5000 cycles, demonstrating exceptional cycling stability and superior electrochemical efficiency.

Reference

1. Dar, M. A.; Majid, S. R.; Satgunam, M.; Siva, C.; Ansari, S.; Arusalan, P.; Ahamed, S. R. *Int J Hydrogen Energy* **2024**, *70*, 10–28.
2. Mortazavi-Derazkola, S.; Ebrahimzadeh, M. A.; Amiri, O.; Goli, H. R.; Rafiei, A.; Kardan, M.; Salavati-Niasari, M*J Alloys Compd* **2020**, *820*, 153186.

Numerical Investigation of High-Efficiency Two-Terminal Rb_1MAFA/In_2S_3 Tandem Perovskite Solar Cells

Ajay Kumar[1]*, Neha Gupta[2], Aditya Jain[3], Kaushal Kumar[4], and Amit Kumar Goyal[5]

[1]*ECE Department, Jaypee Institute of Information Technology, Noida, India, 201309.*

[2]*Department of Applied Sciences, GNIOT Group of Institutions, Uttar Pradesh, India, 201306.*

[3]*ECE Department, SIT, Symbiosis International (Deemed University), Pune, Maharashtra, India, 412115.*

[4]*ECE Department, Graphic Era Deemed to be University, Dehradun, Uttarakhand, India.*

[5]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104.*

***Corresponding author e-mail:** ajay.kumar@jiit.ac.in

ABSTRACT

Traditionally, silicon-based solar cells were widely used to produce solar energy. However, the efficiency of a solar cell is determined by its ability to convert solar energy directly into electricity, a process known as the photovoltaic effect [1]. This paper presents a comprehensive investigation of two-terminal tandem perovskite solar cells, highlighting their advantages in achieving better efficiency and performance compared to traditional single-terminal devices [2]. The proposed device structure consists of Rb_1MAFA and In_2S_3 layers, stacked together to achieve higher efficiency. Simulations were performed using SCAPS-1D software under the AM1.5G solar spectrum and a temperature of 300 K [3]. By meticulously adjusting the thickness and other parameters of both layers, we achieved an efficiency of 32.46%, surpassing that of single-terminal devices. Additional parameters examined include current density, quantum efficiency, absorption coefficient, electric field, and IV characteristics such as Jsc=33.656 mA/cm2, Voc=1.2658 V, fill factor (FF) = 76.20%, and efficiency (η)=32.46%.

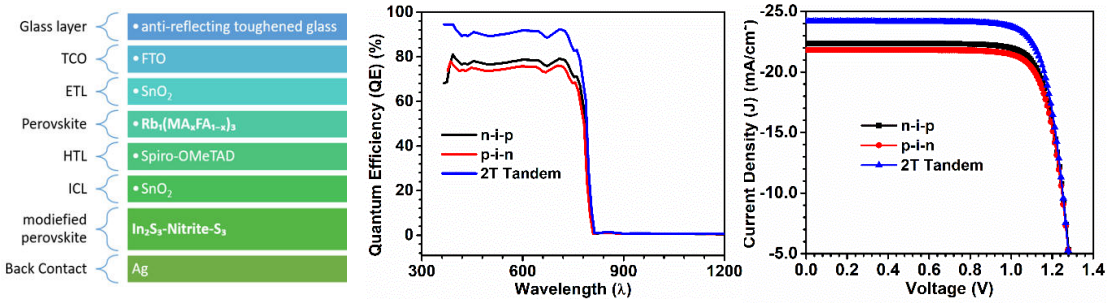


Fig. 1: (a) Device structure of 2T Tandem Solar Cells. (b) Current density 2T Tandem Solar Cells. (c) Quantum Efficiency 2T Tandem Solar Cells.

References:

1. Y. Yang *et al.*, "Effect of ultraviolet aging of backsheet on electrical performance of silicon photovoltaic module," *Solar Energy Materials and Solar Cells*, vol. 262, p. 112558, 2023.
2. P. Wang, Y. Zhao, and T. Wang, "Recent progress and prospects of integrated perovskite/organic solar cells," *Applied Physics Reviews*, vol. 7, no. 3, p. 031303, 2020.

EN-188

Development of Chitosan based nanocomposites for enhanced adsorption of chromium from industrial waste water

Varsha K P [1] and Samarendra Maji[1*]

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology (SRMIST), Kattankulathur, Tamil Nadu-603203*

[*]**Corresponding author e-mail:** samarenr@srmist.edu.in.

ABSTRACT

Heavy metal contamination possesses a serious threat to environment and ecosystem due to its toxicity, persistence and bioaccumulation. Among these pollutants, hexavalent chromium (CrVI) is particularly hazardous because of its high solubility, mobility, carcinogenicity, and widespread discharge from industries such as electroplating, leather tanning, textile processing, and metallurgy that significantly threatens the environment and sustainable human development. The World Health Organization has established maximum permissible limits for Cr(VI) in industrial wastewater is 0.25 mg L^{-1}. Therefore, there is an urgent need to develop efficient polymeric system for the removal of hexavalent chromium. Among the various methods available for the removal of Cr(VI), Adsorption is considered one of the most effective and economical methods owing to its simplicity, high efficiency, and operational flexibility. We demonstrate and design chitosan-based polymer nanocomposite designed specifically for the adsorption of Cr(VI) from aqueous solutions. Chitosan is a naturally abundant and biodegradable biopolymer, was selected as the base matrix due to its rich amino and hydroxyl functional groups that facilitate strong interaction with metal ions. Different magnetic nanofillers were added in to the chitosan matrix to improve its mechanical strength, surface functioning, and ease of desorption. Importantly, the synthesized nanocomposite is designed to overcome common limitations such as poor recyclability, structural degradation, and leaching of the nanofiller. Strong interfacial interaction and enhanced crosslinking within the composite matrix provide great stability and stop material loss during multiple cycles of adsorption and desorption.

Keywords: Chromium, Chitosan, magnetic nanofillers

References

1. L. Yin, K. Wang, L. Jiang, Y. Xi, Z. Xu, Z. Song and H. Zhou, *RSC Advances*, 2025, **15**, 16337–16347.
2. P. C. Bandara, J. Peña-Bahamonde and D. F. Rodrigues, *Scientific Reports*, 2020, **10**, 1–8.

EN-189

Surface Engineered Sulvanite Integrated with Layered Double Hydroxide for Asymmetric Hybrid Supercapacitor

Sachin Sreedhar[1], Shanmugam Ganesan[1]*

[1] *Energy Conversion and Energy Storage Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, 603203, Tamil Nadu, India*

***Corresponding author e-mail:** ganesans2@srmist.edu.in

ABSTRACT

Layered double hydroxides (LDHs) are an emerging material, owing to their unique 2-D flake like morphology giving them a rapid diffusion characteristic. Surface tuning of Cu3VS4 sulvanite was performed to obtain various novel 3-D morphologies, to be integrated with 2-D mesoporous $Ce^{(III)}$–$Mg^{(II)}$–$Y^{(III)}$ LDH by a facile cost-effective approach. The 3-D structure of sulvanite enhances the surface area and number of active sites around the surface, allowing excellent redox behaviour. The integration of 3-D sulvanite with the 2-D LDH gave rise to a unique synergistic effect, resulting in an outstanding specific capacitance of 1456.6 F g^{-1} with 98.8% retention of its initial capacitance after 10 000 charge–discharge cycles, for cubic sulvanite integrated LDH (LD-C). A sulvanite LDH asymmetric supercapacitor hybrid (SLASH) device was fabricated using LD-C, showing the specific capacitance of 52.5 F g^{-1} at 1 A g^{-1}, exhibiting an exceptional power density of 756.8 W Kg^{-1} at an energy density of 67.2 Wh Kg^{-1}. The device exhibited an outstanding durability of 98.9% after 12,000 charge discharge cycles, displaying capable endurance when applied in real world energy storage applications.

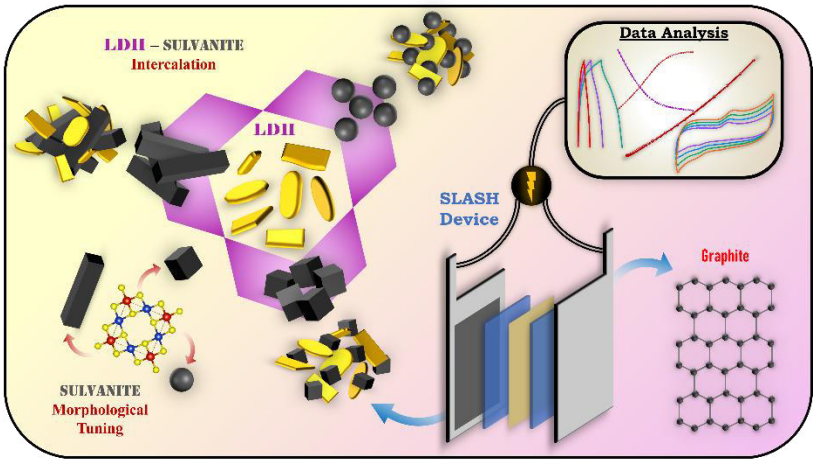


Fig. 1 Graphical Abstract

Keywords: porous coordination polymers, MOFs, supercapacitor, redox mediator, organic potassium salt

References:

1. S. Kitagawa, Chemical Society Reviews, 43 (2014).
2. B. Xu, H. Zhang, H. Mei, D. Sun, Coordination Chemistry Reviews, 420 (2020).

EN-190

A phase-tuned layered 1T W-MoS_2/PEDOT:PSS hybrid: functional engineering towards self-binding supercapacitor cathodes

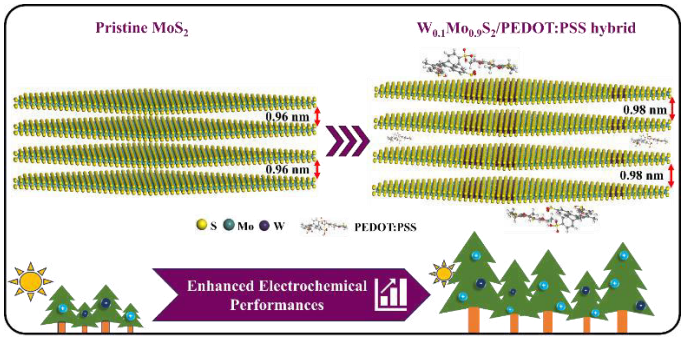
Chandru Gunasekaran[1], Ganesan Shanmugam[1]*

[1]*Energy Conversion and Energy Storage Laboratory, Department of Chemistry, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur, Chengalpattu District, Tamil Nadu - 603 203, India.*

***Corresponding author e-mail**: ganesans2@srmist.edu.in

ABSTRACT

A layered two-dimensional 1T-molybdenum disulfide (MoS_2), substitutionally doped with tungsten (W), and incorporated with poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS), was synthesized via a one-pot hydrothermal method to form $W_xMo_{1-x}S_2$/PEDOT:PSS hybrid composites as self-binding electrodes for supercapacitors. The optimal doping and hybrid construction of $W_{0.1}Mo_{0.9}S_2$/PEDOT:PSS (10W-MS/P) increase the interlayer spacing and stabilize the metallic 1T phase, which enhance the electrical conductivity and structural durability in an electrochemical analysis under a three-electrode configuration using 1 M H_2SO_4 electrolyte. 10W-MS/P exhibits a high specific capacitance (C_m) of 845.14 F g^{-1} and an areal capacitance (C_a) of 4.73 F cm^{-2} at 1 A g^{-1} and the electrode also demonstrates excellent stability, retaining 89% of its capacitance after 10000 cycles. The asymmetric coin cell supercapacitor (ASC-CC), fabricated using a self-binding cathode of 10W-MS/P, delivers an energy density of 6.53 Wh kg^{-1} and a power density of 79.64 W kg^{-1}. After 20000 continuous cycles, the device retains 75% of capacitance and it reveals that the hybrid material possesses significant potential as an efficient and durable electrode for next-generation energy storage applications.



Keywords: Transition Metal Dichalcogenides, Conducting polymer, Doping.

References:

1. Chandru Gunasekaran, Ganesan Shanmugam* and Sachin Sreedhar, Journal of Materials Chemistry A, 2025.
2. Chandru Gunasekaran, Ganesan Shanmugam* and Sachin Sreedhar, Monisha Venkatesan, Electrochimica Acta, 516 (2025) 145725.

EN-191

Recycled Electroactive Materials from Batteries as Catalysts for Green Hydrogen Production

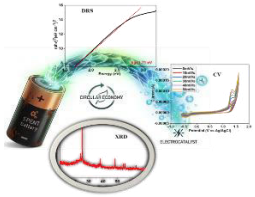
P. Sri Bala Jeya Krishna Sri[1], G. Gopu[1]*

[1]*Nano & computational materials lab, Department of Industrial Chemistry, Alagappa University, Karaikudi, Tamil Nadu, India*

***Corresponding author e-mail:** *gopug@alagappauniversity.ac.in*

ABSTRACT

The rapid increase in battery consumption has resulted in the accumulation of large quantities of spent primary batteries, raising significant environmental and resource management concerns. When these electrochemical devices are improperly disposed of, hazardous metal ions and electrolyte residues may leach into soil and groundwater, posing potential risks to ecosystems and human health. Therefore, recovering and repurposing valuable components from used batteries has become an important approach toward sustainable resource utilization and circular energy technologies. In particular, the reuse of electrode materials for catalytic and energy-conversion applications offers a promising pathway for value-added recycling. In this study, we explore the recovery of primary battery materials containing zinc (Zn), graphite (C), and manganese dioxide (MnO_2) and their subsequent application in hydrogen production. A combined recycling strategy involving mechanical comminution (grinding) followed by a chemical sol–gel synthesis route was employed to isolate and reprocess the active components. The recovered materials were engineered as electrocatalytic materials for oxygen evolution reactions (OER) and hydrogen evolution reactions (HER), enabling their utilization in water-splitting systems for sustainable hydrogen generation. The structural, optical, and electrochemical properties of the synthesized materials were systematically characterized using cyclic voltammetry (CV), Linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), UV–Vis diffuse reflectance spectroscopy (DRS), powder X-ray diffraction (XRD), attenuated total reflectance fourier transform infrared spectroscopy (ATR-FTIR), and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDX). The findings highlight the potential of recycled battery materials as cost-effective electrocatalysts for hydrogen production, supporting both waste reduction and the advancement of clean energy technologies.



Keywords: Battery recycling; Sol–gel synthesis; Electroactive cathode materials; Electrochemical characterization; Hydrogen production

References:

1. Fichtner M, Edström K, Ayerbe E, Berecibar M, Bhowmik A, Castelli IE, et al. *Adv. Energy Mater.* **12** (2022) 2102904.
2. Shan Fang, Dominic Bresser and Stefano Passerini, *Adv. Energy Mater.* **10** (2020) 1902485.

EN-192

Enhancing the Thermoelectric Power Factor via Carrier Energy Filtering in Ag-Decorated Bi_2Se_3 Nanostructures/Carbon Fabric for Wearable Thermoelectric Application

Anjali Krishna A. A[1], C. Suresh Prasanna[2], S. Harish[2], H. Ikeda[3,4], M. Navaneethan[2], M. Krishna Mohan*[1]

[1]Centre of Excellence in Materials and Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603203, Tamil Nadu, India

[2]Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203.

[3]Graduate School of Science and Technology, Shizuoka University, 3-5-1 Johoku, Chuo-Ku, Hamamatsu, Shizuoka, 432-8011, Japan

[4]Research Institute of Electronics, Shizuoka University, 3-5-1 Johoku, Chuo-Ku, Hamamatsu, Shizuoka, 432-8011, Japan

***Corresponding author e-mail:**krishnam1@srmist.edu.in

ABSTRACT

Conventional thermoelectric materials are typically rigid and brittle, which limits their use in flexible and wearable energy harvesting systems for Internet of Things (IoT) devices. In this work, we report a simple and scalable strategy to fabricate textile-based wearable thermoelectric generators (WTEGs) using conductive carbon fabric (CF) as a flexible substrate. Bi_2Se_3 nanoflakes were directly grown on CF through a binder-free hydrothermal method, enabling strong interfacial adhesion and reduced internal resistance while ensuring uniform coverage of the active material on the textile substrate. To further improve the thermoelectric performance, the Bi_2Se_3 surface was modified with Ag nanostructures, including nanoparticles and nanoprisms. These nanostructures introduce interfacial energy-filtering effects that enhance carrier transport by selectively allowing high-energy carriers to contribute to conduction. As a result, the optimized Ag/Bi_2Se_3/CF composite exhibits an in-plane power factor of 8.1 $\mu W\ m^{-1}K^{-2}$, representing a 5.4% improvement compared to pristine Bi_2Se_3/CF. The Seebeck coefficient reaches 15.4 $\mu V\ K^{-1}$ at 303 K and 50.9 $\mu V\ K^{-1}$ at 370 K, indicating improved carrier modulation. A flexible Y-shaped WTEG device was fabricated using Bi_2Se_3/CF as the p-type leg and Cu-Ni fabric as the n-type leg with carbon electrodes. The device generated 0.015 µV under a 3.3 K temperature gradient on human skin and retained good flexibility, showing only 15.8% resistance increase after 1000 bending cycles and stable operation for 30 days.

References:

1. Santosh Kumar, Manjusha Battabyal, Kanikrishnan Sethupathi, Dillip K. Satapathy, ACS Applied Materials & Interfaces, Vol 16/Issue 31, 40848–40857 (2024).
2. Quan Zhou, Hongxiong Li, Chunyu Du, Zhenqiang Ye, Lirong Liang, Guangming Chen, Nano Energy, Volume 118, Part B, 109007 (2023)

EN-193

Enhancing Thermoelectric Properties of Ag_2Se Nanoparticles on Carbon Fabric via ZnO Composite for Wearable Energy Harvesting

Anjali Krishna A A[1,2], S Harish[2], M Navaneethan[2], Y. Hayakawa[1], H. Hamasaki[1], H. Ikedaa,[1*]

[1]*Shizuoka University, Hamamatsu, Shizuoka, 432-8001, Japan*

[2]*SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India*

***Corresponding author e-mail:** ikeda.hiroya@shizuoka.ac.jp

ABSTRACT

Flexible Ag_2Se/ZnO composite films were successfully fabricated using a screen-printing technique on carbon fabric substrates with varying weight ratios of Ag_2Se/ZnO. X-ray diffraction (XRD) analysis confirmed the crystallinity and phase formation of the Ag_2Se/ZnO composites, validating the successful integration of both components. The introduction of ZnO into the Ag_2Se matrix aims to leverage the superior electrical conductivity of Ag_2Se and the excellent thermal stability of ZnO, thus achieving a balanced improvement in the overall thermoelectric performance. Scanning electron microscopy (SEM) observations revealed a uniform surface morphology and well-adhered composite layers across the flexible carbon fabric. Furthermore, electron probe microanalysis (EPMA) confirmed the homogeneous distribution of Ag, Se, Zn and O elements within the films, indicating uniform compositional dispersion achieved through the screen-printing process. The resulting composite films exhibited excellent flexibility and mechanical integrity, making them ideal for applications in wearable and flexible thermoelectric devices. This work provides an eco-friendly and scalable route for fabricating cost-effective thermoelectric films with enhanced structural uniformity and mechanical reliability for flexible energy-harvesting technologies.

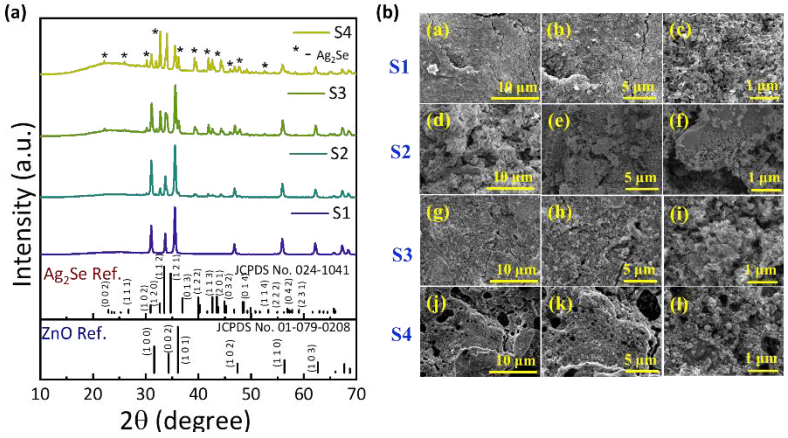


Fig. 1 (a) XRD* and (b) SEM images *of Ag_2Se/ ZnO composite films

Key words – Wearable thermoelectric generator, carbon fabric, Ag_2Se/ZnO composite films, screen printing.

References:

1. C. Suresh Prasanna et. al., *Carbon* 243 (2025): 120486.
2. Palaporn Dulyawich et. al., *Advanced Materials Technologies* 9 (2024): 2301242.

EN-194

Decoupling Thermal and Electrical Transport Through Halide-Chalcogenide Hybridization in Cu_2SnSe_4 Thermoelectrics

C.N. Dhivya Mahalakshmi[1,2], K.P. Mohamed Jibri[1], J. Archana[1] S. Harish[1] H. Ikeda[2] and M. Navaneethan[1*]

[1] *SRM Institute of Science and Technology, Kattankulathur, India, 603203*
[2]*Shizuoka University, Hamamatsu, Shizuoka 432–8011, Japan*
***Corresponding author e-mail:** m.navaneethan@gmail.com

ABSTRACT

Efficient thermoelectric energy conversion requires the simultaneous optimization of mutually coupled electronic and thermal transport parameters. Here, we report a heterostructure engineering strategy in which a 0D halide-derived soft lattice phase is integrated with a chalcogenide thermoelectric matrix to decouple charge and phonon transport. Specifically, composites of Cu_2SnSe_4 and $Cs_3Bi_2I_9$ were synthesized with controlled incorporation (1–7 wt%), forming a hybrid chalcogenide-halide system that exhibits strongly modified transport behaviour. Thermal and electrical transport measurements reveal that the introduction of $Cs_3Bi_2I_9$ induces a pronounced reduction in lattice thermal conductivity while simultaneously improving electronic transport characteristics. Temperature-dependent transport studies (303–653 K) demonstrate that these composites exhibit a synergistic enhancement of electrical conductivity and Seebeck coefficient compared with pristine Cu_2SnSe_4, leading to a substantial increase in the power factor. Analysis of weighted carrier mobility as a function of temperature reveals a characteristic "U"-shaped behaviour for the optimized compositions, indicating a transition in the dominant carrier scattering mechanism. This behaviour suggests that the $Cs_3Bi_2I_9$ phase introduces beneficial electronic band perturbations and energy filtering at the heterointerfaces, which selectively enhances high-energy carrier transport. Concurrently, the presence of the soft halide lattice containing stereochemically active Bi^{+3} lone-pair electrons and heavy iodine atoms introduces strong lattice anharmonicity and suppress phonon propagation. This modulation of charge and heat transport results in a marked enhancement of thermoelectric figure of merit achieving 0.27 at 653K.These findings highlight the potential of halide-chalcogenide hybridization as a novel design for next-generation thermoelectric materials.

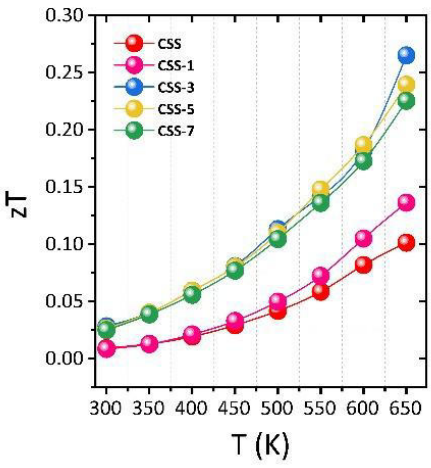


Fig. 1 Figure of merit (zT) for hybrid $Cu_2SnSe_4/Cs_3Bi_2I_9$ composite

Key words – Soft lattice, band perturbations, energy filtering, heterointerfaces stereochemically active

References:

1. C. N., D. M., and K. P., M. J., *Appl. Phys. Lett.*, **126** (2025).
2. J. Li, L. Wei, Z. Ti, L. Ma, Y. Yan, G. Zhang, and P.-F. Liu, *Phys. Rev. B*, **108** (2023) 224302.

EN-195

Fabrication and Testing of High Performance Flexible Symmetric Supercapacitor Using Copper Cobaltite Spinel Nanostructures

Pooja Sanjeev[a,c],Ananth Vajhula [b,c],Punnakal Navaneeth[d], TG Satheesh Babu[b,c], Punathil Vasu Suneesh[b,c]*,

[a] *Department of Physics, Amrita School of Physical Sciences, Coimbatore, Amrita Vishwa Vidyapeetham, India-64112*

[b] *Department of Chemistry, Amrita School of Physical Sciences, Coimbatore, Amrita Vishwa Vidyapeetham, India-641112*

[c] *Amrita Biosensor Research Lab, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India -641112*

[d] *Centre of Excellence for Research in Engineering Materials (CEREM), Deanship of Scientific Research, King Saudi University, Riyadh 11421, Saudi Arabia*

***Corresponding author e-mail**: pv_suneesh@cb.amrita.edu

ABSTRACT

Flexible supercapacitors using materials with high surface area, superior charge transport, and strong mechanical integrity are the best choice for powering flexible and wearable devices. In this work, a Copper Cobaltite ($CuCo_2O_4$), spinel metal oxide was prepared by annealing of copper cobalt hydroxide prepared by urea hydrolysis method. Urea hydrolysis method provides controlled and gradual nucleation, resulting in smaller and more uniform nanoparticle. Subsequent annealing of the hydroxides results in the formation of $CuCo_2O_4$ with a spinel structure**.** The morphology and crystal structure of copper cobaltite was examined using TEM and XRD techniques, confirming the presence of the cobalt copper spinel phase**.** The symmetric supercapacitor fabricated exhibited a high areal capacitance of 28.51 mF cm^{-2} at a current density of 0.5 mA cm^{-2}, energy density of 5.702µWh cm^{-2}, power density of 299.97 µW cm^{-2} and a capacitance retention of 78% after 8000 charge discharge cycles. The flexibility of the fabricated supercapacitor was tested at six different bending angles and the corresponding cyclic voltammograms did not exhibited significant change. These results indicate the potential application of the fabricated supercapacitor for powering wearable energy storage devices.

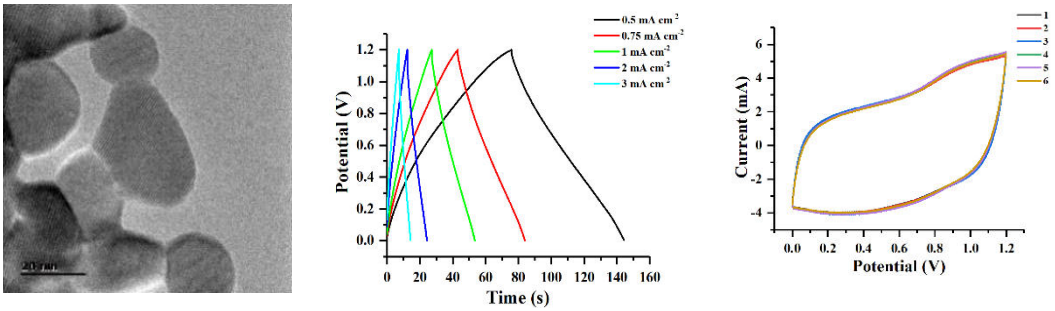


Fig :1 TEM image of copper cobaltite (A) ,Galvanostatic charge discharge curves at different current densities (B), Flexibility test of the fabricated supercapacitor(C)

Keywords : *Copper Cobaltite , Spinel metal oxide, Flexible supercapacitors,Urea hydrolysis*

References

1. Prasath, Jeeva. et. al. Journal of Energy Storage 121 (2025): 116600.
2. Ali, Yasir et al. - Journal of Materials Science: Materials in Electronics 36, no. 19 (2025): 1189.

EN-196

Experimental Investigation of a Passive Battery Thermal Management System Using OM42 Phase Change Material and Aluminum Enhancements

Dr. Prashanth S P[1]*, Tarun Sai M[1], Vinay S[1], P Lohith Prakash[1], Abhay R Karthik[1], Suman Maity[1], Dr. Devendra Dandotiya[1]

[1]*Presidency University, Yelahanka, Rajankunte, Bengaluru 560119*

***Corresponding author e-mail:** prashanth.sp@presidencyuniversity.in

ABSTRACT

This study investigates the effectiveness of a passive Battery Thermal Management System (BTMS) utilizing Phase Change Materials (PCMs) to regulate the temperature of lithium-ion batteries. An experimental setup was designed integrating a specialized organic PCM, OM42, known for its optimal melting point around 42 ℃ and high latent heat capacity, with thermally conductive aluminum fins to counteract the characteristically low thermal conductivity of PCMs. The methodology involved simulating battery heat generation under various charge/discharge rates (0.5C to 3C) and monitoring the thermal response of the PCM using strategically placed thermocouples. The results demonstrated that the PCM-based system effectively absorbed thermal energy during heating cycles and released it during cooling, thereby stabilizing the battery's temperature. At higher C-rates, which generate more heat, the system successfully mitigated sharp temperature increases, affirming the viability of this passive cooling approach. The conclusion underscores that a BTMS incorporating PCM and conductive enhancers provides a compact, energy-efficient, and safe solution for maintaining optimal battery operating temperatures, ultimately extending battery life and improving reliability. This research offers a framework for advancing thermal management technologies in line with the push for more sustainable and innovative energy systems.

References:

3. Joshi, A. K., Kakati, P., Dandotiya, D., Pandiyan, P. S., Patil, N. G., & Panchal, S. (2024). *International Journal of Modern Physics C*, *35*(04), 2450047.
4. Lokhande, Indra Kumar, and Nishant Tiwari. *Journal of Power Sources* 661 (2026): 238553.Name Surname, Name Surname, J. Appl. Physics, vol (year) page no.
5. Nagmule, Siddharth A., and Pramod B. Salunkhe. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science* 237, no. 23 (2023): 5767-5776.
6. Kumar, S.S. and Rao, G.A.P., 2024. *Energy Storage*.
7. Pandiyan PS, Dandotiya D, Alathadi Maloor S, Rajagopalan S. Energy Storage. 2023.

Carbon Ion Implanted $Ti_3C_2T_x$ MXene as a Multifunctional Material for Hydrogen Evolution Reaction and Supercapacitor Devices

Naresh Aneja[1], Akshidha Singla[1], Aman Mahajan[1]*

[1]*Department of Physics, Guru Nanak Dev University, Amritsar, India*

***Corresponding author e-mail:** aman.phy@gndu.ac.in

ABSTRACT

Hydrogen evolution reaction (HER) for energy conversion and supercapacitors (SCs) for consequent storage have attracted significant research interest for sustainable utilization of green and clean energy. Despite their efficient performance, still suffer from limitations which necessitates designing of proficient electrode/interfacial materials which can improve performance, stability and recyclability of devices. To address these issues, two-dimensional (2D) MXenes based materials are gaining interest by virtue of large surface area, high conductivity and tunable surface chemistry. However, the interlayer restacking issue directly hampers their scalability. To this, herein, surfacial modification of $Ti_3C_2T_x$ MXene have been done using carbon ion implantation technique to efficiently increase the surfacial active sites. Finally, by employing a multifaceted approach, the morphology and structure of pristine and ion implanted MXene have been analyzed using X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). Subsequently, the electrochemical investigation towards HER and SCs have been done using linear sweep voltammetry (LSV), cyclic voltammetry (CV), Galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS). The ion implanted electrode exhibit reduced overpotential and Tafel slope with minimal charge transfer resistance and high capacitance value making them suitable for designing efficient MXene based electrochemical energy conversion and storage devices.

Keywords: Hydrogen Evolution Reaction, Supercapacitor, MXene, Carbon Ion Implantation

References:

1. O. J. Kewate, S. Punniyakoti, J. Energy Storage **72**, 108501 (2023).
2. H. Xu, H. Dong, X. Liu, H. Qiao, G. Chen, F. Du, Y. Dall'Agnese, Y. Gao, ACS Appl. Mater. Interfaces **15**, 53549-53557 (2023).
3. A. Singla, R. Dhiman, A. Mahajan, J. Electron Mater. (2024).

EN-198

Ternary MXene/CNT/WO_3 Hybrid Cathode for High Performing Rechargeable Zinc–Air Batteries

Akshidha Singla[1] , Rajnish Dhiman[2] and Aman Mahajan[1]*

[1]*Department of Physics, Guru Nanak Dev University, Amritsar, India*

[2]*Department of Physics, Malaviya National Institute of Technology, Jaipur, India*

***Corresponding author e-mail:** aman.phy@gndu.ac.in

ABSTRACT

The development of efficient bifunctional air cathodes is critical for improving the performance of rechargeable zinc-air batteries (ZABs). Herein, a ternary MXene/CNT/WO_3 hybrid cathode was designed with enhanced oxygen electrocatalytic activity and charge transport properties. The integration of conductive $Ti_3C_2T_x$ MXene, –COOH functionalized multiwalled carbon nanotubes, and WO_3 nanoparticles induces a synergistic heterostructure which promotes rapid electron transfer and abundant catalytic active sites. Electrochemical measurements reveal that the optimized MCW-111 electrode exhibits superior electrochemical behavior and enhanced ORR activity with a limiting current density of 4.7 mA cm^{-2} at 1600 rpm in 0.1 M KOH. An assembled MCW-111 air cathode based ZAB delivers excellent electrochemical performance with an open-circuit voltage of ~1.42 V, stable cycling for ~480 cycles (≈180 h). The device also exhibits remarkable rate capability up to 50 mA cm^{-2}. The superior performance arises from the synergistic integration of MXene, MWCNT-COOH and WO3 which enhances electrical conductivity, catalytic activity, and structural stability. This work highlights the potential of MXene-based ternary heterostructures as promising air cathodes for high-performance rechargeable zinc-air batteries.

Keywords: Zinc-air battery, Oxygen Reduction reaction, Oxygen evolution Reaction, MXene, Interfacial engineering

EN-199

Synergistic α-MnO_2/$Ni(OH)_2$ Heterostructure as a High-Performance Cathode for Aqueous Zinc-Ion Batteries: Separator-Dependent Electrochemical Evaluation

Sugirtha Baskar, Jeya Kiruba Palraj, Helen Annal Therese*

Department of Chemistry, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** helena@srmist.edu.in

ABSTRACT

Manganese oxide-based aqueous zinc-ion batteries (AZIBs) have attracted significant research interest owing to their low cost and environmental compatibility. Nevertheless, unresolved charge storage mechanisms and insufficient long-term cycling stability continue to impede their practical application. To address these limitations, α-MnO_2/$Ni(OH)_2$ composite cathode material was fabricated via a facile hydrothermal route, wherein the incorporation of nickel hydroxide effectively enhances the electrochemical performance of the host α-MnO_2 structure. The optimized cathode delivers a specific capacity of 257 mAh g^{-1} at 1 A g^{-1} using a glass fiber separator, markedly surpassing the 208 mAh g^{-1} at 0.1 A g^{-1} recorded with a Whatman filter paper separator, highlighting the critical role of separator selection in governing ion transport and overall battery performance.

Keywords: α-MnO_2/$Ni(OH)_2$ composite, Ion Transport, Specific capacity

EN-200

Copper Metal Organic Framework Reinforced Sulfonated Polyether Sulfone Composite for Proton Exchange Membrane Fuel Cells

Gandhimathi Sivasubramanian[1], Indra Dhakshnamoorthy[2], Paradesi Deivanayagam[2]*

[1] *Department of Physics, SRM Valliammai Engineering College, SRM Nagar, Kattankulathur-603203 India*

[2] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, India.*

***Corresponding author e-mail:** paradesd@srmist.edu.in

ABSTRACT

Fuel cells serve as zero-emission energy sources that generate electrical energy continuously with a steady fuel supply. Proton exchange membrane fuel cell (PEMFC) using polymer electrolyte is a promising solution to meet rising energy demands. Sulfonated polyether sulfone (SPES) was prepared by sulfonating polyether sulfone (PES) with concentrated sulfuric acid and chlorosulfonic acid. Copper metal-organic framework (Cu-MOF) was synthesized hydrothermally using $Cu(NO_3)_2 \cdot 3H_2O$ as the precursor and trimesic acid as the linker. Varied ratios of Cu-MOF were incorporated into the polymer matrix, and the resulting composite membranes were fabricated by the solvent casting method to enhance the thermal stability and proton conductivity of the SPES matrix for PEMFC applications. SPES and Cu-MOF were structurally characterized by FTIR, XRD and XPS. Morphology and elemental analysis of the composite membrane is investigated by SEM and EDXs analysis. Physicochemical properties such as water uptake, swelling ratio, ion-exchange capacity and electrochemical performance (proton conductivity) confirmed the suitability of the SPES/Cu-MOF composite membrane for fuel cells.

Keywords: Sulfonated polyether sulfone, Cu MOF, PEMFC, Proton conductivity

References:

1. J. Anie Shejoe, M. Siva, M. Berlina, S. Karthikeyan, K. Dinakaran and D. Paradesi, *ACS Omega*, **8** (2023), 27510−27518.
2. M. Siva, S. Ragasudha, M. Aparna, P. Hemalatha, and D. Paradesi, *Ind. Eng. Chem. Res*., **63 (**2024**)**, 17567−17576.

EN-201

Advancements in Activation Methods and Electrode Fabrication of Biomass-Derived Biochar for High-Efficiency Supercapacitors

Velmurugan Palanisamy[1, 2], Ayyadurai Saravanakumar[2 *]

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603 203, Chengalpattu District, Tamil Nadu, India*

[2]*Centre for Research in Environment, Sustainability Advocacy and Climate Change (REACH), Directorate of Research and Virtual Education, SRM Institute of Science and Technology, Kattankulathur – 603 203, Chengalpattu District, Tamil Nadu, India*

*** Corresponding author e-mail:** sara_mnes@yahoo.co.in & saravana7@srmist.edu.in

ABSTRACT

A growing global demand for energy has amplified the need for effective and sustainable energy storage technologies. The supercapacitor (SC) has become a promising energy storage solution owing to its superior power density, increased durability, and environmental sustainability. Biomass-derived carbon compounds, especially activated biochar, are attracting significant attention as sustainable and economical electrode materials for supercapacitors (SCs). This review analyzes the activation techniques employed for biochar, including chemical methods (KOH, NaOH, H_3PO_4, HCl, HNO_3, $ZnCl_2$, metal oxides) and physical methods (steam, CO_2, plasma, ultrasound, microwave). These activation techniques improve the porosity, surface area, and electrochemical properties of biochar. This review highlights the activation methods of biochar, the importance of constituent components in electrode fabrication, and their impact on mechanical stability and ion transport. Activated biochar exhibits remarkable electrical conductivity, tunable surface functionalities, and a hierarchical porous architecture that facilitates the development of the electrochemical double layer. Overall, this review provides a comprehensive overview of biochar activation techniques and electrode fabrication methods, emphasizing their potential to enhance sustainable energy storage solutions.

Keywords: Biomass derived carbon; Biofuel; Activated biochar; Supercapacitor; Activation methods; Electrode fabrication

EN-202

CNF-Reinforced Ag_2Se/PVDF Films with Enhanced Seebeck Coefficient and High Flexibility for Wearable Thermoelectrics

Sakeena V, Mohamed Jibri K P, Mani Navaneethan*

Nanotechnology Research Centre (NRC), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603203, India

***Corresponding author e-mail:** navaneem@srmist.edu.in

ABSTRACT

The growing demand for sustainable energy solutions has accelerated the development of flexible thermoelectric materials capable of harvesting low-grade heat, especially for wearable applications. This study presents a flexible Ag_2Se-based thermoelectric composite film fabricated without compromising electrical conductivity and exhibiting an enhanced Seebeck coefficient through heterointerface-mediated energy filtering. Polyvinylidene fluoride (PVDF) serves as a flexible polymer matrix, while carbon nanofibers (CNFs; 0.25–0.75 wt.%) are incorporated to modulate carrier transport and enhance electrical conductivity. The formation of well-contacted heterojunction interfaces between Ag_2Se, CNFs and PVDF induces selective scattering of low-energy charge carriers, thereby enhancing the Seebeck coefficient without compromising electrical conductivity. The optimized APC1 composite exhibits a Seebeck coefficient of −239.69 μ V K^{-1}, while the APC3 composition achieves a maximum electrical conductivity of 5187 S m^{-1}. Leveraging this performance, a six-leg flexible thermoelectric generator (TEG) was fabricated, delivering an open-circuit voltage of 0.18 mV and a maximum output power of 0.0035 n W under matched load resistance. Under a temperature gradient of 5 K on the human body, the device generated 0.15 mV in real-time operation. These findings demonstrate that heterointerface-engineered Ag_2Se/PVDF/CNF composites provide a viable strategy for high-performance, flexible thermoelectric energy harvesting from body heat.

Keywords: Wearable Thermoelectrics, Seebeck coefficient, Ag_2Se and Energy filtering effect.

References:

1. Owusu, P. A. & Asumadu-Sarkodie, S. A review of renewable energy sources, sustainability issues and climate change mitigation. *Cogent Engineering* **3**, 1167990 (2016).
2. Kwon, C. *et al.* Stretchable Ag2Se Thermoelectric Fabric with Simple and Nonthermal Fabrication for Wearable Electronics. *Small Science* **4**, 2400230 (2024).
3. Shi, Y., Wang, Y., Mei, D., Feng, B. & Chen, Z. Design and Fabrication of Wearable Thermoelectric Generator Device for Heat Harvesting. *IEEE Robotics and Automation Letters* **3**, 373–378 (2018).

EN-203

High-Performance $Mg_2Si_{0.6}Sn_{0.4}$ Solid Solution through Decoupling of Carrier-Phonon Dynamics for Thermoelectric Application

Saran. M[1, 2], Vijay. V[3], Navaneethan. M[3], Justin Jesuraj. P[1, 2] *, Archana. J[1] *

[1]*Center of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology, Kattankulathur, 603 203, India*

[2]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India.*

[3]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India*

***Corresponding authors:** justin.jesuraj@gmail.com, archanaj@srmist.edu.in

ABSTRACT

Achieving simultaneous optimization of electrical transport and thermal conductivity remains a key challenge in thermoelectric materials due to the intrinsic coupling between charge carriers and phonons. In this work, Sb-Bi co-doping is employed in $Mg_2Si_{0.6}Sn_{0.4}$ solid solutions to regulate carrier-phonon interactions and enhance thermoelectric performance. The dual-doping strategy effectively tunes carrier concentration and modifies band structure while influencing acoustic phonon scattering. The optimized composition, $Mg_2(Si_{0.6}Sn_{0.4})_{0.98}Bi_{0.015}Sb_{0.005}$, exhibits improved electrical transport with a high weighted mobility of 123 $cm^2V^{-1}s^{-1}$ and a power factor of ~3 mW. m^{-1} K^{-2}. At the same time, alloy disorder and multi-frequency phonon scattering significantly suppress lattice thermal conductivity to 0.89 Wm^{-1} K^{-1}. As a result, the material achieves a high figure of merit (zT_{max}) of 1.57 at 753 K. These results demonstrate that co-doping induced carrier-phonon interaction modulation provides an effective pathway for improving the performance of n-type Mg_2Si-Sn based thermoelectric materials.

Keywords: Carrier-phonon decoupling; Band structure engineering; Weighted mobility and Alloy disorder phonon scattering.

References:

1. P. Mangelis, A. Sousanis, G. Mesaritis, P. S. Ioannou, A.-K. Søiland, Y. Xu and T. Kyratsi, *ACS Applied Electronic Materials*, 2024, **6**, 2988-2998.
2. G. Yang, L. Sang, C. Zhang, K. See, A. Hamilton, M. Fuhrer, N. Ye, G. J. Snyder and X. Wang, *Advanced Materials*, 2025, 2506417
3. G. Jiang, J. He, T. Zhu, C. Fu, X. Liu, L. Hu and X. Zhao, *Advanced Functional Materials*, 2014, **24**, 3776-3781.

EN-204

A Flexible Triboelectric Nanogenerator Based on Biodegradable MXene@Cellulose Acetate/Ag Nanofibers for Self-Powered Electronics

Seema and Aman Mahajan*

Department of Physics, Guru Nanak Dev University, Amritsar 143005, India

***Corresponding author e-mail:** aman.phy@gndu.ac.in

ABSTRACT

Batteries have a short lifetime, lack structural flexibility, and produce a significant amount of e-waste causing negative environmental impacts. Therefore, sustainable power sources, Triboelectric nanogenerators (TENGs) emerge as promising technology converting the often-wasted mechanical energy to electrical energy. However, TENGs are mostly composed of non-biodegradable polymers. To solve this, MXene@Cellulose Acetate Nanofibers/Ag were fabricated by using electrospinning. The Cellulose Acetate Nanofibers (CA-NFs)/Ag significantly improved the biodegradability, stability and conductivity of the triboelectric negative MXene NFs. The resulting composite functioned well as highly triboelectric negative friction layer in triboelectric nanogenerators (TENGs) when paired with triboelectric positive Kapton. The composite containing 17 wt. % CANFs in conjunction with MXene was extremely efficient during the prolonged operation of a TENGs, generating an output voltage around 200 V at a frequency of 6 Hz. Moreover, FESEM revealed the proper dispersions of composite and enhanced spinnability as beadless nanofibers. Further, XRD was done to confirm the formation of nanocomposite. This work, flexible TENG based on MXene@CA/Ag NFs composite is a promising technology for energy harvesting to enable intelligent self-powered sensing systems and wearable electronics.

Keywords: Biodegradable;Flexible; MXene; Cellulose Nanofibers; Energy harvesting.

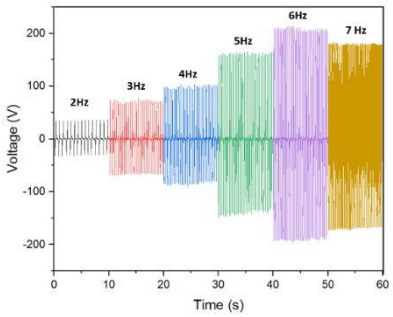


Figure 1. Dependence of output voltage on tapping frequency.

Keywords: Biodegradable;Flexible; MXene; Cellulose Nanofibers; Energy harvesting.

References:

1. Li, Z., Zhu, M., Qiu, Q., Yu, J., & Ding, B. (2018). Multilayered fiber-based triboelectric nanogenerator with high performance for biomechanical energy harvesting. Nano Energy, 53, 726-733.
2. Lv, Q., Ma, X., Zhang, C., Han, J., He, S., Liu, K., & Jiang, S. (2024). Nanocellulose-based nanogenerators for sensor applications: A review. International Journal of Biological Macromolecules, 259, 129268.

EN-205

Potassium Oxychloride Solid State Electrolytes for Energy Storage Applications

Rohit Kumar Kasaudhan, Atul Khanna*

Department of Physics, Guru Nanak Dev University, Amritsar-143005, India

***Corresponding author e-mail:** atul.phy@gndu.ac.in

ABSTRACT

Potassium oxychlorides of starting composition; $K_{2.99}OCl$ and Ca^{2+} doped sample of the starting composition: $K_{2.99}Ca_{0.005}OCl$ were synthesized by wet-chemistry method by heating the starting materials upto 250ºC. The structural and electrical properties of the samples were studied by X-ray diffraction (XRD) and ac impedance spectroscopy techniques. XRD studies confirmed the formation of orthorhombic $KClO_4$ phase. The room temperature ionic conductivities of the samples are 26 $mS \cdot cm^{-1}$ and 55 $mS \cdot cm^{-1}$ for undoped and Ca^{2+} doped samples. It is found that potassium oxychlorides exhibit very high ionic conductivity and are promising materials for applications in all solid-state batteries.

Keywords: potassium oxychlorides, XRD, impedance spectroscopy, ionic conduction

EN-206

Investigation of Ru-doped Higher Manganese Silicide for Thermoelectric Application

J. Karuna[1,3], V. Vijay[2], M. Navaneethan[2], J. Archana[1]*

[1]*Centre of Excellence in Materials and Advanced Technologies, SRMIST*

[2]*Nanotechnology Research Centre, SRMIST*

[3]*Department of Physics and Nanotechnology, SRMIST, India*

***Corresponding author e-mail:** archanaj@srmist.edu.in

ABSTRACT

Higher Manganese Silicide (HMS), an intermetallic Nowotny Chimney Ladder (NCL) phase is a potential mid- to high temperature thermoelectric material owing to its elemental abundance, oxidation resistance and mechanical robustness. However, its thermoelectric efficiency is limited by intrinsically high lattice thermal conductivity (κ_l). In this study, the electronic structure and transport properties of $Mn_{1-x}Ru_xSi_{1.74}$ (x = 0.01, 0.015, 0.02) were systematically investigated to elucidate the isovalent transition-metal d-orbital hybridization in tuning TE performance. Structural analyses through XRD confirmed tetragonal I-42d symmetry with superspace reflections, while HR-TEM revealed occupational modulation and high dislocation density at elevated dopant concentration, consistent with increased lattice strain. The thermoelectric transport measurements (303–803 K) demonstrated a reduced κ (~2.7 $Wm^{-1}K^{-1}$ at 753 K) in x = 0.02 which is due to enhanced phonon scattering from lattice defects as a result of suppressed ionized impurity scattering. The isovalent substitution has maintained both electrical conductivity and Seebeck coefficient, without compromising each other. The optimized composition (x = 0.02) yielded an enhanced power factor (PF ≈ 1483 $\mu Wm^{-1}K^{-2}$ at 753 K) and a peak zT ≈ 0.39, corresponding to a 21% improvement over undoped HMS. The results establish isovalent doping as an effective approach for decoupling σ and κ, providing insights into orbital hybridization driven transport phenomena in NCL-based thermoelectrics.

Keywords: Isovalent doping, Lattice thermal conductivity, transition metal hybridization

EN-207

Interface-Engineered $NiCo_2O_4$@rGO Nanostructures with Superior Redox Activity for Efficient Energy Storage Devices

Kartheka Anandan[1], M. Jothibas[2*]

[1,2] *PG & Research Department of Physics, T.B.M.L College (affiliated to Annamalai University), Porayar, Mayiladuthurai, 609 307, Tamil Nadu, India.*

ABSTRACT

$NiCo_2O_4$@rGO nanocomposites were synthesized using an ultrasonication method to enhance surface area, pore structure, and interfacial charge transport for improved electrochemical energy storage performance. The control of precursor molar concentration shows that $NiCo_2O_4$ synthesized at a 1.5:1 M ratio produces defect-rich nanocrystallites with high lattice strain and numerous redox-active sites, yet suffers from low electronic conductivity. The incorporation of reduced graphene oxide (rGO) significantly changes nucleation and growth dynamics, resulting in a hierarchically porous micro–mesoporous structure with a BET surface area of 104.5 $m^2\ g^{-1}$ and a large pore volume, thereby improving electrolyte accessibility and ion diffusion. The rGO scaffold effectively prevents particle agglomeration, controls lattice strain, and creates continuous electron-transport pathways, leading to a notable decrease in charge-transfer resistance. Spectroscopic and electronic analyses reveal significant interfacial π–d coupling, defect-assisted charge redistribution, and electron transfer from rGO to $NiCo_2O_4$, resulting in Fermi-level upshift and enhanced faradaic kinetics. The $NiCo_2O_4$@rGO electrode achieves a specific capacitance of 1059 F g^{-1} at 1 A g^{-1} due to the integration of high-density redox sites and efficient ion/electron transport from its hierarchical porous structure, demonstrating excellent rate capability and cycling stability. This study shows that BET-driven porosity engineering and interfacial electronic coupling are crucial for enhancing electrochemical performance in spinel oxide–graphene hybrid electrodes.

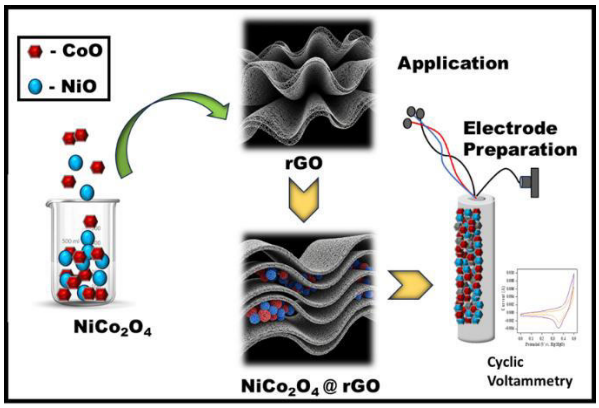


Fig. Graphical representation of $NiCo_2O_4$@rGO formation and electrode assembly for cyclic voltammetry studies.

References

1. Cai L., Li Y., Xiao X., Wang Y., *J. Appl. Physics*, 23 (2017) 2457–2463.
2. Arya K., Kumar A., Sharma A., Singh S., Sharma S. K., Mehta S. K., Kataria R., *J. Appl. Physics*, 65 (2022) 1924–1937.
3. Rao K. A., Mazhar M. E., Ahmad J., Bilal M., Haider S., Khan M. I., Abbas W., Akhtar N., Ahmad M. S., Luque R., *J. Appl. Physics*, 20 (2025) Issue 15.
4. Pore O. C., Fulari A. V., Chavare C. D., Sawant D. S., Patil S. S., Shejwal R. V., Fulari V. J., Lohar G. M., *J. Appl. Physics*, 824 (2023) 140551.

EN-208

Solid-State Derived Crystalline Molybdenum Pyrophosphate for High-Energy and Stable Pseudocapacitive Supercapacitors

Raju Ram, Km.Sweta Chauhan, Sushama Giripunje*

Visvesvaraya National Institute of Technology, Nagpur, Maharashtra, India, 440010

***Corresponding author e-mail:** sushamagiripunje9@gmail.com

ABSTRACT

The growing integration of renewable energy sources demands efficient and reliable energy storage technologies. Supercapacitors have gained considerable attention due to their high power density, rapid charge–discharge capability, long cycle life and environmentally friendly operation, making them attractive for advanced energy storage applications. In this context, metal pyrophosphates have emerged as promising electrode materials owing to their structural rigidity, rich redox chemistry and enhanced chemical stability in alkaline media. Crystalline molybdenum pyrophosphate (MoP_2O_7) was synthesized through a solid-state route and subsequently calcined at 550 °C, yielding a phase-pure structure as confirmed by X-ray diffraction. The well-defined crystalline framework provides abundant and accessible redox-active sites, enabling efficient pseudocapacitive charge storage in alkaline electrolyte. In 2 M NaOH, cyclic voltammetry delivers a remarkably high specific capacitance of 1434.12 F g^{-1} at 5 mV s^{-1}, corresponding to an energy density of 49.79 Wh kg^{-1} and a power density of 1792.65 W kg^{-1}. Chronopotentiometric (galvanostatic charge–discharge) analysis further reveals a specific capacitance of 939.81 F g^{-1} at 3 A g^{-1}. Moreover, the material demonstrates excellent durability, retaining 78.5% of its capacitance after 5000 cycles, confirming sustained electrochemical stability. The combination of high energy and power density, along with robust cyclic stability, underscores the strong potential of MoP_2O_7 for advanced electrochemical energy storage systems.

Keywords: Molybdenum pyrophosphate; Solid-state synthesis; Supercapacitor; Energy Storage.

References:

1. L. Lezama, J.M. Rojo, J.L. Mesa, T. Rojo, R. Olazcuaga, J. Solid State Chem. 115 (1995) 146–151.
2. B. Wen, N.A. Chernova, R. Zhang, Q. Wang, F. Omenya, J. Fang, M.S. Whittingham, Chem. Mater. 21 (2009) 1481–1488.
3. B. Bommu, S. Rajan, Y. Balasubramaniam, A. Velusamy, N. Somasundaram et. al , *Ionics 31*(6) (2025) 5291–5311.

EN-209

Protonated g-C_3N_4 Coupled Ternary System with Dual S-Scheme Charge Transfer Dynamics for Adsorption studies and Visible Light Driven Photocatalytic degradation of Methylene Blue and Ciprofloxacin

K. Bharathi [1,2], G. Bakiyaraj [2*], J. Archana [1,2], M. Navaneethan [1,3]

[1] *Centre of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India*

[2] *Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India*

[3] *Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India*

ABSTRACT

The widespread use of synthetic organic dyes and Pharmaceuticals poses serious environmental threats due to their toxic and persistent nature. To address this issue, the rational design of highly efficient photocatalysts is essential for the effective degradation of such pollutants. In this context, heterostructure photocatalysts have emerged as promising candidates owing to their enhanced charge separation and extended light absorption capabilities, which collectively improve photocatalytic performance. In the present study, a ternary $ZnCr_2O_4/V_2O_5$/protonated g-C_3N_4 (PVZ) heterojunction photocatalyst was synthesized for the degradation of methylene blue (MB) and Ciprofloxacin (Cip) dye under visible light. The PVZ ternary heterostructure was synthesized using the ultrasonication technique. The resulting photocatalyst exhibited superior photocatalytic efficiency, which is attributed to the formation of a dual S-scheme charge transfer mechanism. This configuration facilitated enhanced light absorption, suppressed recombination of photogenerated carriers, and promoted efficient charge separation and migration. The PVZ photocatalyst achieved a remarkable 97% degradation efficiency for MB and 82% for Cip in 50 and 75 min, respectively, significantly outperforming the binary and individual pristine photocatalysts. Radical trapping experiments confirmed that superoxide ($\bullet O_2^-$) and hydroxyl (•OH) radicals played dominant roles in the degradation mechanism. Moreover, reusability studies demonstrated excellent stability and recyclability of the PVZ system, retaining 94% degradation efficiency after three cycles, indicating its strong potential for practical wastewater treatment applications.

Keywords: Dual S-scheme charge transfer, Ciprofloxacin, Reactive oxygen species, Charge separation.

References:

1. M.A. Ashwini, S. Sagadevan, I. Fatimah, S. Paiman, S. Upadhyay, S. Garg, M.R. Johan, Photocatalytic performance of TiO_2/g-C_3N_4 nanocomposite modified with carbon quantum dots for effective dye degradation: Experiments and DFT studies, J. Alloys Compd. 1025 (2025).
2. M. Ikram, A. Haider, M. Imran, J. Haider, S. Naz, A. Ul-Hamid, A. Shahzadi, S. Moeen, G. Nazir, W. Nabgan, A. Bashir, S. Ali, Cellulose grafted poly acrylic acid doped manganese oxide nanorods as novel platform for catalytic, antibacterial activity and molecular docking analysis, Surfaces and Interfaces 37 (2023) 102710.

EN-210

Surfactant-Regulated Bismuth–Nickel Oxide Nanomaterials for Efficient Supercapacitors

S. Gayathri[a], Sethumathavan Vadivel[a]*

[a]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India*

*Corresponding author: vlvelu7@gmail.com

ABSTRACT

Bismuth-nickel oxide is a prominent mixed-metal oxide electrode material (Bi_2O_3 & NiO) for electrochemical energy storage applications. The rapid evolution of energy storage technologies has elevated demand for electrode materials that ensure optimal energy density and long-term stability. In this work, three notable synthesis routes were performed to fabricate bismuth nickel oxide built on materials. In the first route, the direct synthesis of bismuth-nickel oxide (Bi_2O_3 & NiO) as a bulk material. Secondly, the co-reduction of metals by hexamine is used as a template agent to improve redox behaviour and charge transfer mechanism. Thirdly, bismuth-nickel oxide was synthesised with poly(methyl methacrylate) (PMMA) as a sacrificial template, resulting in a porous structure. This electrode material exhibits an additional surface area and stability, which promote rapid charge-discharge cycles and high energy density. This study confirms the performance order in the three-electrode setup: bulk < hexamine < PMMA. The template controlled by hexamine significantly improved the electrochemical performance compared to the bulk material. In contrast, the PMMA-supported route achieved even higher specific capacitance and stability. This indicates template-controlled synthesis could enhance the electrochemical performance and long-term stability for next-generation energy storage devices.

Keywords: Supercapacitor, Energy density, guest-templated, bismuth, asymmetric device

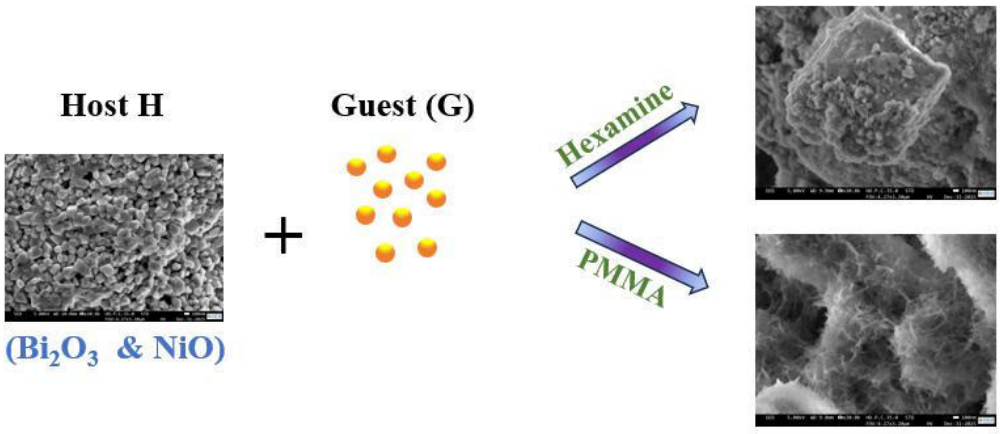


Figure 1. Template-assisted synthesis of bismuth nickel oxides

EN-211

ZnO Anchored g-C_3N_4 Nanosheets as an Efficient Material for Environmental Remediation and Energy Storage Applications

Sivapriya[a], Pradeep Reddy Vanga[a*]

[a]*Department of Physics, Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology, Avadi, Chennai-600062, India.*

***Corresponding author e-mail:** drpradeepreddy@veltech.edu.in

ABSTRACT

Supercapacitors have attracted significant attention because of their fast charge-discharge kinetics, excellent cycling stability, and low production cost. ZnO, and g-C_3N_4 have been widely studied due to their superior electrochemical and photocatalytic properties. In this work, a simple coprecipitation technique was applied to synthesize ZnO@g-C_3N_4 nanocomposite. Different weight ratios of g-C_3N_4 were used to synthesize the ZnO@g-C_3N_4 nanocomposites to optimize the performance. The XRD spectrum confirms the successful formation of ZnO@g-C_3N_4, with no impurity peaks. The FESEM micrographs reveal the uniform dispersion of ZnO nanospheres on the surface of the g-C_3N_4 sheets. The band gap of the prepared nanocomposite was investigated by UV-Vis spectroscopy. The photocatalytic process was performed to degrade the Eriochrome Black T (EBT) dye under UV light. From electrochemical studies, the pure and ZnO@g-C_3N_4 nanocomposite electrodes show the surface pseudocapacitive nature. The ZG1 nanocomposite achieved a specific capacitance 287.2 F g^{-1} at a current density of 1 A g^{-1}. The ZnO@g-C_3N_4 composite demonstrates an effective material for photocatalysis and supercapacitor applications.

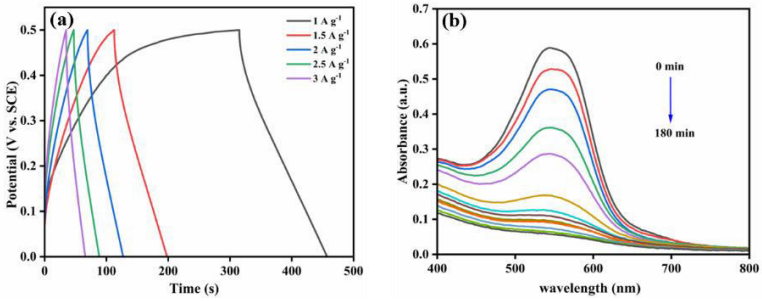


Fig.1 (a) GCD curve of ZG1 nanocomposite at different current density (b) dye degradation spectra.

Keywords: nanocomposites; surface pseudocapacitance; electrochemical energy storage; UV light irradiation; photocatalyst

References:

1. K. Dissanayake and D. Kularatna-Abeywardana, *J. Energy Storage*, 2024, **96**, 112563.
2. A. Shaikh, M. R. Patil, B. S. Jagdale and V. A. Adole, Inorg. Chem. Commun., 2023, **151**, 110570.
3. Y. Luo, Y. Yan, S. Zheng, H. Xue and H. Pang, *J. Mater. Chem. A*, 2019, **7**, 901–924.

EN-212

Electrochemical Performance of $ZnC0_2O_4$ Nanoparticle for Water Splitting Applications

Pubesh B[1,2], M Navaneethan[1], J Archana[2], M Krishna Mohan[2] *

[1]*Nanotechnology Research Centre, SRM Institute of science and Technology (SRMIST), Kattankulathur 603203, India*

[2]*Centre of Excellence in Materials for Advanced Technologies, SRM Institute of science and Technology (SRMIST), Kattankulathur 603203, India*

***Corresponding author e-mail**: krishnaml@srmist.edu.in

ABSTRACT

The spinel oxides (AB_2X_4) with a distinctive structure have been widely explored as an alternative active catalyst for elevate oxygen evolution reaction (OER), but fabricating robust and viable electrodes are major concern nowadays. Herein, $ZnCo_2O_4$ is a promising and extensively studied material for OER. However, owing to its deficient stability during the electrochemical reaction upon high current density makes the material unstable. To rectify this, doping of rare earth metals will enhance the performance by tuning the electronic structure by Co^{+3} site which occupies the octahedral sites of $ZnCo_2O_4$ for both OER and HER with a low overpotential and Tafel slope with long-term stability. In this study, $ZnCo_2O_4$ was synthesized in-situ and grown on NF using a hydrothermal method, then oxidizing heat treatment (350°C) and characterization studies were executed to investigate performance.

Keyword: Electrocatalysis, water splitting, oxygen evolution reaction, hydrogen evolution reaction, Spinel oxide.

References:

1. JianjunShi, Di Yu, Xuehua Yu, Bauyrzhan Sarsenbekuly, Zhen Zhao, Wanli Kang, and Saule B Aidarova. "Spinel $ZnCo_2O_4$ Nanosheets Supported on Ni Foam as Electrocatalysts for the Oxygen Evolution Reaction." ACS Applied Nano materials 2025, 8, 20077—20087.
2. Rajeshvari Samatbhai Karmur, Darshana Anand Upar, Ziyu Mei, Derek Hao, Chuangwei Liu, and Narendra Nath Ghosh. "Electrocatalytic Hydrogen Evolution in Alkaline Medium Using the $ZnCo_2O_4$ WO_3 Heterostructure: Experimental and DFT Insights" Energy & Fuels 2025 39 (5), 2854-2866

EN-213

Enhanced Themoelectric Performance of Layered Chalcogenide Bi_2Se_3 Through Ag Nanoinclusion

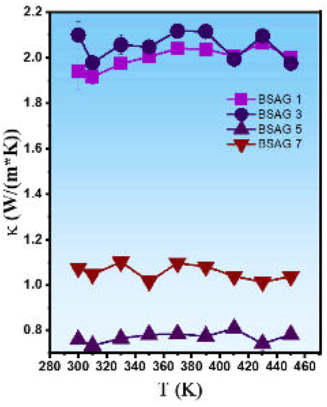
Rasikapriya P V[1], V Vijay[1], J Archana[2], M Navaneethan[1,*]

[1]*Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[2]*Centre of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

ABSTRACT

Thermoelectric technology is undoubtedly one of the important strategies for converting heat into electricity for power generation and cooling. Rapid increase in carbon dioxide and other harmful gases coupled with the depletion of fossil fuels along with the increase in demand of implementation of Internet – of – Things (IoTs), the society is currently in a dire need of sustainable energy conversion, and in this era of industrialisation and urbanisation, thermoelectric technologies play a pertinent role in the conversion of waste heat to electricity. Optimisation of thermoelectric performance in layered chalcogenides such as bismuth selenide (Bi_2Se_3) is a promising route towards the efficient energy conversion technologies. In this work, Ag nanoparticles prepared via Seed mediated Lee – Meisel method and Bi_2Se_3 via hydrothermal method. Obtained nanoparticle is included into Bi_2Se_3 matrix via hand grinding and investigated the influence of metallic inclusions on structural, electrical and thermal transport behavior. Mobility has been enhanced by the increase of Ag content which contribute to the enhancement in electrical conductivity. Furthermore, the intercalation of Ag in the van der Waals gap caused the lattice thermal conductivity to reduce, attributed to intensified phonon scattering at Ag/Bi_2Se_3 interfaces. 5% Ag included sample exhibited a very low thermal conductivity of 0.734 W/mK at a temperature of 313K. This study demonstrates that Ag nanoparticle inclusion substantially reduces the lattice thermal conductivity, making it a viable strategy for achieving high performance Bi_2Se_3.



Keywords: Thermoelectic, Bismuth Selenide, Thermal conductivity, Phonon scattering, Electrical conductivity.

Reference

1 V Vijay, S Harish, J Archana, M Navaneethan et. al. Journal of Colloid and Interface Science 637 (2023) 340 – 353

2 Musah, Jamal-Deen, Xiao Yanjun, A. M. Ilyas, Travis G. Novak, Seokwoo Jeon, Clement Arava, S. V. Novikov et al. "Simultaneous enhancement of thermopower and electrical conductivity through isovalent substitution of cerium in bismuth selenide thermoelectric materials." ACS Applied Materials & Interfaces 11, no. 47 (2019): 44026-44035.

EN-214

Enhanced Atomic Ordering Leads to Carrier Delocalization and High Thermoelectric Performance in Zn doped $AgSbSe_2$

Godlim P M[a], K P Mohamed Jibri[b], J Archana [a]*, M Navaneethan[b]

[a]*Center of Excellence in Materials for Advanced Technologies(CeMAT), Faculty of Engineering and Technology ,SRM Institute of science and Technology (SRMIST), Kattankulathur 603203, India*

[b]*Nanotechnology Research Center (NRC), Faculty of Engineering and Technology, SRM Institute of science and Technology (SRMIST), Kattankulathur 603203, India*

***Corresponding author e-mail:** archanaj@srmist.edu.in

ABSTRACT

In general high thermoelectric performance is achieved through altering electronic structure or by enhancing phonon scattering, which tends to neutralise each other. To attain good performance thermoelectric performance it requires inventive strategies that partially optimize both electronic and phonon transport. $AgSbSe_2$ is an emerging thermoelectric p-type material suitable for mid-temperature applications. In $AgSbSe_2$, the high structural disorder of Ag and Sb on the cationic position in this crystal structure gives rise to very low thermal conductivity. Such random cationic disorderness localise the charge carriers and that leads to inherently low carrier mobility and poor electrical transport properties. It can be tackled through partial substitution of trivalent Sb^{3+} ions with divalent Zn^{2+} ions on the disordered cationic position. This substitution improves the cationic ordering of $AgSbSe_2$ and in turn results to delocalization of the electron and thereby enhances the mobility of the charge carriers. In this work, $AgSbSe_2$ and Zn-doped $AgSbSe_2$ were synthesized and characterized to investigate the improvement of electrical transport properties and the resulting enhancement in thermoelectric performance.

Keywords: Thermoelectrics, Delocalization,Cationic Ordering,$AgSbSe_2$

References:

1. XingTan. Et al. “High Thermoelectric Performance of $AgSb_{1-x}Pb_xSe_2$ Prepared by Fast Nonequilibrium Synthesis.” Applied Material and Interfaces,2020
2. HongdaSong et al. “Decoupling Electron-Phonon Transportin $AgSbSe_2$ via Stepwise Cd-Sb Substitution and Interstitial Se Compensation.” small,2025
3. Subhajit Roychowdhury et al. “Enhanced atomic ordering leads to high thermoelectric performance in $AgSbTe_2$.” Science,2021

EN-215

Tuning of Carrier Concentration and Secondary Phase Interfaces for Enhanced Thermoelectric Performance of $AgInSe_2$

Chellamuthu Kannan [1], Vijay Vaiyapuri [2], Archana Jeyaram[3] , Navaneethan Mani *[4]

Nanotechnology Research Centre (NRC)

Faculty of Engineering and Technology,

SRM Institute of Science and Technology, Kattankulathur 603203, India, Tamilnadu, India, 603203

***Corresponding author e-mail**: navaneem@srmist.edu.in

ABSTRACT

The increasing demand for low-carbon and sustainable energy technologies has stimulated extensive research into thermoelectric (TE) materials that can directly convert waste heat into electricity and vice versa. Among emerging TE systems, diamond-like chalcopyrite compounds have gained considerable attention due to their tunable electronic band structures, favorable carrier transport behavior, and intrinsically low lattice thermal conductivity associated with complex crystal structure. For practical thermoelectric module fabrication, both high-performance p-type and n-type semiconductors are essential. Although p-type diamond-like chalcopyrites have demonstrated excellent thermoelectric performance with figure of merit (zT) values reaching ~1.6, the development of efficient n-type counterparts remains a critical challenge, limiting overall device efficiency. In this regard, n-type $AgInSe_2$, a diamond-like chalcopyrite compound, exhibits intrinsically low thermal conductivity (~1 $Wm^{-1}K^{-1}$ at 303 K), primarily attributed to low-frequency Ag–Se cluster vibrations and enhanced phonon scattering. These features make it a promising candidate for mid-temperature thermoelectric applications. However, its thermoelectric performance is severely constrained by an extremely low intrinsic carrier concentration (~10^{13} cm^{-3}), leading to poor electrical conductivity and a reduced power factor. To overcome this limitation, a synergistic strategy combining defect engineering with $AgIn_5Se_8$ secondary phase modulation was employed to effectively tune the carrier concentration to above ~10^{17} cm^{-3}. Controlled defect formation enhances free carrier generation and optimizes electronic transport, while the introduction of secondary phase interfaces promotes additional phonon scattering, thereby suppressing lattice thermal conductivity. This dual approach enables simultaneous optimization of electrical conductivity and thermal transport properties, resulting in significantly improved thermoelectric performance. The present study demonstrates that defect-engineered $AgInSe_2$ is a promising n-type candidate for high-efficiency diamond-like thermoelectric modules.

Keywords: Thermoelectrics,Chalcopyrite,$AgInSe_2$, Defect engineering, Point defect scattering

References:

1. Qiu, Pengfei, Yuting Qin, Qihao Zhang, "Intrinsically high thermoelectric performance in AgInSe2 n-type diamond-like compounds." Advanced Science 5, no. 3 (2018): 1700727.

EN-216

Investigation of Mg_3Sb_2 a Zintl Phase Material for Thermoelectric Applications

Mohammad Anwar A [1], Vijay Vaiyapuri [2], Archana Jeyaram [1] *, Navaneethan Mani [2]

[1]*Center of Excellence in Materials for Advanced Technologies (CeMAT) Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattangulathur, 603203, India.*

[2]*Nanotechnology Research Centre, SRM Institute of Science and Technology, Kattangulathur, 603203, India.*

***Corresponding author e-mail:** archanaj@srmist.edu.in

ABSTRACT

The global energy demand surged due to the increase in energy consumption which creates demand in cultivating carbon free sustainable energy. Thermoelectrics, a way to produce sustainable energy from recovering waste heat in electric energy via Seebeck effect. Mg_3Sb_2 a Zintl phase material is an evolving state of art n-type material, attains the thermoelectric performance (zT) of nearly ~ 1.5 around 750 K. This material is intrinsically p-type due to the presence of Mg vacancies, and also has low thermal conductivity due to its complex structure. This material has a major demerit of low carrier concentration and less number of valley degeneracy. By adding excess Mg and substitution of Bi on Sb site optimize its band structure and also decrease the lattice thermal conductivity. The carrier concentration was increased by incorporating Se on Sb site, enrich the carrier concentration of -1.82×10^{19} cm^{-3}. The concept solute drag, improves the electrical conductivity between grain boundaries of the materials to enhance its thermoelectric performance in near room temperature regime. Further the excess Mg was replaced by selective dopant to create solute drag to enhance electrical conductivity in between grain boundaries to achieve better performance at near room temperature regions round 400 K. Then a thermoelectric module was designed with the prepared material to convert waste heat into effective sustainable energy.

Keywords: Thermoelectrics, Mg_3Sb_2, Zintl, Solute drag, Band structure, n-type.

References:

1. Alkayyali, Malek, and Fadi Abdeljawad. "Grain boundary solute drag model in regular solution alloys." Physical Review Letters 127.17 (2021): 175503.
2. Luo, Ting, et al. "Nb-mediated grain growth and grain-boundary engineering in Mg3Sb2-based thermoelectric materials." Advanced Functional Materials 31.28 (2021): 2100258.
3. Wang, Longquan, et al. "High-performance Mg3Sb2-based thermoelectrics with reduced structural disorder and microstructure evolution." Nature Communications 15.1 (2024): 6800.
4. Wang, Changjian, and Moneesh Upmanyu. "Solute-drag forces from short-time equilibrium fluctuations of crystalline interfaces." Journal of Applied Physics 137.15 (2025).

EN-217

Flexible Cu_2Se/PVDF Thermoelectric Film for Efficient Human On-Skin Energy Harvesting

S. Raja surya[1], K.P. Mohamed Jibri[1], M. Navaneethan[1,*]

[1]*Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

ABSTRACT

As wearable health monitoring devices become part of our daily lives, providing a continuous and reliable power source remains a key challenge. Harnessing the natural warmth of human skin offers a sustainable way to generate electricity, reducing the need for frequent battery replacement in wearable devices. In this work, Copper Selenide (Cu_2Se), a p-type semiconductor with a bandgap of about 1.9-2.3 eV, was selected for its high electrical conductivity and stable performance near room temperature. Polyvinylidene fluoride (PVDF) was used as a flexible polymer binder, enabling the film to adapt to human body movements. To further enhance the overall thermoelectric performance, the Seebeck coefficient (S) was tuned by incorporating Bismuth selenide (BiSe), an n-type semiconductor with a band gap of around 0.1 eV, forms a naturally occurring heterojunction that reduces the carrier concentration, increases the Seebeck coefficient, and improves the power factor. When placed on human skin, the device generates consistent power from body heat, highlighting its capability for continuous, maintenance-free energy harvesting. This encouraging performance indicates that Cu_2Se/PVDF hybrid films could be promising choices for future self-powered wearable devices.

Keyword: Wearable devices, Electricity, energy harvesting, flexible, Thermoelectric

References:

1. Yang et al. Flexible thermoelectric generator and energy management electronics powered by body heat. Microsystems & Nanoengineering 9:106(2023).
2. Yang et al. Wearable and flexible thin film thermoelectric module for multi-scale energy harvesting. Microsystems & Nanoengineering 9:106(2023).
3. Samanta, M.; Pal, K.; Pal, P.; Waghmare, U. V.; Biswas, K. Localized Vibrations of Bi Bilayer Leading to Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance in Weak Topological Insulator N-Type BiSe. J. Am. Chem. Soc. 2018, 140 (17), 5866–5872. DOI: 10.1021/jacs.8b02691

EN-218

NiFeCo LDH/Transition Metal Sulfide Heterostructures as Bifunctional Electrocatalysts for Water Splitting

T.Jovitha[1],J.Archana[1], P.Justin Jesuraj[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** justinp@srmist.edu.in

ABSTRACT

To design highly active and economically sustainable materials is crucial for advancing electrochemical water-splitting technologies. In this work, the oxygen evolution reaction (OER), which is sluggish and involves a four-electron transfer process to produce oxygen gas, To overcome these challenges, transition metal-based layered double hydroxides (LDHs) are considered promising low-cost and stable non-noble metal catalysts for OER. Furthermore, ternary NiFeCo layered double hydroxides with an optimized metal ratio were synthesized via a two-pot hydrothermal method and integrated with transition metal sulfides grown on nickel foam to construct a heterostructured electrocatalyst. The electrocatalytic performance of the prepared catalyst was investigated in 1 M KOH, demonstrating applicability in alkaline electrolyzer systems and depicting enhanced OER and HER performance. In addition, LSV, CV, Tafel analysis, EIS, and ECSA measurements were carried out. Key parameters, including overpotential, charge transfer resistance, and reaction kinetics, were assessed. Chronopotentiometry confirmed catalytic stability and durability under alkaline conditions.To further improve the catalytic efficiency and achieve a bifunctional electrocatalyst for overall water splitting, a NiFeCo/transition metal sulfide heterostructure was constructed. The incorporation of sulfides can enhance interfacial charge transfer, expose more active sites, and improve hydrogen evolution reaction (HER) activity.

Keywords: Electrocatalysis, Oxygen Evolution Reaction, Hydrogen evolution reaction Transition Metal Sulphides, Alkaline Water Splitting, Heterostructure.

References:

1. Susikumar, T., M. Navaneethan, and P. Justin Jesuraj. "Insights over the in-situ grown copper sulfide/NiFe-LDH composites for alkaline and urea water electrolysis." Inorganic Chemistry Communications 170 (2024): 113523.
2. Susikumar, T., Manikandan Kandasamy, Jayaram Archana, Brahmananda Chakraborty, and P. Justin Jesuraj. "Silver Sulfide-Functionalized NiFe-Layered Double Hydroxide Heterostructure as a Bifunctional Catalyst in Anode-Favoring Electrolysis." Energy & Fuels 39, no. 28 (2025): 13715-13727.

EN-219

Alloying-Driven Atomic Disorder Enables Phonon Suppression and Enhanced Thermoelectric Performance in BiSe

S. Kowsalya [1], K. Arun[2], J. Archana[1], Mani Navaneethan[1,2], Senthil Kumar Eswaran[2,3*]

[1]*Centre of Excellence in Materials for Advanced Technologies, Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[2]*Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[3]*2D Materials and Devices Laboratory (2DML), Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

***Corresponding author e-mail:** senthile2@srmist.edu.in

ABSTRACT

The development of high-performance Te-free thermoelectric materials has become a key research direction for sustainable energy applications. In this context, BiSe, belonging to the $(Bi_2)_m(Bi_2Se_3)_n$ homologous series, exhibits promising near-room-temperature n-type thermoelectric properties. In this study, Sb alloying in BiSe enhances the Seebeck coefficient from −78 μV K^{-1} to −105 μV K^{-1} for the x = 0.3 composition, representing an ~1.35-fold improvement over the pristine sample. Consequently, the x = 0.3 composition attains a power factor of 839 μW $m^{-1}K^{-2}$ at 500K. Furthermore, Sb alloying significantly reduces the lattice thermal conductivity by 57.82%, reaching ~0.38 W $m^{-1}K^{-1}$ at 300 K for the x = 0.3 composition. This reduction is primarily attributed to alloy-induced lattice distortions and enhanced phonon scattering. Additional S doping in the x = 0.3 composition further decreases the lattice thermal conductivity by ~12%, reaching 0.33 W $m^{-1}K^{-1}$, thereby improving the overall thermoelectric performance. These results demonstrate an effective defect-engineering strategy to enhance the thermoelectric properties of BiSe-based materials.

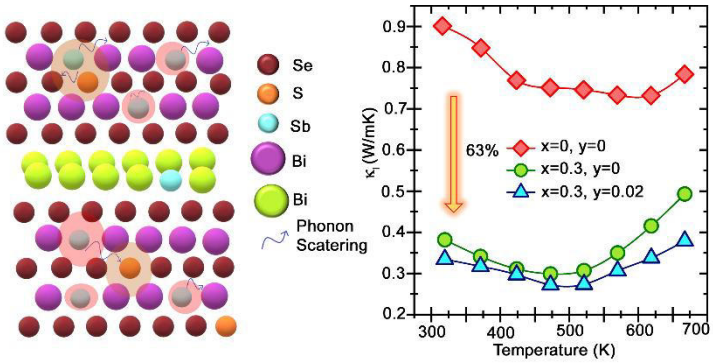


Fig.1. Atomic arrangement of BiSe and lattice thermal conductivity of $Bi_{1-x}Sb_xSe_{1-y}S_y$

References:

1. M. Samanta, K. Pal, P. Pal, U. V. Waghmare, and K. Biswas, J. Am. Chem. Soc., 140 (2018) 5866
2. H. Liu, X.-L. Shi, L. Pan, Y. Mao, M. Li, L. Wang, W.-D. Liu, Q. Liu, Y. Wang, and Z.-G. Chen, Acta Mater., 280 (2024) 120343.

EN-220

Rare-Earth-Induced Spin-State Engineering of Co_3O_4 For Efficient Oxygen Evolution Reaction

A Arokya Hepshiba[1], T Govindaraj[1], M Navaneethan[1], J Archana[2], S Harish[1*]

[1]*Nanotechnology Research Centre,SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203.*

[2]*Center of Excellence in Materials for Advanced Technologies, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** harishs@srmist.edu.in

ABSTRACT

Green hydrogen has received a lot of attention as a clean fuel for future energy systems due to the growing need for sustainable energy sources. In practical, electrocatalysts capable of delivering high current density with efficient charge transfer are highly desirable, as high current density reflects the ability of the catalyst to produce hydrogen efficiently at industrially relevant rates. Therefore, the development of efficient and cost-effective catalytic materials has become an important research focus. As a result, transition-metal oxides have been thoroughly investigated. Among these, Co_3O_4 gained a lot of attention due to its Spinel structure, multiple oxidation states and strong chemical stability. However, the catalytic performance of Co_3O_4 is limited because the low-spin state of Co^{3+} ions leads to a low charge-carrier concentration and poor electrical conductivity, which hinders efficient electron transport during electrocatalysis. Introducing rare-earth elements to modify the material's electronic structure is one potential way to overcome these limitations. This work introduces gadolinium into the Co_3O_4 lattice. Gd incorporation can cause lattice distortion and strain in the crystal structure because of its larger ionic radius. This change will lower the crystal field stabilization energy. As a result, electrons can move into higher-energy orbitals, promoting a high-spin electronic configuration. This adjustment in spin state can improve charge transport and increase the number of active catalytic sites. which improves charge transport and increases the number of active catalytic sites. As a result, the optimized catalyst achieves an lower overpotential of 454 mV to reach a high current density of 500 mA cm^{-2} and exhibits excellent stability, maintaining 500 mA cm^{-2} for 100 hours in chrono-potentiometry measurements.

Keywords: Transition-metal oxides, Gd doping, lattice distortion, lattice strain, lower CFSE, high spin state, better electron mobility.

References:

1. Myeong Gyu Kim and Yun-Hyuk Choi, “Electrocatalytic Properties of Co_3O_4 Prepared on Carbon Fibers by Thermal Metal–Organic Deposition for the Oxygen Evolution Reaction in Alkaline Water Electrolysis,” *Nanomaterials* 13 (2023): 1021.
2. Peijia Wang et al., “Rational Construction of Pt-Incorporated Co_3O_4 as High-Performance Electrocatalyst for Hydrogen Evolution Reaction,” *Nanomaterials* 14 (2024): 898.

Application of Lead-Free $Cs_3Bi_2Br_9$ Halide Perovskite for Solar-Driven Photocatalytic and Photoelectrochemical Water Splitting

K. Nisha[a], T. Govindaraj[b], J. Archana[a*], M. Navaneethan[a,b]

[a]*Centre of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603203, India*

[b]*Nanotechnology Research Centre, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603203, India*

***Corresponding author e-mail**: archanaj@srmist.edu.in

ABSTRACT

Solar-driven photoelectrochemical (PEC) and photocatalytic water splitting generates clean hydrogen from sunlight and water, powering zero-CO_2 energy solutions for sustainable industry, transportation, and storage. Metal halide perovskite materials such as $Cs_3Bi_2Br_9$, with a wide band gap of 2.59 eV, have attracted significant attention in photoelectrochemical (PEC) and photocatalytic applications due to their strong visible-light absorption and suitable optoelectronic properties. However, their limited stability and rapid charge recombination in aqueous environments restrict their efficiency in solar-driven water splitting. To overcome these challenges, I have composited $Cs_3Bi_2Br_9$ with reduced graphene oxide (rGO) at different ratios to optimize performance, where rGO provides some of the advantages like superior electron conductivity. $Cs_3Bi_2Br_9$/rGO composites were developed to address the low photocurrent density of pristine $Cs_3Bi_2Br_9$, primarily caused by poor charge carrier mobility and rapid recombination. rGO extracts photogenerated electrons from conduction band of $Cs_3Bi_2Br_9$, which boosts charge separation efficiency and increasing measured photocurrent densities through enhanced interfacial electron transfer. This work provides a promising strategy for the practical application of $Cs_3Bi_2Br_9$/rGO composites in efficient solar-driven PEC and PC water splitting, enabling enhanced charge separation, improved stability, and sustainable hydrogen production in aqueous environments.

Key Words: Photoelectrochemical, Photocatalytic, Metal halide perovskite, rapid charge recombination, photocurrent densities.

References:

1. Fan, Qiangwen, Dawei Liu, Zhaohong Liao, Debo Wu, Zongbo Xie, Haibo Zhu, and Zhanggao Le. "Ru3+-doped lead-free perovskite Cs3Bi2Br9 for photocatalytic selective oxidation of sulfides to sulfoxides using trace water as an oxygen source." *Journal of Catalysis* 443 (2025): 115945.
2. Poursam, Yasaman, Nemat Tahmasebi, Hamed Derikvand, and Hamze Moayeri. "Utilizing the water instability of Cs3Bi2Br9 perovskite for in situ growth of BiOBr nanosheets on g-C3N4 toward enhanced photocatalytic activity." *ACS Applied Nano Materials* 8, no. 13 (2025): 6465-6478.

EN-222

Rare Earth Incorporated Bimetallic MOF for Efficient Electrocatalytic Watersplitting

Harinisri V [1], T Govindaraj[1] , M Navaneethan[1,2], J Archana[1] , K D Nisha[1]*

[1] *Centre of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[2] *Nanotechnology Research Centre , Facutly of Engineering and Technology, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

Corresponding author e-mail: nishad@srmist.edu.in

ABSTRACT

Metal–organic frameworks (MOFs) are crystalline porous materials known for their tunable structures, high surface area Based on the target of carbon neutrality, it is very important to explore highly active and durable electrocatalysts for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Herein, a series of FeCo based metal organic frameworks (MOFs) with the doping of rare-earth elements 1% Sm were in situ grown on nickel foam by a facile solvothermal process. The representative FeCoMOF showed amazing OER performance with low overpotentials 1.0 M KOH respectively. Moreover, it also exhibited favorable activity and durability for alkaline. This work provided new inspiration for the electron modulation and activity optimization of MOF-based electrocatalysts.

Keywords: Electrocatalysis; BimetallicMOF; Rare earth element doped;

References:

1. Sirati, Muhammad Mukhtar, Shagufta Sirati, Umay Amara, Ajaz Hussain, Dilshad Hussain, Muhammad Hanif, Khalid Mahmood et al. "Samarium-based metal organic frameworks as high performance electrocatalyst for alkaline water splitting." Fuel 362 (2024): 130812.
2. Senthil Raja, Duraisamy, Xui-Fang Chuah, and Shih-Yuan Lu. "In situ grown bimetallic MOF-based composite as highly efficient bifunctional electrocatalyst for overall water splitting with ultrastability at high current densities." Advanced Energy Materials 8, no. 23 (2018): 1801065

Enhanced Electrocatalysis Performance of NiFe LDH through Doping with Rare Earth Element

Manivasuki M[1], J Archana[1], Navaneethan M[2] M Krishna Mohan[1,*]

[1]*Centre of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[2]*Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology (SRMIST),Kattankulathur 603203, India*

[*]**Corresponding author email:** krishnam1@srmist.edu.in

ABSTRACT

Designing highly efficient and noble-metal-free electrocatalysts for the oxygen evolution reaction (OER) continues to be a fundamental limitation owing to its sluggish kinetics and high activation energy barrier in alkaline water splitting. NiFe layered double hydroxide (NiFe LDH) is considered as one of the most promising non-noble metal catalysts, but it's practically limited by insufficient intrinsic activity and moderate electrical conductivity. Herein, Rare Earth (RE) metal doping is employed as an effective strategy to regulate the electronic structure and defect chemistry of NiFe-LDH. The incorporation of RE metal into the NiFe-LDH lattice alters the electronic structure by facilitating electronic redistribution between metal active sites due to the unique partially filled 4f orbitals and tend to donate electron density nature of rare earth elements. Subsequently, the RE-NiFe-LDH catalyst demonstrates superior intrinsic activity, reflected by a reduced overpotential at a standard benchmark current density, a small Tafel slope, and improved by faster charge-transfer kinetics than NiFe-LDH. Moreover, the doped catalyst gives excellent long-term durability and high Faradaic efficiency in alkaline conditions. Overall, this study focuses on rare-earth doping as a promising approach to tune the electronic structure of active sites and enhance the catalytic efficiency of NiFe-LDH for overall water splitting applications.

Keywords: Electrocatalysis, Water splitting, Oxygen evolution reaction (OER), NiFe layered double hydroxide, Rare-earth, Electronic structure modulation, Oxygen vacancies, Charge transfer kinetics.

Reference

1 Li, Meng, Hao Li, Xuechun Jiang, Mengqi Jiang, Xun Zhan, Gengtao Fu, Jong-Min Lee, and Yawen Tang. "Gd-induced electronic structure engineering of a NiFe-layered double hydroxide for efficient oxygen evolution." *Journal of Materials Chemistry A* 9, no. 5 (2021): 2999-3006.

2 Nagappan, Sreenivasan, Hemalatha Gurusamy, Harpriya Minhas, Arun Karmakar, S. Ravichandran, Biswarup Pathak, and Subrata Kundu. "Unraveling the Synergistic Role of Sm3+ Doped NiFe-LDH as High-Performance Electrocatalysts for Improved Anion Exchange Membrane and Water Splitting Applications." *Small Methods* 9, no. 5 (2025): 2401655.

Flexible Ag_2Se Composite Films using Organic Insulating Polymers for Wearable Thermoelectric Applications

Kesavan. K[1], Vijay. V[1], Archana. J[2], Navaneethan. M[1], Harish. S[1*]

[1]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India.*

[2]*Center of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology, Kattankulathur, 603 203, India.*

***Corresponding author e-mail**: aravindharri@gmail.com

ABSTRACT

Silver selenide (Ag_2Se) is a promising thermoelectric material due to its low lattice thermal conductivity and high electrical conductivity. However, its poor mechanical flexibility limits use in flexible devices. In this work, Ag_2Se composites with polyvinyl alcohol (PVA) and sodium alginate were prepared to enhance flexibility and fabricate free-standing films with different polymer concentrations. Among the composites, smaller bending radii were compared to than Na-alginate, indicating superior mechanical flexibility. XRD patterns of the prepared samples confirm the orthorhombic crystal structure of Ag_2Se without any secondary phases. The presence of PVA and Na-alginate was verified using FTIR spectroscopy. SEM images reveal irregular Ag_2Se particles embedded in the polymer matrix, indicating strong interfacial interaction. Among the composites, Na-alginate-based films exhibit higher carrier concentration due to improved particle contact arising from the strong attraction between Na^+ ions and polysaccharides. Conversely, Na-alginate–based composite films exhibited a higher thermoelectric power factor of 9.6 $\mu W/mK^2$ and electrical conductivity of 1989 S/cm at room temperature, exceeding those of PVA-based films. These results highlight a balance between mechanical flexibility and thermoelectric performance, providing valuable guidance for the development of next-generation flexible thermoelectric devices.

References:

1. Wu, H., Shi, X.L., Duan, J., Liu, Q. and Chen, Z.G., 2023. Advances in Ag 2 Se-based thermoelectrics from materials to applications. *Energy & Environmental Science*, *16*(5), pp.1870-1906.
2. Liang, J., Wang, T., Qiu, P., Yang, S., Ming, C., Chen, H., Song, Q., Zhao, K., Wei, T.R., Ren, D. and Sun, Y.Y., 2019. Flexible thermoelectrics: from silver chalcogenides to full-inorganic devices. *Energy & Environmental Science*, *12*(10), pp.2983-2990.

Han, S., Chen, S. and Jiao, F., 2021. Insulating polymers for flexible thermoelectric

Investigation of Rapid Thermal Explosion Synthesis of $CuFeS_2$ for Enhanced Thermoelectric Performance

Elakkiya Chidambaram[1], Murugadass T[1], M. Navaneethan[1, 2], J. Archana[1], K D Nisha[1]*

[1] *Centre of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[2] *Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, India.*

***Corresponding author e-mail**: nishad@srmist.edu.in

ABSTRACT

Owing to the enervation of fossil fuels, there is a vital need to explore advanced, eco-friendly thermoelectric power generation. Disparate costly and toxic bismuth telluride (Bi_2Te_3) or lead telluride (PbTe), the abundant, eco-friendly mineral chalcopyrite ($CuFeS_2$) offers a sustainable pathway for n-type thermoelectric applications. Moreover, most of them are synthesized by high energy and time -efficient synthesis. Herein, demonstrated a rapid and time-efficient method combining thermal Explosion (TE) and Spark Plasma Sintering (SPS) for the synthesis of $CuFeS_2$. A single-phase pristine $CuFeS_2$ composite was successfully obtained through rapid thermal explosion at 1273 K by fluctuating the holding time at 30s, 60s, and 90s. The as-synthesized material was further densified through Spark Plasma Sintering (SPS) at an applied pressure of 40 MPa at 873K. This variation in holding time resulted in structural modifications, which were analysed and reported in this work. The effective strategy approach to refine the microstructure and enhance the thermoelectric properties of $CuFeS_2$, enabling its use in sustainable waste heat recovery.

Keywords: Thermoelectric; chalcopyrite; thermal explosion.

References:

1. Xie, Hongyao, et.al *NPG Asia Materials* 9, no. 6 (2017): e390-e390.
2. Wang, Di, et.al *Nano Letters* 25, no. 14 (2025): 5925-5931.
3. Sootsman, J. R et.al Chem. Int. Ed. 48,8616–8639 (2009).

EN-226

Cocatalyst-Free Solar Driven Photocatalytic Hydrogen Production Using a Bimetallic Copper–Iron BDC MOF

Madhanraj P G[1], T Govindaraj[1] M, Navaneethan[1], J Archana[2,], S Harish[1*]

[1]*Nanotechnology Research Centre, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203.*

[2]*Center of Excellence in Materials for Advanced Technologies, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** harishs@srmist.edu.in

ABSTRACT

Hydrogen generation via solar-driven water splitting represents a highly sustainable pathway for clean energy production. Herein, we report the rational design and synthesis of a bimetallic copper-iron metal-organic framework by varying concentration of Fe (25%,50%,75%) (CuFe-BDC MOF) as a highly efficient catalyst for solar-driven water splitting. The strategic incorporation of Fe into the Cu-BDC architecture systneerajaematically modulates the porosity and electrical conductivity of the framework. Furthermore, Fe doping significantly narrows the optical bandgap, thereby extending the visible-light absorption capabilities and drastically enhancing the catalytic performance. Morphological characterizations reveal a hierarchical, stacked sheet-like structure with high surface roughness, providing an abundance of accessible active sites. This unique architecture facilitates superior light harvesting and rapid interfacial charge-transfer kinetics for both photocatalytic and electrocatalytic applications, as corroborated by electrochemical impedance spectroscopy (EIS). The optimized CuFe-BDC MOF demonstrated a remarkable photocatalytic hydrogen evolution reaction. This work elucidates the critical role of bimetallic synergy in tuning the electronic band structure of MOFs, presenting a robust strategy for the development of high-performance catalysts for next-generation solar-to-chemical energy conversion.

Keywords: Metal-organic frame (MOF), band structure, Photocatalyst, solar driven water splitting.

References:

1. Guo, C., Wang, T., Zhang, L., Chen, T., Guo, C., Hassan, A., ... & Wang, J. (2022). Precise regulation of defect concentration in MOF and its influence on photocatalytic overall water splitting. Nanoscale, 14(41), 15316-15326.
2. Afshariazar, F., & Morsali, A. (2025). Mixed-valence metal–organic frameworks: concepts, opportunities, and prospects. Chemical Society Reviews, 54(3), 1318-1383.

Rational Design of Porous MOF-808 Based Material for Strong Physisorptive Hydrogen Storage

Neeraja Ajith, Ajaijawahar Kaliyaperumal, Karthigeyan Annamalai*, Iyakutti Kombiah

Hydrogen Storage Materials and Nanosensors Laboratory, Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Tamil Nadu, India, 603203

***Corresponding author e-mail:** karthiga@srmist.edu.in

ABSTRACT

The development of hydrogen-based energy systems critically depends on the development of efficient and reliable solid-state hydrogen storage materials. In the present work, a zirconium-based metal-organic framework (MOF-808) was synthesized by facile solvothermal method and systematically investigated as a potential hydrogen storage medium. The physical and chemical properties were carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FTIR) spectroscopy, nitrogen adsorption-desorption measurements and thermogravimetric analysis (TGA) techniques. XRD results confirm the highly crystalline framework, while SEM images reveal well-defined polyhedral microcrystals with uniform morphology. FTIR spectrum exhibit distinct vibrational bands corresponding to carboxylate bonding modes and successful coordination between Zr-O clusters and organic linkers. Thermogravimetric analysis demonstrates that the framework retains its structural stability upto 400ºC of MOF-808 prior to decomposition. Textural analysis derived from BET and BJH methods indicates that the prepared MOF-808 possesses a high surface area of 1211.37 m^2/g, pore volume of 0.11 cm^3/g and average pore radius 24.93 Å, indicating the coexistence of micro and mesoporous domains. The combination of large surface area, accessible pore channels and chemically stable Zr-O coordination framework provide abundant physisorption sites favourable for hydrogen uptake. The synergistic interplay of high porosity, structural integrity and thermally stable inorganic clusters suggests that potential of Zr-MOF-808 as a promising candidate for reversible solid-state hydrogen storage applications. These results establish a strong structural-property correlation and offer valuable insights into the rational design of zirconium-based MOFs for advanced hydrogen energy applications.

Keywords: Hydrogen storage; metal organic frameworks; Zr-MOF-808; physisorbents

References:

1. B. Huang *et al*., J. Ind. Eng. Chem., **143** (2025) 293–302.
2. S. N. Miskan *et al*., Int. J. Hydrogen Energy, **162** (2025) 150750.

EN-228

Investigating the Effect of Co doping on the Thermoelectric Properties of Ti-Ni-Sn

Vaishnavi Ganesan[1], Kowsalya Murugan[1] and Kathirvel Venugopal[1*]

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India.*

***Corresponding Author e-mail:** kathirvv@srmist.edu.in

ABSTRACT

Half Heusler alloys are interesting class of materials for large scale thermoelectric power generation. In the main class of the Half Heusler alloy, the Ti-Ni-Sn based half Heusler thermoelectric materials have attracted attention because of their high *zT* and no content of toxic elements. Despite its interesting thermoelectric properties, the main issue to address in Ti-Ni-Sn is its high thermal conductivity of 5 W m^{-1} K^{-1}. However, the Half Heusler exhibits low thermal conductivity. And a small change in the composition of Ti-Ni-Sn causes a remarkable change in the thermal conductivity. With this motivation, the present work is designed to investigate the effect of Co and V substitution at Ti site on the thermoelectric properties of the parent phase. Here, $Ti_{(1-x)}Co_xNiSn$ and $Ti(1-x)V_xCo_yNiSn$ was synthesized by vacuum arc melting process. The change in valence electron count (induced n-type donor) strongly affects the Seebeck co-efficient and electrical resistivity for $Ti_{(1-x)}Co_xNiSn$ and $Ti(1-x)V_xCo_yNiSn$ system. The systematic analysis on the structural, morphological and thermoelectric properties of the synthesized samples are performed. Co and V incorporation in the parent matrix is expected to promote carrier scattering at high temperatures. Based, on the obtained results, Studies indicates that TiNiSn doped Co and V exhibits a strong potential as a thermoelectric material in the room-mid temperature.

References

1. Quinn, R.J. and Bos, J.W.G., 2021. Materials Advances, 2(19), pp.6246-6266.
2. Katsuyama, S., Matsushima, H. and Ito, M., 2004. Journal of alloys and compounds, 385(1-2), pp.232-237.

EH-001

Innovative Spectrophotometric Assay For 'Vitamin C' Quantification and Its Implementation in A Portable Smartphone-Based Analytical Platform

Chris Mariam George[1], Karuvath Yoosaf[1,2]*

[1]*Department of Applied Chemistry, Cochin University of Science and Technology (CUSAT), Kochi, Kerala, India, 686022*

[2]*Inter University Centre for Nanomaterials and Devices, Cochin University of Science and Technology (CUSAT), Kochi, Kerala, India, 686022.*

***Corresponding author e-mail:** yoosafk@cusat.ac.in

ABSTRACT

Oxidative stress, resulting from an imbalance between the production of reactive oxygen species (ROS) and antioxidant defence in our body, can cause extensive cellular damage. Vitamin C, a key water-soluble antioxidant abundant in fruits, plays a vital role in neutralizing ROS. Accurate quantification of Vitamin C in food matrices is therefore essential to prevent both deficiency and toxicity. Conventional determination methods provide reliable results but often require expensive instrumentation, trained personnel, and laboratory infrastructure. In this study, we developed a spectrophotometric assay for the rapid quantification of vitamin C in fruit juices, and translated the developed assay to a smartphone-integrated colorimetric platform (SICP). The assay exploits the specific redox reaction between ascorbic acid and DCPIP dye, wherein the dye is reduced to its leuco-form, producing a measurable color change. The SICP employs an LED light source with images captured by a smartphone camera for subsequent colorimetric analysis. Results demonstrated a linear relationship between analyte concentration and the lightness values, confirming the quantitative capability of the platform. The results obtained were compared with the established techniques. The proposed assay, based on UV–Vis spectroscopic measurements, showcased accuracy and reproducibility. The smartphone integrated analytical device developed from the proposed assay is portable, cost-effective, and user-friendly, offering an alternative to conventional assays for on-site monitoring of vitamin C in food matrices.

References:

1. W. Z. Zhao, P. P. Cao, Y. Y. Zhu, S. Liu, H. W. Gao, and C. Q. Huang, Quim Nova, vol. 43 (2020), 1421–1430.
2. M. Nejati-Yazdinejad, Int J Food Sci Technol, vol. 42 (2007), 1402–1407.
3. Z. Gazdik et al., Sensors, vol. 8 (2008), 7097–7112.

EH-002

Rapid Spectroscopic Detection of Methanol from Alcoholic Mixtures

Anila Joseph[1], Karuvath Yoosaf[1,2]*

[1]*Department of Applied Chemistry, Cochin University of Science and Technology (CUSAT), Kochi, Kerala, India, 682022*

[2]*Inter University Centre for Nanomaterials and Devices, Cochin University of Science and Technology (CUSAT), Kochi, Kerala, India, 682022.*

***Corresponding author e-mail:** yoosafk@cusat.ac.in

ABSTRACT

Methanol is a toxic alcohol that can be present in beverages either unintentionally as a by-product of improper fermentation or intentionally through adulteration. Even small amounts of methanol can pose serious health risks, including blurred vision, blindness, organ damage, and, in severe cases, death. Because methanol is colorless, volatile, and has sensory properties similar to ethanol, it cannot be identified by smell or taste, making analytical detection essential. Raman spectroscopy is a vibrational spectroscopic technique based on the inelastic scattering of monochromatic light, usually from a laser. When light interacts with a molecule, a small fraction undergoes energy shifts corresponding to molecular vibrational modes. These Raman shifts produce a spectrum that serves as a molecular fingerprint, enabling identification and structural analysis of chemical species. Beyond qualitative identification, Raman spectroscopy is increasingly used for quantitative estimation of analytes in liquid and solid matrices. The intensity of Raman peaks is directly related to the concentration of the corresponding molecular species, provided that experimental conditions remain consistent. In this study, Raman spectroscopic techniques were employed to analyse ethanol–methanol binary mixtures across a wide compositional range. A calibration system was developed using the intensity ratios of the characteristic Raman bands of ethanol and methanol. This calibration model was able to accurately predict the methanol concentration in ethanol–methanol binary mixtures.

References:

1. A. Picard, et al., Extremophiles, vol. 11(2007), no. 3, pp. 445–452.
2. Mammone, et al.,The Journal of Physical Chemistry, vol. 84(1980), no. 23, pp. 3130-3134.
3. H. Vaskova, International Journal of Biology and Biomedical Engineering, vol. 8(2014), no. 1998–4510, pp. 27–34.
4. Pelletier, et al., Applied spectroscopy Vol.57(2003), no. 1,pp. 20A-42A.

Cu doped β-Ga_2O_3 Nanostructures for Environmental Photocatalytic Remediation

Radhika Rajagopal K[1], and N. Gopalakrishnan[1]*

[1]*Thin Film Laboratory, Department of Physics, National Institute of Technology, Tiruchirappalli, India, 620015*

***Corresponding author e-mail:** ngk@nitt.edu

ABSTRACT

Pure and Copper (1, 3 and 5 mol%) doped β-Ga_2O_3 nanostructures were synthesized by hydrothermal method followed by calcination at 1000°C. The monoclinic structure of stable β-phase was confirmed by X-Ray Diffraction. Peak shifting towards lower 2θ values has been observed from XRD data due to Cu doping. The 5 mol% doped sample exhibited peaks corresponding to the secondary phase of $CuGa_2O_4$. FESEM analysis revealed the transformation of cocoon-like shape into spindle and stick-like structures upon increase of Cu concentration, while it transforms into flaky, sheet-like structure in 5 mol% doped sample. The characteristic bands of stretching and bending vibration in Ga-O bonds were analysed using FT-IR spectroscope. It revealed subtle peak shifts and intensity variations in pure and Cu doped samples. However, the 5 mol% sample with $CuGa_2O_4$ phase exhibited noticeable change in the FTIR profile. Optical properties were studied using UV-Visible Spectroscope and Photoluminescence Spectroscope. Photocatalytic efficiency of the samples was tested against a model dye (Rhodamine-B) under UV irradiation for various time durations. All Cu doped samples exhibit enhanced photocatalytic activity than pure β-Ga_2O_3, indicating the improvement of degradation ability of the nanostructures via introduction of Cu dopant. The enhancement of photocatalytic activity by Cu doping has been well supported by structural and optical properties.

References:

1. J. Kim, H. Ryou, J. Lee, S. Kim, and W. S. Hwang, Inorganics 13 (2025) 231.
2. Y. Wang, X. Shi, S. Hou, G. Yang, X. Liu, W. Zhang, W. Li, et al., Appl. Organomet. Chem. 39 (2025) e70305.

EH-004

Band Gap Engineering In B-Ga_2O_3 by Hydrothermal Method for Gas Sensing Performance

Sivani TS[1], Radhika Rajagopal K, N[1]. Gopalakrishnan[1]*

[1]*Thin Film Laboratory, Department of Physics, National Institute of Technology, Tiruchirappalli, India, 620015*

***Corresponding author e-mail:** ngk@nitt.edu

ABSTRACT

Al and In doped β-Ga_2O_3 have been synthesized by hydrothermal method to investigate its band gap variation and gas sensing performance. Initially, Gallium oxide hydroxide (GaOOH) has been synthesized using Gallium nitrate hydrate as precursor and Ammonium hydroxide as stabilizing agent, respectively. As obtained GaOOH powders are then converted into β-Ga_2O_3 by calcination at 1000^°C. Three different concentrations (5,10 and 15 mol%) of Al and In have been incorporated in pure β-Ga_2O_3 by same procedure to engineer its bandgap and to tailor it for gas sensing performance. The synthesized powders were thoroughly characterized using X-Ray Diffraction (XRD), UV-Vis spectroscopy, Field Emission Scanning Electron Microscopy (FESEM) and Energy Dispersive Spectroscopy (EDS) techniques in order to study the structural, optical and morphological properties as well as to confirm the successful incorporation of the dopants. It has been found that as Al concentration increases, β-Ga_2O_3 bandgap increases proportionally while band gap decrease upon In concentration increases. This band gap engineering is expected to optimize the adsorption and charge-transfer processes occurring at the material's surface which will be playing a crucial role in gas sensing performance.

References:

1. Pilliadugula, Rekha, and N. Gopala Krishnan, Materials Research Express ,6.2 (2018)025027.
2. Pilliadugula, Rekha, and N. Gopalakrishnan, Materials Science in Semiconductor Processing,135 (2021)106086.
3. Kim, Sunjae, et al, Journal of Alloys and Compounds ,931 (2023)167502.
4. Li, Zhiwei, et al, ACS Applied Electronic Materials ,3.10 (2021)4630-4639.
5. Kim, Sunjae, et al, RSC advances, 11.13 (2021)7338-7346.
6. Vinoth, E., S. Gowrishankar, and N. Gopalakrishnan, Applied Physics A ,124.6 (2018)433.
7. Vinoth, E., S.Gowrishankar, and N.Gopalakrishnan, Materials and Manufacturing Processes ,32.4 (2017)377-382.
8. Li, Xianke, et al., Journal of inorganic materials ,39.12 (2024)1384-1390.
9. Talwar, Madhura N., et al., Materials Science and Engineering: B ,317 (2025)118195.

Reusable SnO_2/g-C_3N_4/Cellulose Acetate Films for Photocatalytic Treatment of Dye-Contaminated Wastewater

R. Rajeswari[1], S. Thanikaikarasan[1]*, Azhagurajan Mukkannan[2]*

[1]*Department of Physics, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai- 602 105, Tamil Nadu, India.*

[2]*Department of Chemistry, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai- 602 105, Tamil Nadu, India.*

***Corresponding author e-mail:** azhagurajan.e1@gmail.com

ABSTRACT

Flexible and sustainable photocatalytic films are essential for efficient treatment of dye-contaminated wastewater. This work reports a novel free-standing SnO_2/g-C_3N_4/cellulose acetate (CA) composite film fabricated via a simple, green solution-casting method. The polymer-immobilised heterojunction design effectively overcomes issues related to catalyst separation and nanoparticle agglomeration, while enabling easy recovery [1]. The visible-light photocatalytic performance was evaluated using methylene blue (MB) and methyl orange (MO) as model pollutants. XRD, FTIR, and SEM analyses confirmed the uniform incorporation of crystalline SnO_2 nanoparticles and layered g-C_3N_4 sheets within the porous CA matrix, promoting strong semiconductor–polymer interactions and enhanced pollutant–catalyst contact. UV-DRS revealed improved visible-light absorption and a reduced optical band gap, indicating efficient light harvesting. The composite film achieved 91.97% MB and 80.95% MO degradation within 90 min, outperforming individual and binary counterparts. The degradation followed pseudo-first-order kinetics with high-rate constants, reflecting accelerated reaction dynamics [2]. The film exhibited excellent stability and reusability, highlighting its promise as a scalable, eco-friendly photocatalytic platform for wastewater remediation.

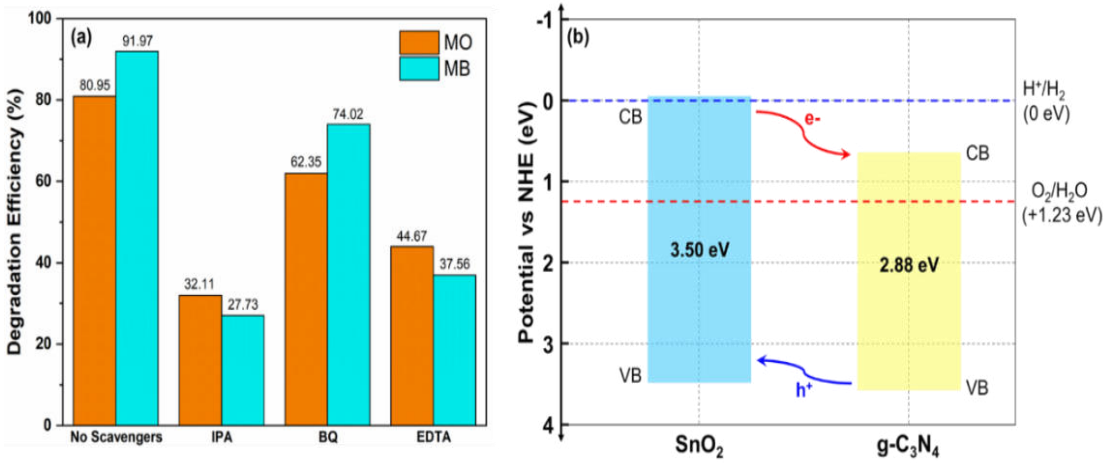


Fig. 1 (a) Scavenger study of MB and MO over the SnO_2/g-C_3N_4 /CA composite film. (b) Photodegradation mechanism illustrating the Type-II interfacial charge-transfer pathway.

Keywords: Photocatalysis, SnO_2/g-C_3N_4 composite, Cellulose acetate film, Dye degradation.

EH-006

Coordination-Induced Self-Assembly of Metallosalens Enables Sustainable Monitoring of Phytic Acid in Agricultural Foods

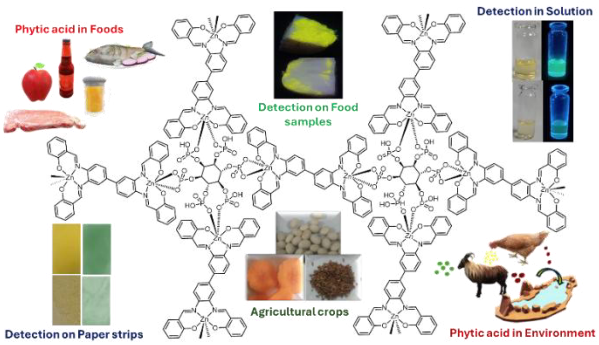
Sourav Mondal[1], Nilanjan Dey[1]*

[1]*Department of Chemistry, Birla Institute of Technology and Science Pilani, Hyderabad, Secunderabad, Telangana 500078, India.*

***Corresponding author e-mail:** nilanjan@hyderabad.bits-pilani.ac.in.

ABSTRACT

Phytic acid (PA), a naturally occurring phosphorylated anti-nutrient present in various food sources, exhibits both health benefits and adverse effects. Due to its strong metal-chelating ability, excessive intake can negatively impact human health, while its persistence in agricultural runoff also contributes to environmental pollution. Therefore, sensitive and reliable detection of PA is crucial for promoting both human well-being and sustainable development. In this study, we developed and synthesized a series of metallosalen complexes containing zinc, copper, and iron centers. The zinc-based complexes exhibited high selectivity toward PA, showing a distinct fluorescence turn-off response accompanied by a visible color change from deep yellow to faint. Mechanistic investigations revealed that the observed quenching originated from PA-induced aggregation of the complexes via coordination through phosphate groups and electrostatic interactions. Notably, the dimeric zinc complex showed a significantly stronger quenching effect than its monomeric counterpart, with a detection limit as low as 2.10 μM. In contrast, replacing zinc with iron resulted in a turn-off-to-turn-on response, attributed to demetallation of the iron complex upon PA addition, whereas the copper-based complex showed negligible interaction. Furthermore, the zinc complex with superior sensitivity was successfully applied for the quantification of PA in vegetable extracts such as carrot, soybean, and sesame seed, achieving excellent recovery rates between 97.2% and 115.2% with relative standard deviations (RSD) of 2-3.7%. Finally, a cellulose-based paper strip embedded with this zinc complex was fabricated for rapid, on-site PA detection.



References:

1. Vucenik, I., J. Nutr. Sci. Vitaminol., 65 (2019) S18–S22.
2. Thavarajah, P., See, C. T., Vandenberg, A., Food Chem., 122 (2010) 254–259.

Optimization of Hydrothermally Synthesized MoS_2 and MoS_2-GO Nanocomposite for Enhanced Uric Acid Detection

Manju Waikhom[1], Neha Batra Bali[2], Monika Tomar[3]*, H Basantakumar Sharma[1]*

[1]*Department of Physics, Manipur University, Canchipur, Imphal-795003, Manipur, India*

[2]*Department of Physics, Hindu College, University of Delhi, Delhi-110007, India*

[3]*Department of Physics, Miranda House, University of Delhi, Delhi-110007, India*

***Corresponding author e-mail:** hbslab.18@gmail.com

ABSTRACT

Uric acid, the end product of purine metabolism in humans, serves as an important clinical biomarker, with abnormal levels linked to disorders such as gout, hyperuricemia and renal dysfunction. Hence, the development of sensitive, reliable and cost-effective platforms for uric acid detection is of significant clinical importance. Molybdenum disulfide (MoS_2), a 2D transition metal dichalcogenide, has attracted considerable attention in electrochemical sensing due to its layered structure, high surface area, tunable electronic properties and excellent biocompatibility. Furthermore, integration of graphene oxide (GO) with $MoS_2$2 can generate synergistic effects by enhancing electrical conductivity, increasing active sites and improving charge transfer kinetics, thereby boosting sensing performance.

In hydrothermal synthesis, the physicochemical properties of MoS_2 are strongly dependent on precursor stoichiometry, where deviations in the Mo:S molar ratio can significantly influence crystallinity, defect density, phase composition, and surface morphology, which in turn have a pronounced impact on the electrochemical performance of the material. In this work, MoS_2 was synthesized via a hydrothermal route by systematically varying the Mo:S precursor ratio to optimize its structural and electrochemical properties. The formation, crystallinity, and phase purity of MoS_2 were confirmed using X-ray diffraction, scanning electron microscopy and Raman spectroscopy. Electrochemical characterization using cyclic voltammetry revealed that a Mo:S ratio of 1:4 exhibited superior electrochemical performance, making it highly suitable for uric acid detection. Subsequently, a MoS_2–GO nanocomposite was fabricated using the optimized MoS2 by varying the GO content. The modified electrode demonstrated enhanced electrochemical response toward uric acid detection. This study highlights the critical role of precursor ratio optimization and composite engineering in developing high-performance MoS_2-based electrochemical biosensors for sensitive and selective uric acid detection.

Reference:

1. Berwal, P.; Rani, S.; Sihag, S.; Singh, P.; Dahiya, R.; Kumar, A.; Sanger, A.; Mishra, A. K.; Kumar, V. Inorganic Chemistry Communications 2024, 159, 111833.
2. Sha, R.; Vishnu, N.; Badhulika, S. Sensors and Actuators B: Chemical 2019, 279, 53–60.

EH-008

Influence of Pyrolysis Temperature on the Characteristics of Borassus Flabellifer Fruit Husk-derived Biochar for Selective Cationic Dye Adsorption from Multi-Dye Mixtures

Mahek Rukadikar, Piyush Kumar Gupta, Abishek Barwar, Susmita Das*

Department of Chemical Engineering, National Institute of Technology Calicut, India

***Corresponding author e-mail**: susmita.82.das@gmail.com

ABSTRACT

Biochar has garnered considerable attention for its cost-effective and eco-friendly potential in removing pollutants from water, with its adsorption capacity largely governed by physicochemical characteristics influenced by pyrolysis temperature. This study investigates the influence of pyrolysis temperatures (250, 350, 550, and 750˚C) on the physicochemical characteristics and adsorption behavior of the biochars derived from Borassus flabellifer fruit husks. The resulting biochars were characterized by using FESEM-EDS, XRD, TGA, FTIR, pHPZC, and BET surface area analysis, revealing that both structural and textural characteristics improved with increasing temperature. The biochars were evaluated for their adsorption performance for anionic dye, such as methyl orange (MO) and cationic dyes, such as rhodamine B (RhB), methylene blue (MB) and malachite green (MG). Experimental results showed negligible adsorption for anionic dye, while nearly 100% removal efficiency was achieved for individual cationic dyes. The biochars were subsequently examined for their ability to selectively adsorb cationic dyes from mixed dye solutions comprising RhB, MG, MO, and MB. The system was optimized by varying biochar dosage (1-5 g/L), solution pH (3-10), and initial dye concentration (100-400 mg/L) for the selective adsorption of cationic dyes. Adsorption mechanisms and rate-limiting steps were elucidated using isotherm and kinetic models. Results indicated that lower pH, lower dye concentrations, and higher biochar dosages led to nearly complete removal. Overall, the findings highlight pyrolysis temperature as a key factor in tailoring biochar characteristics and enhancing their adsorption performance.

Keywords: Borassus Flabellifer fruit husk; Biochar; Pyrolysis temperature; Selective dye adsorption; Cationic dye, multi dye mixtures.

References:

1. B. Zhao, D. O'Connor, J. Zhang, T. Peng, Z. Shen, D. C. W. Tsang, and D. Hou, J. Cleaner Prod. 174, 977–987 (2018).
2. O. Dokkathin, P. Onsri, P. Thaveemas, A. S. Lobo, S. Kaowphong, W. Watcharin, S. Techasakul, D. Dechtrirat, and L. Chuenchom, ACS Omega 10, 43981–43994 (2025).

EH-009

High-Sensitivity Piezoelectric PVDF - Coal GO Composite for Wearable Arterial Pulse Monitoring application

S. Dinesh Kumar[1]*, Suman K Jhajharia[2], Deepa Xavier[3], V. Subramanian[3], M K Padmanabhan[4] and Roop L. Mahajan[2]

[1]*Virginia Tech India Research and Education Forum, Indian Institute of Technology Madras Research Park, Chennai – 600 113, Tamil Nadu, INDIA*

[2]*Department of Mechanical Engineering, Department of Materials Science and Engineering, Virginia Tech, Blacksburg, VA 24061, USA*

[3]*Microwave Laboratory, Department of Physics, Indian Institute of Technology Madras, Chennai, Tamil Nadu, 600 036, INDIA*

[4]*Dr. MGR Educational and Research Institute (Deemed to be University), Chennai, Tamil Nadu, 600 095, INDIA*

***Corresponding author e-mail:** dinesh.s@vtindia.in

ABSTRACT

Flexible and wearable sensors capable of continuous cardiovascular monitoring are critical for next-generation healthcare. In particular, cuff-less and non-invasive blood pressure and arterial pulse monitoring can overcome the limitations of conventional sphygmomanometers and invasive arterial cannulation, enabling comfortable and continuous assessment of cardiovascular health. In this work, we report a high-sensitivity, flexible, and self-powered piezoelectric sensor based on a poly (vinylidene fluoride) (PVDF)–coal-derived graphene oxide (C-GO) composite for real-time arterial pulse monitoring. To enhance the piezoelectric performance of PVDF through electroactive β-phase and minimizing dielectric loss and leakage currents, non-conductive C-GO is used as a nanofiller. The polymer composite films are fabricated using a solution casting method, followed by mechanical stretching and electrical poling to induce piezoelectricity. Structural and phase transformations are systematically investigated using X-ray diffraction and FTIR spectroscopy, enabling quantification of the β-phase fraction as a function of C-GO concentration. The dielectric, ferroelectric, and piezoelectric properties of the PVDF–C-GO composites are evaluated to identify the optimal concentration of C-GO for enhanced sensitivity and stable performance. By utilizing coal as the precursor, the synthesized C-GO provides a cost-effective and environmentally sustainable alternative to conventional graphite-derived graphene oxide. The PVDF–C-GO composite film demonstrates excellent flexibility and dynamic response, making it suitable for wearable health monitoring applications. The self-powered sensor is conformally attached to the brachial and radial arteries to capture real-time arterial pulse waveforms. The acquired signal is amplified and integrated using analog front-end circuitry, processed by a microcontroller, and wirelessly transmitted via Bluetooth to a smartphone for real-time monitoring. The proposed PVDF–C-GO composite sensor shows strong potential for wearable, cuff-less arterial pulse and cardiovascular monitoring applications.

Reference:

1. Y. Luo, et al., ACS Nano. 17 (2023) 5211–5295.

EH-010

Synthesis and Characterization of Transition Metal Doped Gallium Nitride for Gas Sensing Application

Pragathi Murugan, Surya Sathiyamoorthy, Samreen Fathima and Balaji Manavaimaran*

Department of Materials Science, University of Madras, Guindy Campus, Chennai- 600 025

***Corresponding author e-mail:** drbalajimaran@gmail.com

ABSTRACT

Ammonia (NH_3) gas detection is critical for industrial safety, environmental monitoring, and healthcare applications, as ammonia production exceeds 100 million tons annually and poses significant health risks at concentrations as low as 50 ppm [1]. Conventional Chemi resistive sensors require elevated operating temperatures (typically >200°C), severely limiting practical deployment and increasing power consumption [2]. Gallium nitride (GaN), a III-nitride wide bandgap semiconductor with a direct bandgap of 3.4 eV and exceptional thermal stability, represents a superior platform for room-temperature gas sensing, particularly in nanostructured form where enhanced surface-to-volume ratio facilitates efficient molecular adsorption [3,4]. Transition-metal doping, specifically iron incorporation into the GaN lattice, strategically modulates electronic structure and introduces catalytic sites to enhance charge-transfer mechanisms toward NH_3 adsorption through engineered band-gap modification. This work presents synthesis and optimization of Fe-doped GaN nanostructures with varied iron concentrations up to 10 wt% through sequential solvothermal-chemical vapor deposition (CVD) route. The solvothermal processing of gallium nitrate precursor is subjected to high-temperature ammonia nitridation at 950°C with controlled $Fe(NO_3)_3$ incorporation to achieve systematic Fe substitution into the GaN lattice. X-ray diffraction (XRD) confirms retention of hexagonal wurtzite GaN structure with composition-dependent lattice parameter modulation indicative of successful Fe incorporation in GaN. UV - visible spectroscopy, FESEM and EDAX has been used to understand the optical, morphological and elemental analysis. Chemi resistive gas-sensing performance toward NH_3 at room temperature is evaluated across all dopant concentrations. The optimized Fe-doped GaN composition exhibits room-temperature NH_3 sensing characteristics. Furthermore, the correlation between Fe doping concentration in GaN and ammonia sensing behavior, including response kinetics and selectivity, will be discussed in detail to elucidate the mechanistic pathways underlying the enhanced gas-sensing performance.

Keywords: Fe-doped GaN; ammonia gas sensor; room-temperature detection; solvothermal

References:

1. B. Shen, F. Li, Y. Xie, J. Luo, and P. Fan, Phys., 312 (2020) 112172.
2. Z. E. Slaiby and A. Ramizy, J. Optoelectron. Biomed. Mater., 12 (2020) 17–23.
3. P. Muzammil, S. M. Basha, et al., J. Supercond. Nov. Magn., 33 (2020) 2767–2771.

Machine Learning–Driven Assessment of Urbanisation and Land Surface Temperature Dynamics in Hyderabad (1994–2024) Using Multi-Temporal Landsat Data

Mallapuram Bala Chennaiah*, M Sumalatha

Department of Mechanical Engineering, V.R. Siddhartha School Engineering, Siddhartha Academy of Higher Education (Deemed to be University), Vijayawada, AP-520 007.

***Corresponding author e-mail:** chennai303.mech@vrsiddhartha.ac.in

ABSTRACT

Monitoring environmental change in fast-urbanizing regions requires the ability to process and interpret large volumes of satellite data with high spatial, spectral, and temporal variability. This study integrates remote sensing and machine learning to analyse Land Use/Land Cover (LULC) change and Land Surface Temperature (LST) dynamics in Hyderabad from 1994 to 2024 using multi-temporal Landsat 5 TM, Landsat 7 ETM+, and Landsat 8 OLI/TIRS imagery on the Google Earth Engine (GEE) platform. Three supervised classifiers—Support Vector Machine (SVM), Artificial Neural Network (ANN), and Classification and Regression Trees (CART)—were evaluated using a training sample sensitivity analysis at five sample levels (20 –100 samples per class). SVM achieved the highest accuracy across all epochs (Overall Acc uracy: 92.8–95.2%; Kappa: 0.89–0.93), outperforming ANN (OA: 88.4–90.1%; Kappa: 0.82–0.86) and CART (OA: 82.4–84.1%; Kappa: 0.76–0.78), while requiring fewer training samples to stabilise. SVM-classified maps show that built-up area increased more than 306% over the 30-year period (250 km² in 1994 → 1015 km² in 2024), while barren land decreased by 54.5%, vegetation declined by 21.8%, and water bodies increased by 62.5%. Integration of LULC and LST revealed a strong positive relationship between urbanisation and surface heating, with mean LST over built-up zones rising from 28.4°C in 1994 to 36.2°C in 2024, while vegetated and water-dominated zones remained cooler at 26–29°C and 23–26°C, respectively. The results demonstrate that machine-learning-based classification is essential for efficiently handling large geospatial datasets and reliably quantifying environmental transformation, offering evidence-based inputs for urban climate resilience and sustainable planning.

EH-012

Synthesizing High-Performance Zr-MOFs via Mixed-Linker Strategy to Enhance Rhodamine B Removal

Yi-Cyun Liu[1], Duo-Syuan Lin[1], Ming-Wei Chen[1], Chao-Wei Huang[1*]
[1]*Department of Engineering Science, National Cheng Kung University, Tainan 70101, Taiwan*
***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

Zr-based Metal-Organic Frameworks (Zr-MOFs) were synthesized using a mixed-ligand defect engineering strategy to enhance Rhodamine B (RhB) adsorption [1]. The study employed three 10 mol% substitution strategies (IML, HML, and TML) on a UiO-66-NH2 framework. The best performer was the HML-derived IP-10 (isophthalic acid substituted), which achieved the maximal BET surface area (1331.87 m2/g) and a superior RhB adsorption capacity of qe = 24.29 mg/g. The enhanced performance is attributed to optimal pore structure and hydrogen bond-assisted chemisorption[2]. Kinetic analysis confirmed the dominance of chemisorption, fitting the pseudo-second-order model [3]. IP-10 also recorded the highest intraparticle diffusion rate constant (ki = 2.8133 mg·g-1·min-1), underscoring its efficient pore accessibility. This demonstrates the potential of rational mixed-ligand design for effective environmental remediation.

References:

1. S. Jiang, L. Xu, Y. Lyu, J. Zhang, F. Wu, X. Zhang, W. Xiong, B. He, and H. Yi, Sep. Purif. Technol., 363 (2025) 132056.
2. D.-S. Lin, J.-H. Lin, T.-Y. Wang, M.-W. Chen, L.-H. Kao, W.-Y. Chen, K. Manatura, H. Yang, V.-H. Nguyen, and C.-W. Huang, J. Taiwan Inst. Chem. Eng., (2025) 106246.
3. Y.-S. Ho, J. Hazard. Mater., 136 (2006) 681–689.

EH-013

Interfacial charge transport-Engineered ZnO–g-C_3N_4 Nanocomposites for Enhanced Ammonia Detection

Pavithra Shanmugam, Subha Krishna Rao
Centre for Nanoscience and Nanotechnology Sathyabama Institute of Science and Technology, Jeppiarnagar, Chennai 600119, Tamil Nadu, India.
***Corresponding author e-mail:** subhha2010@gmail.com

ABSTRACT

High-performance gas sensors room temperature and fast response are critically important for environmental monitoring and industrial safety. Beyond conventional metal oxide-based sensors, hybrid heterostructures have emerged as promising candidates due to their tunable electronic structure and enhanced surface reactivity. Here, we report the gas sensing characteristics of a ZnO–g-C_3N_4 heterostructure and establish a clear correlation between interfacial charge transport and sensing performance. Structural analysis confirms the formation of a well-defined heterojunction between hexagonal wurtzite of ZnO nanoparticles on g-C_3N_4, providing an extended interfacial sensing area. Optical studies showed enhanced visible light absorption and a reduced band gap for the ZnO–g-C_3N_4 composite compared to pure ZnO. The enhanced sensing performance is attributed to the synergistic effect of the heterojunction formation, increased surface area, and efficient charge transfer at the ZnO–g-C_3N_4 interface. These results suggests that ZnO–g-C_3N_4 nanocomposites are promising for high-performance gas sensing applications.

Keywords: ZnO–g-C_3N_4 heterostructure, optical sensing, Fiber optic sensor, Ammonia.

References:

1. S. K. Rao, J. Alloys Compd., 838 (2020) 155603.

Synthesis and Characterization of Room Temperature, Surfactant-Free GO-Cuo Nanosheets for Photocatalytic Degradation and Antibacterial Efficacy

Saathvika Lakshmanan, Gopalakrishnan Nammalvar*

Thin film Laboratory, Department of Physics, National Institute of Technology,

Tiruchirappalli-620 015, India.

***Corresponding author e-mail**: ngk@nitt.edu

ABSTRACT

A facile, surfactant-free approach was employed to synthesize copper oxide (CuO) nanosheets anchored on graphene oxide (GO) via a simple ultrasonication-assisted method. The resulting nanocomposite was comprehensively characterized (XRD, FTIR, Raman and FESEM). The photocatalytic performance for the degradation of methylene blue (MB), methyl orange (MO) and methyl red (MR) was investigated. For the chosen concentration (10 mg/ 50 ml), methylene blue showed a decolourization of 96% in 120 min while it was 88% for methyl red (120 min) and 93% for methyl orange (120 min). The antibacterial efficacy was tested via the agar diffusion method, demonstrating enhanced zones of inhibition versus pure CuO or GO. The enhanced performance is attributed to synergistic effects: GO acts as a conductive support enhancing charge separation while CuO serves as the active photocatalyst generating reactive oxygen species (ROS) and the absence of surfactants preserves active surface sites. The novelty of this work lies in (i) surfactant-free synthesis, avoiding potential surface blockage by capping agents (ii) intimate coupling of CuO and GO nanosheets for improved charge separation (iii) dual-functionality (photocatalysis + antibacterial) in a single system. The material exhibits significant potential for wastewater remediation and for developing antimicrobial surface applications.

References:

1. Arnab Ghosh, Milon Miah, et.al., Journal of alloys and compounds, vol. 862, (2021), 158549.
2. Haixue Chen, Wei Ji, et.al., J. Mater Sci: Mater Electron, vol.32, (2021), 27564-27575.
3. Farhana Anjum, Mohamed Shaban, Muhammad Ismail*, et.al., ACS Omega, Vol.8, (2023), 17667-17687.

EH-015

Experimental Spatiotemporal Studies on Fire Spread Over Thin Solid Fuels: Observations and Mechanisms

Vinayak Malhotra[1]* and Thunaipragasam Selvakumaran[1]

[1]*Department of Aerospace Engineering, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** vinayakm@srmist.edu.in

ABSTRACT

Severe issues related to the fire-spreading phenomenon have led researchers worldwide to try different approaches for simplification. The increase in fire-related accidents has escalated the need for better operating solutions. The work presents experimental simulations conducted on transitional fire spread to improve knowledge of the spread of heterogeneous fires in both space and time. Different configurations were tested at varying surface orientations with a fixed number of external energy sources per direction. The results reflect the turbulent nature of fire spread and the disorderly burning process. The spread rate analysis highlights distinct heat source and sink effects, uncertainty involved with collective burning, along with combustion instability in the form of irregular energy transfer. The results can be utilised in designing effective fire suppressants and retardants within given fire safety norms. To gain true replication, experiments were conducted on dynamic models, linear time-invariant (LTI), linear time-variant (LTV), and the effect of spatial non-linearity was studied on non-linear dynamic models, viz., NLTI (Non-linear time-invariant) and NLTV (Non-linear time variant), to determine spreading fire behaviour and features.

References:

1. R. F. R. Lopes, M. MohammadReza, J. P. C. Rodrigues, and M. Almeida, Fire Saf. J., 141 (2023).
2. R. H. Ismail and O. H. Kharufa, Int. J. Saf. Secur. Eng., 13 (2023) 151.
3. T. Chu, W. Zeng, G. Wang, C. Chen, G. Zhang, D. Yuan, J. Wang, A. Usmani, and L. Jiang, J. Build. Eng., 99 (2025).

Novel Highly Porous Carbon Hygrogel for Selective Electrochemical Sensing Application

Sowhanthi Chandrasekar[1], Gunasekaran Venugopal[1]*

[1]*Advanced Nanomaterials and System Lab, Department of Materials Science, School of Technology, Central University of Tamil Nadu, Thiruvarur – 610 005, Tamil Nadu, India.*

***Corresponding author e-mail:** gunasekaran@cutn.ac.in

ABSTRACT

In this study, a novel electrochemical sensor based on a green synthesized porous carbon hydrogel is proposed for the sensitive and selective detection of p-Nitrophenol ($C_6H_5NO_3$). p-Nitrophenol (p-NP) is a hazardous pesticide-derived food contaminant formed as a degradation product of organophosphate pesticides and frequently detected in agricultural products and residues in food, widely used in fruits, vegetables, cereals. When these pesticides break down (sunlight, moisture, microbes), p-NP is formed and remains on crops and is strongly electroactive. Sensitive detection of p-nitrophenol, a toxic pesticide-derived food contaminant, is essential for food safety and can be effectively achieved by porous carbon hydrogel electrochemical sensors. The synergistic combination of porous carbon hydrogel matrix enhances the electroactive surface area and facilitates rapid electron transfer, which significantly improves the sensor performance. Porous Carbon Hydrogel characterized by XRD, Fourier Transform Infrared Spectroscopy, Cyclic Voltammetry and Differential Pulse Voltammetry (DPV) techniques. DPV studies reveals the electrochemical oxidation of p-NP on porous carbon hydrogel followed by a diffusion-controlled and quasi-reversible mechanism involving electron transfer process. The sensor exhibits a wide linear range of sensitivity, limit of detection (LOD) and limit of quantification (LOQ). The sensor demonstrates the selectivity against some common interferents. The practical applicability of the sensor is validated by successful quantification of p-NP in real food samples, with high recovery rates and minimal matrix effects. These findings highlight the potential of the porous carbon hydrogel platform for reliable electrochemical detection of p-NP in complex food matrices.

Keywords: Porous Carbon Hydrogel, p-Nitrophenol, Food Contaminant, Electrochemical Sensor, Cyclic Voltammetry, Differential Pulse Voltammetry.

References:

1. Yang, C., Li, P., Wei, Y., Wang, Y., Jiang, B., & Wu, W. (2023) 14(5), 1003.
2. Bashir, S., Hina, M., Iqbal, J., Rajpar, A. H., Mujtaba, M. A., Alghamdi, N. A., Wageh, S., Ramesh, K., & Ramesh, S. (2020) 12(11), 2702.
3. Zhao, M., Wu, T., Han, J., Li, F., & Zhao, H. (2025), 1–12.

EH-017

Electrocoagulation for Sustainable Tannery Wastewater Treatment: Modeling, Optimization, and Reactive Species Analysis

Shiv Om Meena*, Sanjeev Kumar Meena, Vikas K. Sangal

Department of Chemical Engineering, Malaviya National Institute of Technology, Jaipur – 302017

***Corresponding author e-mail:** someena.chem@mnit.ac.in

ABSTRACT

Tannery wastewater contains high organic loads and toxic contaminants that challenge conventional biological treatment. This study investigates electrocoagulation (EC) as a sustainable process for the treatment of synthetic tannery wastewater with a focus on Total Organic Carbon (TOC) and Chemical Oxygen Demand (COD) removal. Response Surface Methodology using Box–Behnken Design was employed to optimize key operating parameters (pH, current, and reaction time) for maximum performance with minimum energy demand. Under optimized conditions, EC achieved 86.1% COD and 48.2% TOC removal with an energy consumption of 12.2 kWh/m³. Kinetic studies showed pseudo-first-order behaviour for pollutant removal. An ANN-based predictive model further improved process forecasting, with the Levenberg–Marquardt model (10 neurons) showing highest accuracy. Scavenger tests confirmed the dominance of •OH, SO4•–, and O2•– radicals in pollutant degradation. FTIR and XRD characterization validated the stability of the produced sludge. Overall, EC with iron electrodes is an efficient and clean technology, offering a promising pathway for sustainable wastewater treatment.

Keywords: artificial neural network, chemical oxygen demand, electrocoagulation, tannery wastewater,

References:

1. M., S. K., M., S. O., and S., V. K. Journal of the Indian Chemical Society, 101(8), 101212 (2024).
2. Y., F., W., X.-B., S., Y., W., C., Z., R., H., N., P., F., and J., Y. Collagen and Leather, 5(1), 24 (2023).
3. Z., J., W., Q., T., Y., Z., J., G., and H. Journal of Leather Science and Engineering, 4(1), 10 (2022).

Enhanced Performance of Tungsten Oxide Gas Sensors through Bismuth Doping: A Pathway to Reduced Operating Temperature

D. Kanchan Kumar[1], A. Govind[2], P. Bharathi[2], J. Archana[1], M. Navaneethan*[1,2], S. Harish*[1,2]

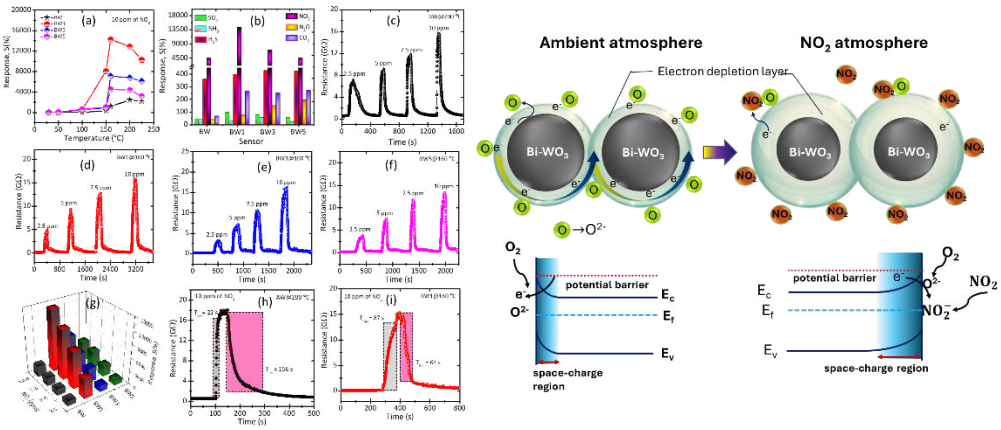
[1] *Centre of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India.*

[2] *Nanotechnology Research Centre (NRC), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India.*

***Corresponding authors' e-mail:** m.navaneethan@gmail.com; aravindharri@gmail.com

ABSTRACT

Engineering defect states in metal oxide semiconductors (MOS) provides an effective route to tailor their electronic structure and chemical activity for low-power gas sensing. Nevertheless, achieving both high response and rapid recovery remains a persistent challenge for MOS-based NO_2 sensors. This study, assess the role of bismuth (Bi) into tungsten trioxide (WO_3) to address these limitations. Notably, the 1 mM% Bi-doped sensor delivers an exceptional response of 14303% towards 10 ppm NO_2 at 160 °C, representing a seven-fold improvement over pristine WO_3. The device further exhibits excellent repeatability, high selectivity, and outstanding long-term stability (97% retention over 8 weeks). Further, Bi introduction accelerates the recovery process, reducing the response-reset time to 64 s compared to 156 s for the pristine sensor. These enhancement stems from the oxygen-vacancy-induced increase in surface reactivity, which strengthens gas-solid interactions. Overall, this study demonstrates the promise of defect-engineered WO_3 for reliable environmental NO_2 monitoring.



Keywords: Defect Engineering, Bi-doped WO_3, Metal oxide semiconductor, Chemiresistive NO_2 sensing, Low-Temperature gas sensors.

EH-019

Enhanced Electrochemical Response of Sol-Gel TiO_2/rGO Electrodes for PFAS Sensing

Abishek M[1], Roshan S[1], Pravin T U[1], Dharani Priya P K[2], Muthuvel V[2], Anil Kumar K K[1], Arul H[2]*

[1]*Department of Electronics and Instrumentation Engineering, Kumaraguru College of Technology, Coimbatore, Tamil Nadu, India- 641049*

[2]*Department of Physics, School of Foundation Sciences, Kumaraguru College of Technology, Coimbatore, Tamil Nadu, India- 641049*

***Corresponding author e-mail**: arul.h.sci@kct.ac.in

ABSTRACT

The development of energy-efficient, sensitive and reliable electrochemical sensors for monitoring Per- and polyfluoroalkyl (PFAS) substances concentrations has garnered considerable attention in recent years. PFAS represent a diverse group of synthetic fluorinated compounds for their environmental longevity and bioaccumulative potential, necessitating rapid on-site detection. In this work, we have discussed the PFAS sensing properties of a reduced graphene oxide (rGO)–TiO_2 nanocomposite serves as the core of an electrochemical sensor designed for sensing in aqueous samples. TiO_2 synthesized via Sol-gel chemistry and rGO derived from the Hummers method were prepared as a nanocomposite. This nanocomposite was applied to glassy carbon via spin coating, yielding stable electrodes. XRD, UV-DRS, Raman, FE-SEM, TGA and Electrochemical sensing analysis were done for the samples. From SEM, it is evident that the rGO and TiO_2 had interconnection bridges between adjacent nanocomposites, which is anticipated to enhance electron–hole separation by facilitating electron transfer. The electrochemical results indicated that the TiO_2-rGO enhanced the electrochemically active surface area for the prepared electrode and significantly improved the electrochemical response. The rGO matrix accelerates carrier mobility, while TiO_2 facilitates targeted analyte binding through surface hydroxyls and defects. Tested on synthetic PFAS solutions, this platform exhibited robust signal amplification under ambient conditions, positioning spin-coated TiO_2–rGO as a viable, economical tool for initial PFAS assessment in polluted waters and advancing portable environmental diagnostics. As a PFAS sensor, the composite showed excellent results with its resistance changing multiple times under exposure to PFAS. A fast response time and recovery time were observed.

References:

1. S. Bandi et al., Bull. Mater. Sci., 41 (2018) 115.
2. X. Li et al., Sens. Actuators B, 230 (2016) 330.
3. N. Chaurasiya et al., Sens. Diagn., 2 (2023) 1215.
4. D. R. Dreyer et al., Chemical Society Reviews, 39 (2010) 228.
5. Z. Wang et al., Environmental Science & Technology, 51 (2017) 2508.

EH-020

Low-Cost Spin-Coated ZnO–rGO Thin-Film Electrodes for Portable Electrochemical Detection of PFOA in aqueous Systems

Roshan S[1], Abishek M[1], Sanjay S[1], Dharani Priya P K[2], Muthuvel V[2], Anil Kumar K K[1], Arul H[2]*

[1]*Department of Electronics and Instrumentation Engineering, Kumaraguru College of Technology, Coimbatore, Tamil Nadu, India- 641049*

[2]*Department of Physics, School of Foundation Sciences, Kumaraguru College of Technology, Coimbatore, Tamil Nadu, India- 641049*

***Corresponding author e-mail:** arul.h.sci@kct.ac.in

ABSTRACT

Perfluorooctanoic Acid (PFOA) are environmentally persistent contaminants for which routine monitoring remains dependent on laboratory-based chromatographic methods that are costly and unsuitable for on-site analysis. A Zinc Oxide-Reduced Graphene Oxide (ZnO-rGO) nanocomposite sensor is synthesized, fabricated and evaluated electrochemically for PFOA detection. ZnO nanoparticles were synthesized via a Sol-gel route and reduced graphene oxide (rGO) was prepared by the Hummers method. Cubic Phase Zinc Oxide and Hexagonal Phase reduced Graphene Oxide were combined to form a nanocomposite, which was then spin-coated onto a glassy carbon substrate to produce the sensing electrode. Powder X-Ray Diffraction, Fourier Transform Infrared Spectroscopy, Molecular Vibration Analysis (Raman) Spectroscopy, UV-DRS Reflectance Spectroscopy, X-ray Photoelectron Spectroscopy, Thermo-Gravimetric Analysis (TGA) and Field-Emission Scanning Electron Microscopy and Electrochemical sensing Analysis were done. ZnO particles were integrated within a reduced graphene oxide matrix to form a ZnO–rGO composite. Electrochemical studies demonstrated that ZnO–rGO electrodes exhibited lower charge-transfer resistance compared to pure ZnO electrodes, indicating improved conductivity and electron transport. All measurements were conducted using a standard three-electrode configuration. The ZnO–rGO electrode produced a higher current response in PFOA-containing solutions than ZnO or graphene oxide electrodes, confirming enhanced electrochemical activity and surface interaction. The sensor electrode was fabricated through a simple, solution-based spin coating process, enabling straightforward electrode preparation. Measurements were performed on laboratory-prepared PFOA solutions, and parameters such as detection limit and long-term stability were also evaluated. These results indicate that ZnO–rGO composites are promising candidates for preliminary electrochemical detection of PFOA in aqueous systems.

References:

1. O. Jongprateep et al., Scientific Reports, 14 (2024) 14224.
2. M. E. Naghani et al., Scientific Reports, 13 (2023) 1496.
3. Haiwei Fu et al., Sensors and Actuators B 254 (2018) 239.
4. Gloria B. Post et al., Environ. Res., 116 (2012) 93.
5. Patrick Severin Sfragano et al., Biosens Bioelectron X,28 (2025) 100726

EH-021

Evaluation of Raw and Boiled Eggshell Powders as Renewable Biosorbents for Efficient Uranium (VI) Removal

Akash B V[1], Vaishnavi S[2], Kirthika J[2], Dr. Ilaiyaraja Perumal[1]*

[1]*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology Chennai Campus, Tamil Nadu, 600127, India.*

[2]*Centre for Advanced Materials and Innovative Technologies, Vellore Institute of Technology Chennai Campus, Tamil Nadu, 600127, India.*

***Corresponding author e-mail:** ilaiyaraja.perumal@vit.ac.in

ABSTRACT

Uranium contamination in wastewater poses significant environmental and health problems due to its high toxicity and mobility, highlighting the need for affordable and sustainable treatment materials. Among various alternatives, converting agro-waste into functional adsorbents has gained increasing attention because of its low cost and environmental benefits. Eggshell waste, abundant and naturally rich in $CaCO_3$, offers a promising and eco-friendly option for large-scale uranium removal. Building on this concept, the present study investigates the adsorption performance of raw and boiled eggshell powders for U(VI) removal from aqueous solutions. Comprehensive characterization using FTIR, XRD, SEM–EDS, BET and pHPZC analyses was conducted to elucidate the structural, morphological and surface chemistry differences between the two materials. This systematic evaluation focuses on assessing the suitability of eggshell-derived materials as low-cost biosorbents, with emphasis on how surface properties, functional groups and $CaCO_3$ composition influence U(VI) uptake. Additionally, kinetic and isotherm modeling was employed to gain insight into the interaction mechanisms between U(VI) ions and eggshell surfaces. Overall, this work advances the development of sustainable, waste-derived materials for radioactive wastewater treatment and demonstrates a practical route for converting eggshell waste into a value-added environmental adsorbent.

Keywords: Uranium (VI), Eggshell waste, Adsorption.

EH-022

Conducting Polymer-Based Flexible Electrodes for Non-Invasive Electrochemical Biomolecule Detection

Nivethitha Kumarasamy[1], Bernaurdshaw Neppolian[1]*

[1]*Energy and Environmental Remediation Laboratory, Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India.*

***Corresponding author e-mail:** neppolib@srmist.edu.in

ABSTRACT

Early and accurate detection of biomolecules is crucial for diagnosing and monitoring human health conditions. In this context, non-invasive and minimally invasive sensing techniques have gained significant attention due to their patient-friendly nature and real-time monitoring capability. Biomolecules produced in the human body regulate metabolic activities through a balanced internal environment known as homeostasis. Any disruption in this balance alters biomolecule concentrations, leading to various pathological conditions. Therefore, precise analysis of biomolecular concentrations plays a vital role in clinical diagnostics. Electrochemical sensing has emerged as a simple, cost-effective, and highly sensitive technique with excellent multiplexing capability for biomolecule detection. Recently, flexible electrode materials have attracted growing interest due to their lightweight nature, mechanical flexibility, biocompatibility, and seamless integration with biological tissues. These features enable their application in wearable and disposable biosensors, skin-mounted sensor patches, and smart healthcare devices. Among flexible electrode materials, conducting polymers have received considerable attention owing to their unique electrical and structural properties. Unlike conventional insulating polymers composed of sp3-hybridized carbon atoms, conducting polymers consist of sp2-hybridized carbon frameworks with π-conjugated systems, enabling efficient charge transport. Their electrical conductivity can be further enhanced through doping during oxidative or electrochemical polymerization. Additionally, the tunable surface chemistry, high electroactive surface area, and excellent mechanical stability of conducting polymers significantly improve sensor sensitivity, selectivity, and reproducibility. Based on these advantages, conducting polymer-based flexible electrodes were fabricated and systematically evaluated for their electrochemical performance, demonstrating their potential as efficient platforms for advanced biomolecule sensing applications.

References:

1. M. Daniel, C. Yazhini, S. Peters, T. Sadhukhan, K. Sekar, and B. Neppolian, Chem. Mater., 36 (2024) 6925.
2. M. Eswaran, S. Rahimi, S. Pandit, B. Chokkiah, and I. Mijakovic, Fuel, 345 (2023) 128182.
3. B. Sriram, S. Shajahan, Y. Hsu, S.-F. Wang, and M. A. Haija, ACS Appl. Nano Mater., 6 (2022) 1.

EH-023

MXene-Modified Metal-Organic Frameworks for Non-Invasive Electrochemical Detection of Serotonin

Bhuvaneshwari Shanmugaraj, Bernaurdshaw Neppolian*

Energy and Environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India.

***Corresponding author e-mail:** neppolib@srmist.edu.in

ABSTRACT

Non-invasive and reliable detection of biomolecules is critically important for early diagnosis and monitoring of neurological disorders. Among various neurotransmitters, serotonin (5-Hydroxytryptamine) plays a pivotal role in regulating mood, cognition, and physiological functions. However, its abnormal concentration is associated with disorders such as depression, anxiety, and neurodegenerative diseases. Despite its significance, accurate detection of serotonin remains challenging due to its low physiological concentration, interference from coexisting biomolecules, and instability in biological environments. Electrochemical detection has emerged as a promising approach owing to its high sensitivity, rapid response, and suitability for miniaturized and non-invasive sensing platforms. Two-dimensional MXenes have recently attracted considerable attention for electrochemical serotonin sensing due to their high electrical conductivity, large surface area, and abundant surface terminations. Nevertheless, pristine MXenes suffer from intrinsic limitations such as restacking, surface oxidation, limited active sites, and conceded long-term stability, which restrict their sensing performance. To overcome these challenges, we report a novel MXene-modified metal-organic framework (MXene@MOF) nanocomposite designed to synergistically enhance electrochemical serotonin detection. MOF-modified MXene prevents restacking while increasing active sites and surface area for efficient serotonin oxidation. The developed MXene@MOF-based sensor demonstrates excellent analytical performance, including a low detection limit, high sensitivity, and robust operational stability. This work highlights a strategic materials-engineering approach that addresses the inherent limitations of MXenes while unlocking their full potential for non-invasive electrochemical serotonin sensing.

References:

1. M. Daniel, C. Yazhini, S. Peters, T. Sadhukhan, K. Sekar, and B. Neppolian, Chem. Mater., 36 (2024) 6925.
2. K. Amarnath, T. S. Gopal, A. C. J. Malathi, S. Pandiaraj, M. Alruwaili, A. Alshammari, A. N. Alodhayb, C. Abeykoon, A. N. Grace, and V. G. Kumar, ACS Appl. Nano Mater., 8 (2025) 12661.

Electrochemical Monitoring of Nitrofurantoin as an Emerging Antibiotic Pollutant Using Transition Metal Chalcogenides

Sundari Devi Saminathan, Bernaurdshaw Neppolian*

Energy and Environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603 203, India.

***Corresponding author e-mail:** neppolib@srmist.edu.in

ABSTRACT

The extensive use of antibiotics and their incomplete metabolism have led to the persistent accumulation of pharmaceutical residues in natural ecosystems, posing serious risks to environmental and public health. Among these emerging contaminants, nitrofurantoin is a widely prescribed nitrofuran antibiotic, which has attracted growing concern due to its chemical stability, bioaccumulation tendency, and potential toxicity. Consequently, the development of rapid, sensitive, and reliable analytical tools for its on-site monitoring is critically required to mitigate future environmental threats. Electrochemical sensors have emerged as promising platforms for pollutant detection owing to their cost-effectiveness, high sensitivity, operational simplicity, and excellent selectivity. In this regard, transition metal chalcogenides (TMCs) have gained significant attention as electrode materials because of their intrinsic catalytic activity, abundant redox-active sites, and high surface-to-volume ratio, which facilitate strong interactions with functional groups present in antibiotic molecules. However, the practical sensing performance of pristine TMCs is often limited by poor conductivity, surface passivation, and sluggish charge-transfer kinetics. To overcome these limitations, heteroatom modulation and compositional engineering like oxides and sulphides, offer an effective strategy to tailor the electronic structure, enhance active-site density, and improve adsorption-driven electrochemical responses. In this work, we present a novel TMC-based electrochemical sensing platform for the ultrasensitive and selective detection of nitrofurantoin. The proposed design demonstrates improved charge-transfer behaviour, and superior sensing performance, highlighting its potential for real-time environmental monitoring of antibiotic pollutants.

References

1. S. P. Selvam, S. Vinothini, S.-M. Chen, and T. W. Chiu, ACS Appl. Nano Mater., 8 (2025) 23701.

EH-025

Synthesizing High-Performance Zr-MOFs via Mixed-Linker Strategy to Enhance Rhodamine B Removal

Yi-Cyun Liu[1], Duo-Syuan Lin[1], Ming-Wei Chen[1], Chao-Wei Huang[1]*

[1]*Department of Engineering Science, National Cheng Kung University, Tainan 70101, Taiwan*

***Correspoonding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

Zr-based Metal-Organic Frameworks (Zr-MOFs) were synthesized using a mixed-ligand defect engineering strategy to enhance Rhodamine B (RhB) adsorption[1]. The study employed three 10 mol% substitution strategies (IML, HML, and TML) on a UiO-66-NH2 framework. The best performer was the HML-derived IP-10 (isophthalic acid substituted), which achieved the maximal BET surface area (1331.87 m^2/g) and a superior RhB adsorption capacity of qe = 24.29 mg/g. The enhanced performance is attributed to optimal pore structure and hydrogen bond-assisted chemisorption[2]. Kinetic analysis confirmed the dominance of chemisorption, fitting the pseudo-second-order model[3]. IP-10 also recorded the highest intraparticle diffusion rate constant (ki = 2.8133 $mg \cdot g^{-1} \cdot min^{-1}$), underscoring its efficient pore accessibility. This demonstrates the potential of rational mixed-ligand design for effective environmental remediation.

References:

1. Jiang, S.; Xu, L.; Lyu, Y.; Zhang, J.; Wu, F.; Zhang, X.; Xiong, W.; He, B.; Yi, H. Sep. Purif. Technol. 363 (2025) 132056.
2. Lin, D.-S.; Lin, J.-H.; Wang, T.-Y.; Chen, M.-W.; Kao, L.-H.; Chen, W.-Y.; Manatura, K.; Yang, H.; Nguyen, V.-H.; Huang, C.-W. J. Taiwan Inst. Chem. Eng. (2025) 106246.
3. Ho, Y.-S. J. Hazard. Mater. 136 (2006) 681–689.

EH-026

Bimetallic MOF Derived Metal Oxide Based Chemiresistive No_x Gas Sensor

S. Poovarasan[1] , H.Yuvaraj[2], R.T. Rajendrakumar[1]*

[1]*Advanced Materials and Devices Laboratory, Department of Nanoscience and Technology, Bharathiar University, Coimbatore – 641046, Tamil Nadu.*

[2]*Department of Chemistry (SF), PSG College of Arts and Science, Coimbatore 641 014, Tamil Nadu*

ABSTRACT

Zn-Fe bimetallic MOF was synthesized by in-situ solvothermal method. We optimized Zn-Fe MOF composite by stoichiometric variations. Synthesized composites were modified MOF into metal oxides via thermal treatment and characterized by physicochemical characterization techniques. All of the synthesized oxides were highly selective for NOx gas across other VOCs. Zn-Fe 1:1 composite sensor material showed high sensitivity for 5ppm NOx gas a response of 15% with 100 sec of response and recovery time. LOD of the sensing material was 1ppm. Sensor exhibits good stability during the stability check over 30 days. Then, the sensing mechanism was discussed in depth.

Comparative Screening of Metal Oxides for Nitrate Removal from Aqueous Solutions

Subhasini D. C.[1], Meenal S. Deo*[1]

[1] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** meenald@srmist.edu.in

ABSTRACT

Global nitrate contamination, spurred by agricultural and industrial activities, poses severe risks to groundwater. The World Health Organization (WHO) has established a maximum contaminant level (MCL) for nitrate in drinking water, setting the safe limit at 50 mg/L1. Prolonged exposure to elevated nitrate levels in drinking water has tremendous health effects on human beings and demands research for efficient nitrate removal adsorbents. The remarkable adsorption properties and efficacy of metal oxide nanoparticles have gained considerable interest in their potential for water treatment applications2. Our study aimed to examine nitrate ion removal by various metal oxides (Mn_2O_3, Co_3O_4, NiO, CuO, ZnO and P25) in an aqueous solution. The metal oxide nanoparticles were synthesized by the co-precipitation method, and the morphology, crystal structure, and surface area of the synthesized nanoparticles were characterized by X-ray diffraction (XRD), High-Resolution Transmission Electron Microscopy (HRSEM), and Brunauer-Emmett-Teller (BET). The optimal adsorbent dosage, and the effect of contact time, initial nitrate concentration, and co-existing anions on nitrate adsorption were studied in a batch model. The experimental data were fitted to widely used adsorption kinetic models and adsorption isotherms. Desorption and regeneration studies were carried out to examine the ability to release and recover nitrate ions from the adsorbent. Also, the influence of co-existing ions on the adsorption of nitrate was studied. Our study highlights the potential of metal oxide nanoparticles as a viable and promising adsorbent for nitrate ion removal in water, offering an effective solution for the water treatment process.

References:

1. World Health Organization. Guidelines for Drinking-Water Quality, Vol. 33. World Health Organization, 2022.
2. Ghosh, N.; Das, S.; Biswas, G.; Haldar, P. K. Water Sci. Technol. 85 (2022) 3370–3395.

EH-028

Plasma-Induced g-C_3N_4/BC-Derived LIG Electrodes for AChE-Assisted Pesticide Detection

Saranvignesh Alagarsamy[1], and Ying-Chih Liao[1]*

[1]*Department of Chemical Engineering, National Taiwan University, Taiwan*

***Corresponding author e-mail:** saranvignesh1507@gmail.com

ABSTRACT

A sustainable biosensor platform was developed through the strategic integration of natural precursors, surface modification, and ambient-condition processing. Bacterial cellulose (BC), chosen for its biodegradability and structural purity, was first functionalized with matcha extract to enhance its carbonization potential. Nitrogen-rich graphitic carbon nitride (g-C_3N_4) was then incorporated to introduce electronic functionality and nitrogen doping capacity. To further activate the surface and promote uniform dispersion of g-C_3N_4, the composite was treated with low-temperature plasma, creating defect sites favorable for graphitic conversion. Laser-induced graphene (LIG) formation was subsequently achieved using CO_2 laser irradiation, producing porous, conductive films with interconnected carbon networks. Silver nanoparticles (AgNPs) were deposited to boost electrocatalytic properties, and acetylcholinesterase (AChE) was immobilized to impart selective recognition of organophosphate pesticides via enzyme inhibition.

The resulting Ag-PA-LIGgC_3N_4 biosensor demonstrated high sensitivity, excellent selectivity, and strong operational stability under voltammetric analysis. This multi-step, yet chemical-free and eco-compatible process offers a practical route toward high-performance, flexible electrochemical sensors. The work underscores the feasibility of combining natural dopants, mild plasma activation, and laser patterning to develop biodegradable sensing devices suited for environmental and agricultural diagnostics.

References:

1. Tun, W. S. T.; Saenchoopa, A.; Daduang, S.; Daduang, J.; Kulchat, S.; Patramanon, R. RSC Adv. 13 (2023) 9603–9614.
2. Butler, D.; Kammarchedu, V.; Zhou, K.; Peeke, L.; Lyle, L.; Snyder, D. W.; Ebrahimi, A. Sens. Actuators B Chem. 378 (2023) 133090.

Removal of Reactive Dyes from Water by PANI–$CoCl_2$ Composite: Kinetic, Isotherm, and Thermodynamic Studies

Lingeswari Dheenathayalan[1]*,

[1]*Karpagam Academy of Higher Education, Coimbatore, Tamilnadu, India, 641005*

***Corresponding author e-mail:** udlingeswari@gmail.com

ABSTRACT

This research examines the decolourisation of organic dyes, particularly reactive dyes, from aqueous media using a PANI–$CoCl_2$ composite as an adsorbent. Polyaniline (PANI) is recognized as an efficient conducting polymer owing to its proton-doping capability, excellent redox reversibility, high chemical stability, tunable electrical conductivity, cost-effectiveness, and ease of synthesis. The structural features and surface morphology of the PANI–$CoCl_2$ composite were characterized through scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy. The findings indicate that the dye adsorption performance is significantly affected by various operational parameters, including adsorbent dosage, contact duration, solution pH, agitation speed, initial dye concentration, and temperature. The regeneration and reuse potential of the adsorbent were assessed through recyclability studies. Kinetic analysis revealed that the adsorption of reactive dyes onto the PANI–$CoCl_2$ composite follows a pseudo-second-order kinetic model. Furthermore, equilibrium adsorption data exhibited the best agreement with the Langmuir isotherm model, as validated by correlation coefficients obtained using ANOVA analysis. Thermodynamic parameters, including changes in Gibbs free energy, enthalpy, and entropy, were also determined to elucidate the feasibility and underlying nature of the adsorption process.

Keywords: Adsorption, reactive dyes, ANOVA, PANI-CoCl2, kinetics.

References:

1. Haradhan Kolya, Chun-Won Kang, Discover water, 5(2025), 1-20
2. Zhaona Liu, Make Li, Yangyang Zheng, Huacheng Zhang, Polymers (Basel), 17(2025):2357.
3. Marwa Magdya, Mohamed M. Aboelnga, RSC Adv., 15(2025), 19843-19858

EH-030

Tailoring the Physico-Chemical Characteristics of SnO_2-Based Binary & Ternary Oxide Nanocomposites for Selective Gas Sensing: A New Strategy by Light Activation

Venkatesh M[1,3], Madeswaran S[2], Atul Thakre[3]*

[1]*Department of Physics, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu-632014, India.*

[2]*TP Solar Ltd, Tirunelveli, Tamil Nadu-627352, India*

[3]*Centre for Functional Materials, Vellore Institute of Technology, Vellore, Tamil Nadu-632014, India.*

***Corresponding author e-mail:** atul.thakre@vit.ac.in

ABSTRACT

Inherent lower selectivity and high operating temperature of metal oxide resistive gas sensors pose critical limitations, restricting their practical deployment in real-world applications. Although SnO_2 nanoparticles are electron-rich oxides, surface reactions often limit effective interactions between gas molecules and the oxides at room temperature. To address these challenges, heterostructures offer a promising strategy, leveraging the individual oxides' catalytic properties to enhance sensor response, sensitivity, and selectivity toward several volatile organic compounds (VOCs). In this study, we propose novel CuO/ZnO/SnO_2 heterostructures synthesized by the solid-state reaction method, and this work aims at selective VOC detection, wherein light activation further amplifies sensor sensitivity compared to conventional thermal activation. X-ray diffraction analysis confirms the preservation of the rutile tetragonal structure of SnO_2, and the incorporation of CuO and ZnO does not induce any phase transformations, resulting in well-defined heterostructures. Raman spectroscopy reveals the characteristic rutile SnO_2 structure, with the most intense peak observed at 624 cm^{-1} corresponding to the A1g mode, alongside the formation of CuO and ZnO. The surface adsorption–desorption kinetics and pore size distribution were systematically investigated to gain deeper insight into the interactions between gas molecules and SnO_2-based heterostructure oxide materials. Furthermore, X-ray photoelectron spectroscopy (XPS) and electron paramagnetic resonance (EPR) analyses corroborate the presence of abundant oxygen vacancies and chemisorbed oxygen species, with the observed spin-orbit splitting of 8.4 eV confirming SnO_2 formation. The heterostructures' charge transport and interface mechanisms were studied using UV light-illuminated I-V characteristics and Hall measurements. The effect of humidity was also studied between the range of 20% - 85% RH. Collectively, these SnO_2-based heterostructures exhibit superior surface reactivity and enhanced physicochemical properties, establishing them as highly promising candidates for next-generation VOC sensors in real-world applications.

Keywords: Selectivity, Light activation, Oxygen vacancies, Humidity effect, Heterostructures.

EH-031

Electrocatalytic Reduction of Carbon Dioxide Over Copper Delafossite Complex Electrode Surface

Subramanian Sakthinathan[1,2]*, Sivaramakrishnan Vinothini[1,2], Te-Wei Chiu[1,2]*

[1]*Department of Materials and Mineral Resources Engineering, National Taipei University of Technology, No. 1, Sec. 3, Chung-Hsiao East Road, Taipei, 106, Taiwan.*

[2]*Institute of Materials Science and Engineering, National Taipei University of Technology, No. 1, Sec. 3, Chung-Hsiao East Road, Taipei, 106, Taiwan.*

***Corresponding author e-mail:** sakthinathan1988@gmail.com, tewei@ntut.edu.tw

ABSTRACT

Carbon dioxide (CO_2) is primarily responsible for the greenhouse effect attributable to human and industrial activity. Various methods are currently under investigation for CO_2 reduction and conversion. Furthermore, CO_2 is converted to valuable products, including methane, ethane, carbon monoxide, and hydrogen, via electrocatalytic reduction. A catalyst plays a leading role in the electrochemical reduction of CO_2 into valuable chemicals and fuels. Therefore, the preparation of highly active, low-coat catalysts is of interest to both academia and industry. The electrochemical reduction of CO_2 was performed on electrodes in an H-type cell, and the faradaic efficiency of this system was evaluated. In this work, we have prepared copper delafossite complexes $CuLaO_2$, $CuCeO_2$, $CuSmO_2$, $CuGdO_2$, and $CuTbO_2$. The surface morphology was characterized and confirmed using appropriate physical and chemical methods. Electrochemical studies and CO_2 reduction performance will be performed using electrochemical impedance spectroscopy, cyclic voltammetry, linear sweep voltammetry, controlled-potential electrolysis, and chronoamperometry. $CuCeO_2$ complex catalyst produces high H2, some formic acid, acetic acid, and also very small CO in an H-type (pH 7) cell. It is the best candidate for CO_2 reduction when parameters such as potentials, pH, cell type, and interface design are optimized. Moreover, Cu-CeO_2 catalysts combine both Cu (Cu^{+}/Cu^{0}) and CeO_2 (Ce^{4+}/Ce^{3+}), readily form oxygen vacancies (Ce^{3+} sites), and have highly active sites that attract CO_2 molecules. However, $CuCeO_2$ exhibited high electrocatalytic activity for CO_2 reduction, with low overpotential, high Faradaic efficiency, high current density, good stability, high surface area, and interconnected electrical conductivity. Moreover, the results obtained will be compared with those previously reported for catalysts and conversion efficiency. The other compounds, $CuLaO_2$, $CuSmO_2$, $CuGdO_2$, and $CuTbO_2$, have limited data on their catalytic performance for CO2 reduction; from a practical perspective, $CuCeO_2$ is the most well-established for this process.

References:

1. R. Z. Xiong, H. M. Xu, H. R. Zhu, Z. J. Zhang, G. R. Li, Chem. Eng. J., 505 (2025) 159210.
2. Q. Zhu etal, Nat. Commun, 3851 (2019).
3. K. Kim, P. Wagner, K. Wagner, A. J. Mozer, Energy Fuels, 36 (2022) 4653-4676.

EH-032

SecureVision-Pro: A Real-Time AI Surveillance Suite for Violence, Hazard, and Safety Detection with Audio-Visual Intelligence

M.Hema[1], H.Varshini[1]*, Tharun.B[1]

[1]*Easwari Engineering College, Ramapuram, Tamilnadu, India, 600089*

***Corresponding author e-mail:** varshinih1804@gmail.com

ABSTRACT

The surveillance systems are believed to be very effective in keeping the people safe and the operations safe, but most of the conventional systems are merely the monitors and lack multiple modes and real time on the threat detection end. This paper presents the prototype which is an artificial intelligence AI -based surveillance system called SecureVision-Pro that merges visual and audio based methods of detecting an incident in a holistic and accurate way. It relies on the YOLOv11 to identify real-time violent activities, fire, smoke, and falls, as well as personal protective equipment PPE violation with the help of strong facial-recognition engine DeepFace and violent audio gunshots, screams, explosions, etc. detection with the help of Librosa-based models. The live CCTV streams, webcams, recorded video, and the audio streams will be easily processed with a modular architecture. The output layer offers annotated visual feeds, multi-channel real-time alerts and structured email and audio alerts through the form of JSON reports. Experimental analysis shows that the multi-modal fusion methodology is significantly superior at decreasing the false alarms, maintaining consistent frame rates and constant load, and producing alerts with a low-latency. The findings of these tests are the predeterminants of the inclusion of SecureVision-Pro in the list of the potential solutions to the issue of monitoring the smart cities and controlling the safety of industries, along with home surveillance.

References:

1. Redmon J. et al., IEEE CVPR, vol. (2016), pp. 779–788.
2. Bochkovskiy A. et al., arXiv preprint, (2020).
3. McFee B. et al., Librosa: Audio and Music Signal Analysis, SciPy Conf., (2015).
4. LeCun Y. et al., Nature, vol. 521 (2015), pp. 436–444.
5. Zhao Z. et al., IEEE Access, vol. (2021), pp. 102345–102356.

Real-Time Cyberbullying Detection and Reporting System with Multimodal Analysis and Secure AI-Powered Interface

Shreya Gloria Victoria F*, Sanjay R, G.Maria Kalavathy

SRM Easwari Engineering College, Ramapuram, Tamilnadu, India, 600089

***Corresponding author e-mail:** shreyagloria032004@gmail.com

ABSTRACT

Cyberbullying on social media has emerged as a serious global issue, made more difficult to detect due to the brevity, informality, and ambiguity of online communication. Traditional detection methods often struggle to differentiate overlapping and vague expressions, leading to reduced accuracy. To overcome these limitations, this work introduces a hybrid cyberbullying detection framework that integrates Neutrosophic Logic into a Multi-Layer Perceptron (MLP) classifier.

The proposed system ensures user security through MATLAB-based face detection and verification at the login stage. Once authenticated, users are redirected to the analysis interface, where Twitter data is collected using keywords, hashtags, or user handles. The preprocessing module removes stop words, hashtags, links, and emojis. The text is then tokenized using the BERT Tokenizer, and contextual embeddings are generated with the bert-base-uncased model to capture the semantic meaning of sentences.

For classification, a one-against-one strategy is employed to improve performance in ambiguous cases. The embeddings are fed into an MLP enhanced with Neutrosophic Logic, which assigns values of truth (T), indeterminacy (I), and falsity (F) to better manage uncertainty and vagueness in language.

The experimental evaluation of the proposed framework demonstrates promising outcomes. The integration of BERT embeddings with the Neutrosophic-MLP classifier significantly improved detection accuracy compared to conventional machine learning models such as SVM and Random Forest. The system was tested on a benchmark cyberbullying dataset as well as a collected set of real-time Twitter posts. Results indicated an overall accuracy of over 90%, with noticeable improvements in precision and recall for ambiguous cases where existing methods often misclassify.

References:

1. Al-Khasawneh H. et al., IEEE Access, vol. (2022), pp. 1–12.
2. Atif M. et al., Journal of Information Science, vol. (2021), pp. 1–10.
3. Al-Wesabi F. et al., IEEE Access, vol. (2022), pp. 1–15.
4. Almufareh M. et al., Computers & Security, vol. (2021), pp. 1–12.
5. Umer M. et al., Future Generation Computer Systems, vol. (2020), pp. 1–11

EH-034

Biogenic CdS Nanostructures Using Hibiscus Rosa-Sinensis, Azadirachta Indica, Aloe Barbadensis Miller, And Citrus Sinensis: Encapsulant-Driven Morphological, Optical, and Photocatalytic Properties

Labhesh Baid[1]*, K. S. Ojha[1]

[1]*NIT Raipur, Raipur, Chhattisgarh, India, 603203*

***Corresponding author e-mail:** Labheshbaid777@gmail.com

ABSTRACT

CdS nanostructures were successfully synthesized using a hydrothermal method, incorporating Hibiscus rosa-sinensis (Hibiscus/Gurhal), Azadirachta indica (Neem), Aloe barbadensis miller (Aloe vera) leaf, and Citrus sinensis peel (orange peel) extracts as natural encapsulating agents. The synthesized nanostructures exhibited distinct morphological features, confirmed by HRSEM, with snowflake-like, cauliflower-like, starflower-like, and sago-like nanostucture formations. X-ray diffraction (XRD) analysis indicated a hexagonal phase with average crystallite sizes ranging from 9.59 nm, 7.43nm, 8.71, and 9.03 nm, respectively, for Hibiscus rosa-sinensis (Hibiscus/Gurhal), Citrus sinensis peel, Azadirachta indica (Neem), Aloe barbadensis miller (Aloe vera) leaf, and capped CdS. Elemental analysis through EADX and mapping confirmed the purity of the synthesized CdS, with no detectable impurities. Optical investigations using UV-Vis spectroscopy revealed a noticeable variation from 2.15 to 2.25 eV[1], and all samples shows redshift compared to the bulk CdS bandgap, while photoluminescence spectra exhibited emission peaks in the UV, blue, and yellow-green regions at 371, 468, and 564 nm, respectively. Additionally, FTIR spectroscopy was employed to analyze the vibrational characteristics of the plant-extract-assisted CdS samples [2]. The photocatalytic performance of these nanostructures was explored for environmental remediation, demonstrating the promising efficiency of acetaminophen degradation under visible light irradiation. The use of eco-friendly plant extracts in the synthesis process not only enhances the stability and morphology of CdS nanostructures but also presents a sustainable approach for advanced photocatalytic applications.

References:

1. M. H. K. Al-Mamoori, D. K. Mahdi and S. M. AlShrefi, AIP Conf. Proc., 2018, 1968, 030018.
2. B. S. M. Al Balushi et al., Appl. Surf. Sci., 2018, 457, 559–565.

EH-035

Utilizing CO_2 for Synthesis of Organic Carbonates via Direct Carbonylation of Glycerol

Wan-I Chen, Ya-Chen Yu, Bing-Hung Chen*

Department of Chemical Engineering, National Cheng Kung University, Tainan, 70101, Taiwan

***Corresponding author e-mail:** bkchen@ncku.edu.tw

ABSTRACT

This study investigates the CO_2 utilization to produce glycerol carbonates via the direct carbonylation of glycerol with CO_2 over ZnO-based catalysts. Owing to the high stability of both glycerol and CO_2, the direct carbonylation reaction is difficult to proceed, requiring high-temperature and high-pressure conditions, which significantly increase equipment and operational costs [1, 2]. Several factors influence the reaction outcome, including reaction temperature, pressure, solvent ratio, and catalyst dosage. Typically, the carbonylation reactions in this work were carried out at 5 MPa CO_2 at 180°C with 2-cyanopyridine and ethanol as dehydrating agents. ZnO/ZrO_2 catalysts were synthesized with the incipient wetness impregnation method to facilitate the reaction (Figure 1). Specifically, $Zn(NO_3)_2 \cdot 6H_2O$ was used as the precursor, while ZrO_2 served as the support. ZnO was loaded onto ZrO_2 via the wet impregnation method, forming a ZnO/ZrO_2 catalyst. The catalyst was characterized using various analytical techniques, including XRD, SEM, EDS, Nitrogen physisorption analyzer, CO_2-TPD, and ICP-OES. The yield of glycerol carbonate was adopted as the response variable, while the optimal reaction condition was sought via the response surface methodology (RSM) with a central composite design (CCD) [3]. Explicitly, a quadratic polynomial equation to describe the yield of glycerol carbonate was obtained by fitting the experimental data. The optimal condition was thus extracted from the established further verified with independent sets of experiments performed in the proximity to the optimal condition.

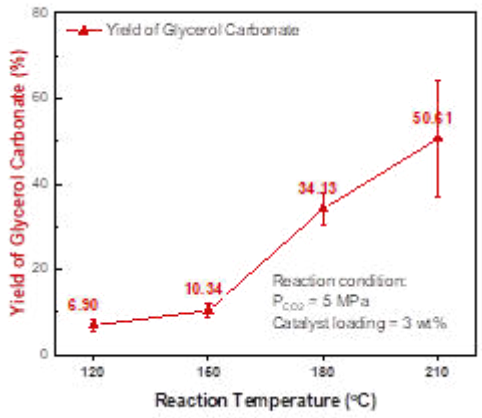


Fig 1. Effect of reaction temperature on the yield of glycerol carbonate via the direct carbonylation of glycerol with CO2.

References:

1. J. Liu and D. He, J. CO_2 Util., 2018, 26, 370–379.
2. S. Lukato, G. N. Kasozi, B. Naziriwo and E. Tebandeke, Curr. Res. Green Sustain. Chem., 2021, 4, 100199.
3. D. C. Montgomery, Design and Analysis of Experiments, 10th ed., Wiley, 2019.

EH-036

Photocatalytic Degradation of Norfloxacin Antibiotic under UV Light Using Brookite TiO_2/N-Doped Graphene Nanocomposites

Amritha C. Jayasankar[1], Mohamed Haseen K. P.[2], Muhsina P. P.[2], Binitha N. Narayanan[1,3]*

[1]*Department of Chemistry, University of Calicut, Malappuram, Kerala, India, 673635*

[2]*Department of Chemistry, Markaz Arts & Science College, Malappuram, Kerala, India, 679571*

[3]*Inter University Centre for Hydrogen & Energy Storage, University of Calicut, Malappuram, Kerala, India, 673635*

***Corresponding author e-mail:** binitha@uoc.ac.in

ABSTRACT

A brookite-phase TiO_2/N-doped graphene (TiO_2/NG) nanocomposite was synthesized through a facile sol-gel and hydrothermal method and evaluated for the photocatalytic degradation of norfloxacin (NOF) under UV irradiation. Although brookite TiO_2 has been comparatively less explored, it exhibits superior photocatalytic performance owing to efficient charge separation and favorable conduction band alignment. Moreover, its formation under mild synthesis conditions enhances the scalability of the process. Incorporation of nitrogen-doped graphene (NG) enhances light absorption, introduces additional active sites, and promotes rapid charge transport, thereby suppressing electron–hole recombination. Comprehensive characterization using XRD, FTIR, Raman spectroscopy, UV–Vis DRS, SEM, TEM, and XPS confirmed the successful formation of brookite TiO_2 and effective nitrogen doping in the less defective few-layered graphene. The TiO_2/NG nanocomposite demonstrated excellent photocatalytic degradation efficiency toward NOF, highlighting the strong synergistic interaction between brookite TiO_2 and NG. Overall, this work presents a cost-effective and efficient strategy for developing advanced photocatalysts for environmental remediation applications.

References:

1. S. Sun, T. Sun, D. Zhang, J. Liu, L. Ren, C. Chen, W. Yao and Z. Shi, J. Photochem. Photobiol. A: Chem., 2026, 471, 116710.
2. Z. Huang, P. Zhu, M. Liu, X. Xin, B. He and X. Li, Sep. Purif. Technol., 2025, 356, 129959.
3. Adnan et al., Heliyon, 2025, 11, e41320.

Synthesis and Morphological Investigation of Carbon Nanotube Reinforced Nd Doped Yttrium Oxide Nano Composite on The Effect of Calcination Temperature for Environmental Gas Monitoring

S. Surya[1], S. Gokul Raj[1],*, G. Ramesh Kumar[2], Ashok Kumar Srivastava[3], K. Ramachandran[3]

[1]*Department of Physics, Pondicherry University, Kalapet, Puducherry 605014, India.*

[2]*Department of Science and Humanities, University College of Engineering Arni.*

[3]*Department of Physics, SRMIST, FET, Vadapalani Campus, Chennai 600026.*

***Corresponding author e-mail:** sgokulraj@gmail.com

ABSTRACT

Carbon nanotube (CNT) reinforced neodymium-doped yttrium oxide (Nd:Y_2O_3) nanocomposites were successfully synthesized via a facile co-precipitation method and subsequently calcined at different temperatures of 500°C, 750°C, and 1000°C to investigate the effect of thermal treatment on their structural, morphological, optical, and gas sensing properties. Thermogravimetric and differential scanning calorimetric (TG–DSC) analyses confirmed the thermal stability and appropriate phase formation of the synthesized nanocomposites. X-ray diffraction (XRD) studies revealed the formation of a single-phase cubic Y_2O_3 structure with no secondary phases, indicating successful incorporation of Nd^{3+} ions and CNTs. The crystallite size was found to increase with increasing calcination temperature; however, even at the highest temperature of 1000 °C, the crystallite size remained < 25 nm, highlighting the nanocrystalline nature of the material. Raman spectroscopy further confirmed the presence of CNTs and provided insight into defect states, while X-ray photoelectron spectroscopy (XPS) validated the elemental composition and oxidation states of Y, Nd, O, and C. Morphological investigations using scanning and transmission electron microscopy (SEM and TEM) revealed well-dispersed CNTs within the Nd:Y_2O_3 matrix and a quasi-spherical nanoparticle morphology. Optical properties were examined using UV–visible absorption and photoluminescence (PL) spectroscopy, indicating defect-related emissions influenced by calcination temperature. Finally, the synthesized nanocomposites were evaluated for environmental gas sensing applications, where the synergistic effect of CNT reinforcement, controlled crystallite size, and surface defects resulted in enhanced sensing performance. These results demonstrate the potential of CNT-reinforced Nd:Y_2O_3 nanocomposites as promising materials for efficient environmental gas monitoring.

References:

1. K. Durgadevi et al., Diamond Relat. Mater., 2025, 112, 112997.
2. J. Hubbard et al., Nanomaterials, 2021, 11, 2168.
3. G. Asgari et al., RSC Adv., 2020, 10, 7718–7731

EH-038

Plasmon-Mediated Energy Distribution and SERS Activity of Copper-Coated Glass Substrates

Gyan Prakash Dewangan*, Ayush Khare, Prabhat k. Dwivedi2 Mainak Basu31National
Institute of Technology Raipur, Chhattisgarh, India 492010

***Corresponding author e-mail:** gpdewangan.phd2025.phy@nitrr.ac.in

ABSTRACT

Surface Enhanced Raman Spectroscopy (SERS) is very impressive and non-invasive analytical techniques that enable detection of very low concentration of analyte with extreme sensitivity, however there are widely used noble metal substrates like gold (Au) and silver (Ag) but these materials limits the large-scale production and cost-efficient applications. In this work we present a copper thin film coated glass substrate as a cost-effective SERS platform and systematically explore its optical energy distribution characteristics to recognize the origin of Raman signal enhancement. Copper thin films were deposited in the normal and FTO glass substrate using DC sputtering technique and evaluated using Rhodamine as a analyte material. Raman analysis reveals a noticeable enhancement in signal intensity from the copper-coated substrate compared to bare and FTO glass, confirming its SERS activity. In addition to spectroscopic analysis, the optical response of the copper thin film was studied by analyzing the distribution of incident energy in terms of reflection, transmission, and absorption. The results indicate that enhanced optical absorption and reduced transmission at the excitation wavelength contribute significantly to localized electromagnetic field confinement at the metal–dielectric interface, thereby promoting Raman signal amplification. The correlation between optical energy dissipation and SERS performance provides deeper insight into the plasmonic behavior of copper thin films. This combined spectroscopic and optical energy analysis demonstrates that copper-coated glass substrates can function as efficient, low-cost alternatives to noble-metal-based SERS platforms, with potential applications in chemical sensing and biosensing.

References:

1. S. Li et al., J. Mater. Res. Technol., 26 (2023), 1537–1552
2. S. Mabbott, Y. Xu, and R. Goodacre, Anal. Methods, 9-33 (2017) 4783–4789

An Edge-Cloud Enabled Smart Agriculture Infrastructure Using ESP32 and AWS for Intelligent Irrigation

Vishal. M, Adarsh. PA, Praveen. D, Shalini. M*

SRM Institute of Science and Technology, Vadapalani, Tamil Nadu, India, 600 026

***Corresponding author e-mail:** shalinim@srmist.edu.in

ABSTRACT

This paper presents a hybrid edge–cloud Smart Agriculture Infrastructure that integrates an ESP32 microcontroller with Amazon Web Services (AWS) to enable intelligent irrigation control and real-time environmental monitoring. The proposed system combines IoT-based sensing, local edge-level decision-making and cloud-driven analytics to achieve reliable, scalable and energy-efficient precision irrigation. Environmental parameters including soil moisture, temperature, humidity and light intensity are continuously monitored using integrated sensors, while threshold-based irrigation control is executed locally on the ESP32 to ensure uninterrupted operation during network disruptions. Sensor data is securely transmitted to AWS IoT Core using the MQTT protocol, where event-driven AWS Lambda functions process and store data in Amazon DynamoDB for real-time analytics and historical trend analysis. A web dashboard hosted on Amazon EC2 provides live visualization and remote control, while AWS Simple Notification Service (SNS) delivers instant alerts during critical environmental conditions. Experimental evaluation under real-world conditions demonstrates an average cloud data latency of 2.1 seconds, relay activation time below 200 milliseconds and alert delivery within 4–5 seconds. The system achieved over 98% data synchronization accuracy and operated reliably during simulated network outages. Compared to traditional irrigation methods, the proposed solution resulted in an estimated 40–50% reduction in water consumption while significantly reducing manual supervision. The results validate the effectiveness of the proposed hybrid architecture in improving irrigation precision, resource efficiency and operational reliability, making it a practical and scalable solution for sustainable smart agriculture.

References:

1. Dhanaraju M, Manoharan K, Ramesh S, Agriculture Journal, vol. 12 (2022), page no. 5.
2. Goon S, Saha P, Roy R, International Research Journal of Engineering and Technology (IRJET), vol. 9 (2022), no. 6, pp. 1278–1283.
3. Singh G, Sharma R, Patel V, Siberian Journal of Life Sciences and Agriculture, vol. 14 (2022), no. 6, pp. 23–29.
4. Choudhary P, Patel A, International Journal of Scientific Research in Engineering and Management (IJSREM), vol. 6, (2022), no. 9, pp. 110–116.
5. N. Siva Kumar and M. Anbarasu, Journal of Emerging Technologies and Innovative Research (JETIR), vol. 10, (2023), no. 4, pp. 212–218.

EH-040

A Machine Learning-Based Vocal Screening Method for Respiratory Conditions

B. Chandra*, Divya Darshini D, Harshini S J

Easwari Engineering College, Ramapuram, Chennai, Tamilnadu, India, 600089

***Corresponding author e-mail:** Chandra.klnce@gmail.com

ABSTRACT

Diseases of the respiratory system continue to be among the top causes of morbidity and mortality worldwide. Therefore, accurate and timely detection of lung abnormalities is an essential need. Traditional auscultation using stethoscopes is inherently subjective and may not detect subtle irregularities in complex lung sound patterns. The study designs and develops a deep learning framework to reconcile these limitations by developing a computerized framework for the characterization and early diagnosis of pathological lung sounds. The workflow begins with the recordings of lung sound signals, which are heavily preprocessed utilizing the MATLAB toolbox. Conclusively, a hybrid framework is employed whereby CNN learns spatial patterns from the spectrograms, and RNN learns temporal patterns and trajectories of the learned progression from the signals. This hybridization increases the positivity of both models, all while the work enables persistent classification of abnormal respiratory events. Clinical research evidence indicated that the proposed system exhibited high specificity and sensitivity to differentiate states that were abnormal from states that were normal and outperformed traditional machine learning classifiers. The framework could permit earlier identification of abnormalities and permit yet better opportunities to monitor the health of the lung in asthma, chronic obstructive pulmonary disease, and the remainder of the chronic diseases of the lungs.

References:

1. Anaadumba, R., Belabbaci, N. A., & Alam, M. A. U., IEEE/ACM Conference on Connected Health: Applications, Systems and Engineering Technologies (CHASE), 2025, pp. 149–153.
2. Han, T.-T., Trung, K. L., Nguyen Anh, P., & Do Trung, A., IEEE Access, 13 (2025), pp. 93017–93032.
3. Kumar, R. et al., IEEE Access, 12 (2024), pp. 189515–189534.
4. Rivero, A. J. L., Corbacho, C. C., Arias, T. R., Martín-Merino, M., & Vaz, P., IEEE Access, 12 (2024), pp. 160516–160528.
5. Almubark, I., IEEE Access, 13 (2025), pp. 8225–8238.

EH-041

Multifunctional Ni–Zn Ferrite ($Ni_{0.5}Zn_{0.5}Fe_2O_4$) Nanoparticles for Efficient Photocatalytic Removal of Pharmaceutical and Agrochemical Pollutants from Wastewater

Jashwini Asokan[1], Shalini Govindaraj M*[1]

[1]*Department of Physics, School of Advanced Sciences (SAS), Vellore Institute of Technology (VIT), Chennai, TN 600127, India*

***Corresponding author e-mail:** shalini.mg@vit.ac.in

ABSTRACT

The increasing persistence of pharmaceutical residues and agrichemicals in water systems poses serious risks to aquatic ecosystems and human health, necessitating efficient and sustainable remediation strategies. In this work, $Ni_{0.5}Zn_{0.5}Fe_2O_4$ nanoparticles (NZ-asp) were synthesized through a facile hydrothermal method and employed as visible-light-active photocatalysts for the degradation of emerging contaminants such as the antibiotic drug Metronidazole ($C_6H_9N_3O_3$) and the herbicide Atrazine ($C_8H_{14}ClN_5$). The nanoparticles were systematically characterized using XRD, FTIR, XPS, Raman spectroscopy, SEM, UV–Vis spectroscopy, and VSM to evaluate their structural, optical, morphological, and magnetic properties. Single phase spinel formation with crystallite size 13 nm was observed, which increased to 23 nm upon annealing at 750°C (NF-750). The photocatalytic performance was investigated under visible light irradiation, demonstrating rapid degradation of both pollutants through reactive oxygen species–mediated oxidation pathways. The enhanced activity arises from efficient charge separation, an optimal band gap, and abundant active sites in the substituted ferrite structure. Its magnetic nature enables easy recovery and reuse, making $Ni_{0.5}Zn_{0.5}Fe_2O_4$ a stable and sustainable photocatalyst for pharmaceutical and agrochemical wastewater treatment.

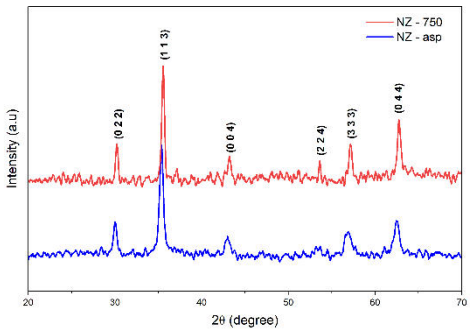


Fig 1. XRD patterns of NZ - asp and NZ - 750 nanoparticles

References:

1. Altendji, K., Hamoudi, S., Environ Sci Pollut Res 32(2025), 1361–1374.
2. Azeezat A Rasheed-Adeleke et al., Nano Ex. 6(2025), 045015.
3. Cai, Hao, et al., Chem Eng J 505 (2025), 159577.

EH-042

Investigation on the Remediation of Malachite Green Dye from Aqueous Solutions Using Industrial Boiler Ash as Sustainable Adsorbent

Venuprasanth_Margabandu[1], Gurram Srihari[1], Marada Kavyamrutha Vardhini[1], Bhukya Akash[1], Bhuvaneshwari Soundararajan [1]*

[1]*Department of Chemical Engineering, National Institute of Technology, Calicut, Calicut – 673601, India*

***Corresponding author e-mail:** sbuvana@nitc.ac.in

ABSTRACT

Water pollution caused by synthetic dyes is considered as a serious environmental concern in contemporary wastewater treatment. In this study, industrial boiler ash (IBA) was evaluated as a low-cost and effective adsorbent for the remediation of malachite green (MG) dye from aqueous solutions. The physiochemical properties of IBA were characterized using FESEM-EDS analysis, BET surface area method, TG analysis, FT-IR and XRD techniques. Adsorption experiments were conducted to investigate the effects of operational parameters, including IBA dosage (0.1-0.5 g/L), solution pH (4-10), initial MG concentration (10-50 mg/L), and contact time (0-180 min). The experimental results showed a maximum removal efficiency of 99.52% at pH 4, IBA dosage of 0.3 g/L, and 10 mg/L of MG. The experimental data were further fitted with various isotherm and kinetic models. The MG adsorption process was best described by the Langmuir isotherm and the pseudo-second-order kinetic model, indicating a strong chemical adsorption process, with a maximum monolayer adsorption capacity of 163.33 mg/g. Regeneration studies were further confirmed the environmental sustainability and reusability of IBA adsorbent. Overall, the findings highlight the applicability of IBA as an economical, sustainable, and efficient adsorbent for dye-laden wastewater treatment, supporting circular economy strategies in environmental remediation.

Keywords: Adsorption; Functional Materials; Industrial Boiler Ash; Malachite Green; Wastewater Treatment

EH-043

Layered Hierarchically Porous Carbon-Composite Polymer Foam Filtration Column for Oil-in-Water Demulsification

Jyotiraman De[1,2], Dharmveer Yadav[1,3], Sumit Saxena[1,2], Shobha Shukla*[1,2]

[1]*Water Innovation Centre: Technology Research & Education, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, MH, India – 400076*

[2]*Nanostructures Engineering and Modelling Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, MH, India – 400076*

[3]*Centre for Research in Nanotechnology and Science, Indian Institute of Technology Bombay, Mumbai, MH, India – 400076*

***Corresponding author e-mail:** sshukla@iitb.ac.in

ABSTRACT

Increasing industrialization continues to elevate oily wastewater discharge, posing significant environmental and health hazards that necessitate the implementation of effective remediation strategies. Although numerous techniques have been developed for oil–water separation, the cost-effective treatment of stable, fine oil-in-water emulsions remains a formidable challenge owing to their intrinsic stability and the small size of dispersed oil droplets. Thus, a cost-effective and highly efficient separation system incorporating coalescence-promoting media is required to enable demulsification and oil removal from water, particularly for emulsions with droplet sizes smaller than 1–2 μm that cannot be effectively addressed by conventional filtration methods. This study utilizes a superhydrophobic/superoleophilic, carbon-incorporated polymer foam arranged in a filtration column to expedite oil droplet coalescence in oil-in-water emulsions. The carbon-composite polymer foam exhibited strong chemical stability over a wide pH range, with negligible changes in wettability when exposed to brine, 2 M HCl, and 2 M NaOH. The device was designed to reduce residual oil concentrations from 70–100 ppm to below 10 ppm, meeting stringent discharge limits for treated water. The modular device can also be operated in both gravity-driven and pressure-driven flow modes. Overall, the layered hierarchical porous foam column provides a practical and scalable strategy for coalescence-assisted water polishing of stable oil-in-water emulsions.

References:

1. W. Lu, W. Xiong, Y. Zhang, X. Li, C. Pan, G. Fan, Y. Long, Surfaces Interfaces, 84 (2026) 108619.
2. J. Zhao, M. Li, W. Liao, Y. Shao, Q. Du, D. Li, Y. Nan, Z. Zhang, D. Sun, J. Hazard. Mater., 500 (2025) 140385.
3. J. Chen, Y. Ni, Y. Gou, T. Zhu, L. Sun, Z. Chen, J. Huang, D. Yang, Y. Lai, J. Hazard. Mater., 461 (2024) 132674.

EH-044

Enhanced No_2 Gas Sensing Performance of MoO_3 Thin Film Deposited by Pulsed Laser Deposition (PLD)

Praveenkumar P[1], E. Vinoth[1], J. Archana[2], M. Navaneethan[1], S. Harish[1]*

[1]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203.*

[2]*Center of Excellence in Materials for Advanced Technologies, Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203.*

***Corresponding author e-mail**: harishs@srmsit.edu.in

ABSTRACT

Nitrogen dioxide (NO_2) is a highly toxic and reactive air pollutant emitted primarily from combustion sources, posing serious risks to human health even at trace concentrations. The great stability and robust surface reactivity of metal oxide semiconductors (MOS) make them a popular choice for chemiresistive gas sensors. To examine the effectiveness of the sensor for NO_2 gas sensing applications, α-MoO_3 thin films were successfully produced using pulsed laser deposition (PLD) on SiO_2/Si substrates. X-ray diffraction verified the development of highly crystalline orthorhombic α-MoO_3. Analysis using X-ray photoelectron spectroscopy and photoluminescence revealed the presence of mixed Mo^{5+}/Mo^{6+} oxidation states and oxygen vacancies, which are essential for gas adsorption and charge transfer. At an operational temperature of 200 °C, the produced MoO_3 thin film had an exceptionally high response of 15000 % towards NO_2 gas, surpassing the sensitivity of several room-temperature MoO_3 based sensors. Defect-mediated adsorption sites and optimized crystallinity work in concert to produce the improved sensing performance. This work shows that well designed PLD-grown MoO_3 thin films with superior NO_2 sensing capabilities are a promising option for realistic, useful ambient air-quality monitoring systems.

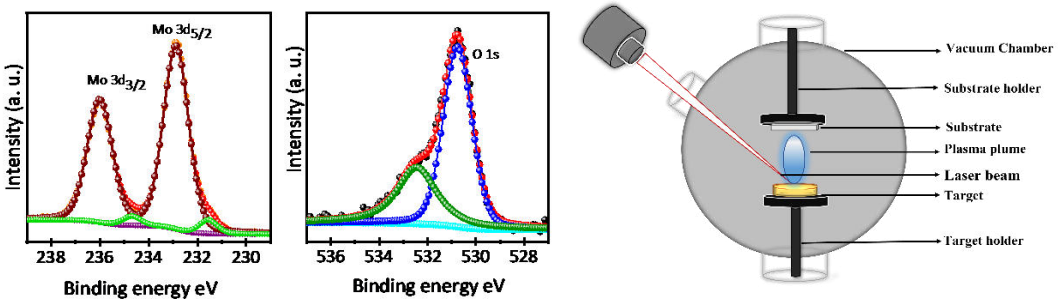


Fig. 1 (a) XPS analysis of MoO_3 deposited on SiO_2/Si and (b) Schematic representation of Pulsed Laser Deposition

Keywords: Pulsed Laser Deposition (PLD), NO_2, α-MoO_3, gas

References:

1. S. S., P. B., and J. P. S., ACS Appl. Nano Mater., 8(38) (2025).
2. P. B., A. K., I. T. J., M. A., B. D. B., B. R. M., Sens. Actuators B Chem., 341 (2021).

Recovery Of Valuable Metals from Effluent of Tannery Industry

Mohamed Aslam K A, Krishnapriya R, Anakha S R, Ramya Sankar M S*

Department of Chemical Engineering, Saintgits College of Engineering (Autonomous), Kottayam, Kerala – 686532

***Corresponding author e-mail:** ramya.sankar@saintgits.org

ABSTRACT

Tannery industries generate large volumes of wastewater containing toxic and valuable heavy metals, particularly chromium and lead, which pose serious environmental and health risks if discharged without adequate treatment. The recovery of these metals is essential not only for pollution control but also for resource conservation and sustainable wastewater management. This study investigated the electrochemical removal and recovery of chromium and lead from tannery effluent using a closed batch electrochemical reactor system. Synthetic tannery effluent was first prepared to simulate real industrial wastewater conditions, and three key operating parameters current density, pH, and operating time were selected for optimization. Based on literature based upper and lower limits of the selected parameters, 21 experimental trials were designed and generated using Minitab software and subsequently conducted to evaluate the combined effects on metal removal efficiency. The electrochemical system fabricated with graphite electrode coated with coconut shell–derived material as the anode and a stainless-steel electrode as the cathode. Statistical analysis using Minitab software was applied to identify the optimal operating conditions with low values of p and f test, under which significant removal and recovery of chromium and lead were achieved in synthetic effluent. The optimized parameters by the ANOVA analysis were subsequently applied to real tannery wastewater, and the results confirmed effective heavy metal removal, demonstrating the feasibility, reliability, and sustainability of the proposed electrochemical treatment method for industrial wastewater management and resource recovery.

Keywords: Electrochemical treatment; Tannery wastewater; Heavy metal removal; Chromium recovery; Lead recovery; Synthetic effluent; Process optimization; Minitab design of experiments; Closed batch reactor; Sustainable wastewater management

References

1. M. N.-E. Alam, M. A. S. Mia, F. Ahmad, M. M. Rahman, An overview of chromium removal techniques from tannery effluent.
2. S. L. Kakakhel, G. Lutfullah, M. I. Bhanger, A. Shah, A. Niaz, Electrolytic recovery of chromium salts from tannery wastewater.

EH-046

Enhanced CO_2 Methanation Over Ni-Doped $AlPO_4$ Catalysts in A Fixed-Bed Reactor

Ganesh Srinivasan, Thamizharasi Pugazhenthi, Purushothaman S P,

N.R. Sasirekha*

Catalysis Laboratory, CAS in Crystallography & Biophysics, University of Madras, Guindy Campus, Chennai 600025, Tamil Nadu, India

***Corresponding author e-mail:** nrsasirekha@gmail.com

ABSTRACT

CO_2 is one of the major environmental pollutants, and its mitigation has attracted significant attention over the years due to rapid increase in greenhouse gas emissions in the atmosphere. Scientists are actively involved in developing carbon capture, utilization, and storage (CCUS) technology for large point sources, where fossil fuels are used for power generation. Even though storage is a better option to manage CO_2 concentration, utilizing CO_2 by converting it into value-added chemicals and feedstocks via electrochemical, photochemical, and photoelectrochemical pathways, and by hydrogenation, is a promising approach. Catalytic methanation of CO_2 has tremendous scope in converting CO_2 into methane that allows the conversion of H_2 into synthetic natural gas. The most challenging part lies in the activation of CO_2 because of its high stability and the highly stable C=O bond. Both homogeneous and heterogeneous catalysts are used for CO_2 hydrogenation, but heterogeneous catalysts offer advantages such as ease of separation, high catalytic activity and selectivity. In this work, a microporous aluminophosphate-based ($AlPO_4$) molecular sieve was synthesized by the hydrothermal method and loaded with Ni metal by incipient wetness impregnation method. All the catalysts were characterized by XRD, BET, HR-SEM, FT-IR, and UV-visible DRS to study their physico-chemical properties. The catalytic activity of the prepared materials was tested for catalytic hydrogenation of CO_2 in a fixed-bed reactor. All the products were analyzed by Gas Chromatography using a TCD detector. The reaction parameters such as time, temperature, GHSV, and ratio of CO_2/H_2, and loading of Ni active metal were optimized. The catalysts were found to be highly active towards the hydrogenation of CO_2.

References

1. Wang, Baowei, et al. H2/CO, Applied Surf. Sci., 526 (2020) 146461.
2. W. Liu, et al., Microporous Mesoporous Mater., 348 (2023) 112416.
3. B. Wang, et al., J. Mater. Chem. A, 7 (2019) 13164–13172.
4. Modak, A. Ghosh, A. Bhaumik, B. Chowdhury, Adv. Colloid Interface Sci., 290 (2021) 102349.
5. P. Gao, L. Zhang, S. Li, Z. Zhou, Y. Sun, ACS Cent. Sci., 6 (2020) 1657–1670.

Electrospun PZT-PVDF composite: A Pathway to Flexible Acoustic Sensors

Karthika P Moni[1], Sneha S Kumar[1], Maneesh Chandran*[1]

[1]*Department of Physics, National Institute of Technology Calicut, Kozhikode, Kerala, India, 673601*

***Corresponding author e-mail:** maneesh@nitc.ac.in

ABSTRACT

Flexible acoustic sensors have attracted significant interest for applications in structural health monitoring, wearable electronics, and human–machine interfaces due to their requirements for high sensitivity, mechanical flexibility, and lightweight form factors. Piezoelectric acoustic sensors are particularly promising because of their self-powered operation. Lead zirconate titanate (PZT) exhibits excellent piezoelectric and ferroelectric properties, while PZT nanofibers with high aspect ratios enhance piezoelectric charge generation. Hence, integration of PZT nanofibers into a β-phase PVDF matrix yields flexible composite films with enhanced piezoelectric performance. Herein, we report the synthesis of PZT nanofibers using sol-gel based electrospinning technique, which were then incorporated into PVDF at different weight percentages to fabricate flexible films through solution casting. XRD analysis was employed to examine the coexistence of PZT and the β-phase of PVDF at different PZT weight percentages, while FTIR analysis was used to evaluate the β-phase content of PVDF. XRD and Raman spectroscopy confirmed the formation of phase-pure perovskite PZT, whereas a stoichiometric composition of $Pb(Zr_{0.52}Ti_{0.48})O_3$ was assessed using EDXS. The morphology of the nanofiber was analyzed using FESEM images, and the average diameter of the nanofiber was found to be ~ 300 nm. The prepared composite films can be employed as an active layer of a flexible acoustic sensor for converting low-frequency mechanical vibrations into electrical signals. The acoustic sensing performance of the composite was evaluated using impedance tube measurements.

References:

1. M. Eledath and M. Chandran, J. Mater. Res., 36 (2021) 4725–4745.
2. D. Ji et al., Nat. Rev. Methods Primers, 4 (2024) 1.
3. J. S. Yun et al., Nanomater. Nanotechnol., 6 (2016) 20.
4. X. Chen et al., Physica A, 199 (2013) 372–378.
5. F. Yousefi and H. Esfahani, Ceram. Int., 50 (2024) 53171–53182.
6. X. Chen, J. Li, G. Zhang, and Y. Shi, Adv. Mater., 23 (2011) 3965–3969.

EH-048

A Stable Piezoelectric Pressure-Sensing Device Based on Riboflavin-Poly(vinylidene fluoride) Composite Nanofibers for Potential Applications in Athlete Training

Akhilesh Kumar Sharma, Gurneet Kaur, Manjeet Jassal*, Ashwini K. Agrawal*

Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India, 110016

***Corresponding author e-mail:** manjeetjassal@gmail.com, ashwini@textile.iitd.ac.in

ABSTRACT

Piezoelectric pressure sensors are being extensively explored for their applications in wearable electronics. However, the long-term stability of the piezoelectric output voltage along with high sensing properties are still challenges for piezoelectric pressure sensors. To overcome this challenge, riboflavin nanorods (Vb NRs) were used as a filler in different concentrations for electrospinning of poly(vinylidene fluoride) (PVDF)-Vb composite nanowebs (Vb_xPVDF_{100-x}) and investigated for their morphology, structural, dielectric, mechanical, and piezoelectric pressure-sensing performance. Vb NRs incorporated into PVDF for the fabrication of piezoelectric pressure sensors help to stabilize dipoles due to dipole–dipole interaction, hydrogen bonding, and van der Waals forces between the various functional groups of Vb NRs and PVDF. Analysis via FTIR and dielectric characterization confirms that 2 wt % Vb NRs in PVDF nanofibers exhibit the highest β phase (67%) and dielectric constant (7.90 at 1 kHz) among all the samples. This sample exhibited high pressure sensitivities of 4.16 ± 0.184 and 1.23 ± 0.009 V/kPa in the pressure ranges of 2.5–10 and 10–20 kPa, respectively. Peak power generation through the piezoelectric device was 163 μW/g on continuous application of cyclic pressure. The piezoelectric voltage of the device was found to be stable for over 15 months, which is the highest duration of stability reported in the literature, to the best of our knowledge. Furthermore, the pressure sensor was integrated into the insole of a shoe and evaluated for its application in monitoring the physical activities of an athlete.

References:

1. Jang, H. S. Adv. Funct. Mater. 2025, 35 (8), 2415501.
2. Latief, U. ACS Appl. Nano Mater. 2025, 8 (9), 4784– 4800.
3. Siddiqui, A. Sens. Actuators, A 2024, 375, 115503.
4. Lakra, H. Polym. Compos. 2025, 46 (S1), S186– S209.

EH-049

Development of Synergistic rGO–ZnO Hybrid Nanocomposites for Flexible Wearable Ethanol Sensors

Krishanu Dey, Ramakrishna Nayak, Adarsh Nigam and Amit Kumar Goyal*

[1]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India*

***Corresponding author e-mail:** amit.goyal@manipal.edu

ABSTRACT

The rapid advancement of non-invasive wearable diagnostic devices has necessitated the development of high-performance sensing materials that are capable of operating efficiently at room temperature. Nanocomposites of Reduced Graphene Oxide (rGO) combined with Zinc Oxide (ZnO) have emerged in recent years as a powerful material for the detection of various volatile organic compounds (VOCs), particularly in applications requiring high sensitivity and selectivity. This material leverages the synergistic effects of rGO's high conductivity and large surface area along with ZnO's high chemical sensitivity. Thus, it provides a good gas absorption properties. This has resulted in good carrier mobility and reduced operating temperatures required for room temperature sensing compared to pure ZnO based sensors. Studies have shown that rGO-ZnO hybrids exhibit enhanced sensor response, good repeatability, selectivity and sensitivity. This material has the capability to address the growing demand for non-invasive detection using flexible and wearable devices. Therefore, the present work explores the capability of rGO-ZnO hybrid nanocomposites for alcohol sensing applications. A resistive-type rGO–ZnO sensor was fabricated using a scalable screen-printing technique, making it suitable for wearable and non-invasive platforms. A homogeneous sensing ink composition was prepared by dispersing the rGO–ZnO nanocomposite, followed by controlled stirring and sonication to achieve stable viscosity and uniform dispersion. The prepared ink was then screen-printed onto the electrode-patterned substrate and subsequently dried to ensure good film adhesion and electrical stability. The fabricated sensor was electrically characterized by exposing it to ethanol vapour at different concentration levels (varying %), and key sensing parameters such as sensor response and recovery times, repeatability, and sensitivity were systematically evaluated to assess its suitability for room-temperature, wearable alcohol monitoring applications. This work demonstrates the potential of rGO–ZnO nanocomposites for scalable, room-temperature wearable sensing. It opens avenues for intelligent sensor optimization and real-time non-invasive diagnostics.

References:

1. Komorizono, R. R. Leite, S. De la Flor, E. Llobet, V. R. Mastelaro, Materials Science in Semiconductor Processing, 181, (2025) 109229.
2. M. Won, J. Sim, G. Oh, M. Jung, S. P. Mantry, DS. Kim, Sensors, 24(5), (2024) 1691.
3. H. R. Madvar, M. Moayedi, Z. Kordrostami, Thin Solid Films, (2024) 140498.
4. S. Aravind, A. Nigam, and A. K. Goyal, IEEE Sensors Letters, 9(5), 6004804 (2025).
5. D. Li, J. Lu, X. Zhang, D. Jin, H. Jin, Nanomaterials, 13(5), (2023) 917.
6. K. Goyal, N. Gupta, A. Kumar, and R. Mahadeva, IEEE Sensors Letters, 9, (2025), 6005609.

EH-050

Toxicological Evaluation of PET Micro-Nano Plastics

Meenakshi Podwal[1], Sharine Priscilla[1], Sajneshri Patil [1], Sushilkumar Ningthoucha[1], Aditya Bagkar[1]Sahabudeen Sheik Mohideen*[1]

[1] *Department of Biotechnology School of Bioengineering, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu District, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** sahabuds@srmist.edu.in

ABSTRACT

Polyethene terephthalate (PET) micro-nano plastics are prevalent plastic pollutants resulting from their vast application in packaging, textiles and consumer goods. Environmental exposure results in the ongoing physicochemical alteration of PET via weathering processes, which substantially affects its biological interactions and toxicity. The absence of standardised environmentally pertinent PET micro- and nano plastics continues to pose a significant issue in experimental toxicology. This research emphasises the regulated synthesis-stimulated weathering and the physicochemical analysis of PET micro- and nano plastics to facilitate accurate toxicity evaluations. PET micro- and nano-plastics were synthesised using a controlled chemical fragmentation method to produce particles with diameters ranging from micro- to nanoscale. To replicate environmental ageing, the synthesised particles underwent UV weathering and Thermal weathering, mimicking photodegradation and temperature-induced changes that occur in natural circumstances. A thorough physicochemical characterisation of the synthesised and aged PET particles was conducted using SEM, dynamic light scattering and zeta potential. The production of precisely characterised PET micro- nano plastics offers a solid foundation for examining size and surface-dependent biological reactions, such as cellular uptake, oxidative stress induction, inflammatory signalling and disruption of barrier integrity in both in vitro and in vivo models. This study develops a replicable approach for generating environmentally relevant Pet-micro -and nano plastics, facilitating enhanced evaluation of their potential environmental and human health concerns.

References:

1. Andrady, A. L., Mar. Pollut. Bull., 62 (2011) 1596–1605.
2. Lambert, S., Wagner, M., Chemosphere, 161 (2016) 510–517.
3. Zhang, Q., Xu, E. G., Shi, H., Environ. Sci. Technol., 54 (2020) 2820–2829.
4. Villacorta, A., Rubio, L., Alaraby, M., López-Mesas, M., Fuentes-Cebrian, V., Moriones, O. H., Marcos, R., Hernández, A.,J. Hazard. Mater., 454 (2023) 131493.

Synthesis, Ageing, and Toxicity of Polypropylene Microplastic

Sanjeshri Patil[1], Sharine Priscilla[1], Meenakshi Podwal[1], Sushilkumar Ningthoucha[1], Aditya Bagkar[1], Sahabudeen Sheik Mohideen*[1]

[1] *Department of Biotechnology School of Bioengineering, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu District, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** sahabuds@srmist.edu.in

ABSTRACT

The rising accumulation of plastic debris has brought microplastics (MPs) and nano plastics (NPs) into a global environmental priority. Polypropylene (PP) microplastics are emerging environmental contamination of growing concern due to their extensive use, environmental persistence, and potential antagonistic biological effects. PP micro- and nano plastics persist in diverse environmental compartments, including aquatic, terrestrial, and atmospheric systems, where they interact with chemical pollutants and biological entities. PP- micro and nano-plastic were created through a controlled chemical fragmentation technique, which results in particle with diameters of micro- to nanoscale. To mimic environmental ageing, the produced particles were subjected to UV weathering and Thermal weathering which replicates photodegradation and temperature-mediated alterations that takes place naturally. The ability of aged PP particles to interact with co-contaminants and biological macromolecules may amplify their bioavailability and toxicity. Toxicological marks indicates that PP particles can induce oxidative stress, inflammatory responses, membrane damage, and metabolic disruption across multiple trophic levels. This study presents a reproductive and environmentally relevant strategy for generating and ageing polypropylene micro and nano plastic that convincingly reflect natural weathering processes. The Resulting particles provides a robust platform for assessing interactions with co-contamination and biological systems, thereby improving the reliability of laboratory-based evaluation of microplastic fate, toxicity, and potential environmental and human health risks.

References:

1. Andrady, A. L., Mar. Pollut. Bull., **62** (2011) 1596–1605.
2. Galloway, T. S., Cole, M., Lewis, C., Nat. Ecol. Evol., **1** (2017) 0116.
3. Sekar, V., Sundaram, B., Sci. Total Environ., **1012** (2026) 181175.
4. Rochman, C. M., Browne, M. A., Halpern, B. S., Hentschel, B. T., Hoh, E., Karapanagioti, H. K., Thompson, R. C., Nature, **494** (2013) 169–171.

EH-052

Tire Wear Particles: Controlled Generation and Characterization

Sushilkumar Ningthoucha[1], Sharine Priscilla[1], Meenakshi Podwal[1], Sanjeshri Patil[1], Aditya Bagkar[1], Sahabudeen Sheik Mohideen*[1]

[1] *Department of Biotechnology School of Bioengineering, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu District, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** sahabuds@srmist.edu.in

ABSTRACT

Tire wear particles produce 5,900,000 tonnes of environmental microplastics annually, but their physiochemical interactions with living organisms are uncertain. TWPs from tyre rubber, additives, and surrounding contaminants are complex and heterogeneous, making it challenging to gather consistent and comparable data across environmental samples and establish appropriate toxicity assessment. At the tire–road interface, TWPs are heterogeneous agglomerates of synthetic and natural rubber, carbon black and silica fillers, vulcanisation agents like sulphur and zinc oxide, heavy metals like Zn, Cd and Ba, oils, plasticisers and antioxidants, as well as pavement minerals, brake wear fragments, road dust and paint residues. These TWP spans from the nano- to micrometer scale, are denser than water, and can be transported via air, stormwater runoff, and riverine fluxes into soils, freshwater and marine systems, where they significantly burden both atmospheric and aquatic environments and contribute to inhalation risks and trophic transfer through food webs. Their complex composition and aging-dependent leaching of metals, PAHs, 6PPD-quinone and other tire-derived chemicals have been associated with oxidative stress, inflammation and ecotoxicity in aquatic and terrestrial organisms, yet environmental concentrations, size distributions, and mixture effects remain poorly constrained. Thus, the current study will generate environmentally relevant TWPs under controlled settings that simulate tire abrasion processes and characterise them to better understand their environmental and biological effects.

References:

1. Z. Gao, J. V. Cizdziel, K. Wontor, C. Clisham, K. Focia, J. Rausch, and D. Jaramillo-Vogel, Front. Environ. Sci., 10 (2022) 1022697.
2. P. J. Kole, A. J. Löhr, F. G. A. J. Van Belleghem, and A. M. J. Ragas, Int. J. Environ. Res. Public Health, 14 (2017) 1265.
3. B. Rosso, E. Gregoris, L. Litti, F. Zorzi, M. Fiorini, B. Bravo, C. Barbai, A. Gambaro, and F. Corami, Environ. Pollut., 326 (2023) 121511.
4. V. Spanheimer and D. Katrakova-Krüger, Sci. Rep., 11 (2021) 11961.

Unveiling LiF-Engineered MXene: A Novel $Ti_3C_2T_x$/ZnO Hybrid Composite for Highly Selective and Sensitive Chemiresistive NH_3 Detection via Schottky Barrier Modulation at Ambient Temperature

Gowri Shonali Natarajamani[1], Veera Prabu Kannan[2], Sridharan Madanagurusamy[1,3*]

[1]*Functional Nanomaterials & Devices Lab, Centre for Nanotechnology & Advanced Biomaterials and School of Electrical & Electronics Engineering, SASTRA Deemed to be University, Thanjavur, 613 401, India,*

[2]*Department of Metallurgical and Materials Engineering, IIT Madras, Chennai 600036, Tamil Nadu, India.*[1,3]*School of Arts, Sciences, Humanities & Education, SASTRA Deemed to be University, Thanjavur, 613 401, India.*

***Corresponding author e-mail:** m.sridharan@ece.sastra.edu*

ABSTRACT

The imperative for ammonia sensors to exhibit high selectivity and sensitivity, capable of detecting low ppm levels, is paramount for addressing toxicity risks, industrial hazards, and medical concerns. Nevertheless, MXene-based sensors often encounter performance constraints owing to residual Al impurities from the MAX phase, which hinder charge transport and surface reactivity. In this study, we developed a high-performance $Ti_3C_2T_x$/ZnO hybrid sensor through an innovative LiF-HCl-assisted Minimally Intensive Layer Delamination (MILD) etching method, eliminating the need for hazardous HF. Optimization of the LiF concentration significantly enhanced surface functionalization, resulting in high-purity, fully delaminated $Ti_3C_2T_x$ nanosheets with abundant active sites for gas adsorption and redox reactions. A $Ti_3C_2T_x$/ZnO hybrid composite was produced via DC reactive magnetron sputtering and drop-casting, establishing a Schottky junction to promote charge transfer. The resultant L3-$Ti_3C_2T_x$/ZnO sensor demonstrated a 50-fold enhancement in NH_3 sensitivity, a 4.5-fold acceleration in response at 5 ppm compared to pristine ZnO, and an ultra-low detection threshold of 0.1 ppm (4.52 ± 1.1). It exhibited rapid response (44 s) and recovery (26 s) times, high selectivity, remarkable stability over 60 days, and resilience to humidity fluctuations at 300 K. The superior sensing performance arises from synergistic charge modulation and interfacial redox activity in the L3-$Ti_3C_2T_x$/ZnO Schottky junction, enabling efficient hazardous gas monitoring.

Keywords: $Ti_3C_2T_x$, ZnO Films, NH_3, Chemiresistive Gas Sensors, Schottky barrier, Sustainable sensor

Reference:

1. G. S. Natarajamani, V. P. Kannan, and S. Madanagurusamy, J. Mater. Chem. A, 13 (2025) 16414–16436.

EH-054

Eco-Friendly Synthesis of Polyphenol Stabilized ZnO Nanoparticles from Pomegranate Peel Waste for Biomedical Energy Harvesting and Pre-Clinical Simulated Wound Monitoring Application

Akash Ghosh[1], Logesh Kumar Sellappan*[2], Janeni Natarajan*[3]

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*Indian Institute of Technology Madras, Chennai, Tamilnadu, India, 600036*

[3]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding authors e-mail:** logesh20feb@gmail.com and janenin@srmist.edu.in

ABSTRACT

The development of a Cost-Effective, bio-friendly nanomaterials through sustainable green synthesis routes has gained significant importance for Pre-Clinical Simulated Wound Monitoring application. In this study, Zinc Oxide (ZnO) nanoparticles were successfully synthesized using pomegranate peel extract as a natural reducing and stabilizing agent, providing a cost-effective and environmentally benign alternative to conventional chemical synthesis methods. The rich polyphenolic and antioxidant compounds present in pomegranate peel facilitated efficient nucleation, surface functionalization, and stabilization of ZnO nanoparticles. Comprehensive physicochemical characterization was carried out to evaluate nanoparticle quality and structural properties. Fourier transform infrared spectroscopy confirmed the presence of bioactive functional groups responsible for reduction and capping, while X-ray diffraction analysis revealed sharp and intense diffraction peaks corresponding to the hexagonal wurtzite crystal structure, indicating high crystallinity and phase purity. Field emission scanning electron microscopy demonstrated fine, quasi-spherical nanoparticles with minimal agglomeration, and energy dispersive X-ray analysis confirmed strong Zn and O elemental composition with negligible impurities. UV-Visible spectroscopy showed strong band-edge absorption with high absorbance intensity, indicating superior nanoparticle formation and uniformity. Zeta potential analysis revealed a highly stable colloidal system with strong negative surface charge, while particle size distribution analysis confirmed low polydispersity and reduced aggregation. These results collectively demonstrate that pomegranate peel extract enables the synthesis of highly stable, well-dispersed, and crystalline ZnO nanoparticles, making them highly suitable for efficient electromechanical energy conversion and advanced MedTech sensing applications.

References:

1. S. Chakraborty, A. Banerjee, and P. Ghosh, Carbohydr. Polym., 325 (2025) 121456.
2. G. De Marzo, F. Rizzi, and M. Rossi, ACS Appl. Mater. Interfaces, 14 (2022) 38921–38932.

EH-055

Investigating the Effects of Microplastics Isolated from Personal Care and Cosmetic Products in Drosophila Melanogaster

Harini S[1], Haritha S[1], Sruthi S[1], Sharine Priscilla[1], Meenakshi Podwal[1], Sajneshri Patil[1], Sushilkumar Ningthoucha[1], Sahabudeen Sheik Mohideen*[1]

[1]*Department of Biotechnology, School of Bioengineering, SRM institute of Science and Technology, Kattankulathur, Chengalpattu District, Tamilnadu, India, 603203*

***Corresponding author e-mail**: sahabuds@srmist.edu.in

ABSTRACT

Microplastics are minute plastic particles ranging in size from 1µm to 5mm. Their persistence in the environment, potential for bioavailability, and associated toxicity have raised growing environmental and public health concerns. Personal care and cosmetic products are recognized as a significant source of primary microplastics, as they are extensively used and commonly released into aquatic environments. These microplastics are added as microbeads, to increase product volume and serve the purpose of cleansing and exfoliation. This study focuses on the extraction and characterisation of microplastics from personal care and cosmetic products and tests their toxicological effects. Plastic microbeads were extracted using chemical digestion of the organic matrix and density separation methods from commercially available face scrubs in India. The presence of polyethylene microbeads was confirmed by physicochemical analysis of the extracted polymer using techniques such as Fourier Transform Infrared Spectroscopy (FTIR) and SEM-EDX. Following characterization, the biological impact of the extracted microplastics will be evaluated using *Drosophila melanogaster*, an *in vivo* experimental model for toxicity assessment due to its short lifecycle, genetic tractability, and high conservation of metabolic and stress response pathways with humans.

References:

1. Geyer, R., Jambeck, J. R., Law, K. L., Environ. Sci. Technol. Lett., 3 (2017) 320–326.
2. Xu, Y., Wang, J., Wang, S., Li, W., Environ. Pollut., 333 (2024) 122148.
3. Wang, L., Chen, Y., Zhang, X., Li, J., Zhao, H., Sci. Rep., 13 (2023) 41457.
4. Yadav, P., Rani, M., Chaudhary, S., Toxicol. Environ. Health Sci., 17 (2025) 275–289.
5. Chahal, S., Macairan, J.-R., Hernandez, L. M., Bui, H.-N. N., Smith, A., Larsson, H. C. E., Tufenkji, N., Environ. Health, 3 (2025) 747–756.

EH-056

Sustainable Valorization of Onion Peel Into Heteroatom-Doped Activated Carbon for Safranin-O Adsorption

M.Bhavani lakshmi[1], A.Alibasha[1], Quazi Arif Islam[2], Tanmay Chatterjee [3], Archana V [4], Mihir Ghosh[1*]

[1] *Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India*

[2] *Department of Chemistry, Birla Institute of Technology and Science, Pilani – Hyderabad Campus, Jawahar Nagar, Kapra Mandal, Hyderabad, Telangana 500078, India*

[3] *Department of Chemistry, Alipurduar University, P.O. – Alipurduar Court, District – Alipurduar, West Bengal 736122, India*

[4] *Department of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram (IISER TVM), Maruthamala P.O., Vithura, Thiruvananthapuram, Kerala 695551, India*

***Corresponding author e-mail:** mihirg@srmist.edu.in

ABSTRACT

Onion peel waste was converted into mesoporous activated carbon (OPP-1) via H_3PO_4 activation and pyrolysis at 600 °C. The material exhibited high surface area (535.5 $m^2\ g^{-1}$), mesoporosity, hydrophilicity, and heteroatom-enriched functionalities (C, O, N, P). Structural analyses (Raman, SEM, TEM, EDX, XPS) confirmed graphitized domains, porous morphology, and abundant active sites. OPP-1 displayed selective adsorption toward cationic dyes, achieving near-complete removal of Safranin-O (99.99%) and high efficiencies for Methylene Blue, Brilliant Green, and Methyl Violet, while anionic dyes were less adsorbed. Adsorption followed Langmuir isotherm and pseudo-second-order kinetics, driven by electrostatic attraction, pore filling, hydrogen bonding, and π–π interactions. OPP-1 remained highly reusable over 10 cycles, demonstrating its potential as a sustainable adsorbent for wastewater remediation.

Keywords: H_3PO_4 Activation, Waste onion peel, Safranine-O dye, Adsorption, Recyclability.

References:

1. G. Xu, J. Han, B. Ding, P. Nie, J. Pan, H. Dou, H. Li, X. Zhang, Biomass-derived porous carbon materials with sulfur and nitrogen dual-doping for energy storage, Green chemistry 17(3) (2015) 1668-1674.
2. F. Mbarki, T. Selmi, A. Kesraoui, M. Seffen, Low-cost activated carbon preparation from Corn stigmata fibers chemically activated using H3PO4, ZnCl2 and KOH: Study of methylene blue adsorption, stochastic isotherm and fractal kinetic, Industrial Crops and Products 178 (2022) 114546.
3. M. Rjeb, A. Labzour, A. Rjeb, S. Sayouri, M.C. El Idrissi, S. Massey, A. Adnot, D. Roy,Contribution to the study by X-ray photoelectron spectroscopy of the natural aging of the polypropylene, Moroccan Journal of Condensed Matter 5(2) (2004).
4. M. Thommes, K. Kaneko, A.V. Neimark, J.P. Olivier, F. Rodriguez-Reinoso, J. Rouquerol, K.S. Sing, Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution (IUPAC Technical Report), Pure and applied chemistry 87(9-10) (2015) 1051-1069.

EH-057

Fabrication and Performance Evaluation of WS_2/Ag NPs/ PVA Nanocomposite Dry Electrodes for Continuous ECG Monitoring

Arun Karthick S*[1]

[1]*Feynman Nano Laboratory, Department of Biomedical Engineering, Sri Sivasubramaniya Nadar college of Engineering, Kalavakkam, Chennai, Tamilnadu, India, 603110*

***Corresponding author e-mail**: arunkarthicks@ssn.edu.in

ABSTRACT

Long-term continuous biosignal monitoring is essential for early disease diagnosis and wearable healthcare applications; however, conventional wet silver/silver chloride (Ag/AgCl) electrodes suffer from gel dehydration, skin irritation, and signal degradation over prolonged use. This study aims to develop and evaluate a flexible, biocompatible dry electrode based on a tungsten disulfide/silver nanoparticle/polyvinyl alcohol (WS_2/Ag NPs/PVA) nanocomposite for reliable electrocardiogram monitoring. WS_2 was synthesized via a hydrothermal method and characterized using X-ray diffraction and field emission scanning electron microscopy. Ag NPs were incorporated through chemical reduction, followed by polymer blending with polyvinyl alcohol to achieve homogeneous dispersion. The composite solution was cast into films and dried at 60 °C for 8 h. Electrical impedance spectroscopy was performed to assess skin–electrode contact impedance. Later, electrocardiogram signals acquired using the fabricated electrode were compared with those obtained from commercial Ag/AgCl electrodes. Signal pre-processing included bandpass filtering (0.5–50 Hz), 50 Hz notch filtering, wavelet-based denoising (Daubechies 6), signal-to-noise ratio estimation, baseline wander analysis, R-peak detection, and heart rate variability metrics such as standard deviation of normal-to-normal intervals and root mean square of successive differences. The nanocomposite electrode demonstrated lower contact impedance and reduced baseline drift compared with commercial electrodes, while maintaining stable R-peak detection and comparable signal-to-noise ratio. These findings confirm that the WS_2/Ag NPs/PVA dry electrode offers a reusable, irritation-free, and high-fidelity alternative for long-term wearable cardiac monitoring, advancing the development of non-invasive smart healthcare systems.

References:

1. Liu H, Tian G, Zhao Q, Chen J, Liu Y, Liang C, Qi D, Advanced Fiber Materials, 7 (2025) 266-280.
2. Zhang XH, Yan CK, Cao HB, Tan H, Wang Z, Chalcogenide Lett., 19 (2022) 817-824.
3. Ferri J, Llinares R, Segarra I, Cebrian A, Garcia-Breijo E, Millet J, Electrochemistry Communications, 136 (2022) 107244.

EH-058

Polymorphic and Cocrystalline Architectures of Acetamiprid: Structural Elucidation, Enhanced Solubility, and Green Field Assay

Jubin Chacko, Palash Sanphui*

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu 603203

***Corresponding author e-mail**: palashi@srmist.edu.in

ABSTRACT

Acetamiprid, a widely used neonicotinoid insecticide, exhibits limited aqueous solubility and has been associated with inhibition of seed germination, posing challenges in agrochemical applications for crop protection. This study explores polymorphs and cocrystals of acetamiprid as crystal engineering strategies to enhance solubility while mitigating phytotoxic effects on seed germination. Novel polymorphs and multicomponent crystals were synthesised via solvent evaporation and mechanochemical methods, characterised using powder X-ray diffraction (PXRD), differential scanning calorimetry (DSC), Fourier-transform infrared spectroscopy (FTIR), and single-crystal X-ray diffraction (SCXRD). We prepared four cocrystals, such as ACTD-MALI, ACTD-TAR, ACTD-3HBA, and ACTD-4HBA. ACTD–MALI exhibited substantially improved aqueous solubility and a higher intrinsic dissolution rate. The influence of solid-state modification on biological performance was assessed through seed germination and early seedling growth studies. The parent acetamiprid form resulted in noticeable suppression of germination and reduced seedling vigour at equivalent concentrations. In contrast, the ACTD–MALI cocrystal showed a significantly lower inhibitory effect on both germination percentage and initial root and shoot development. The improved dissolution characteristics of ACTD–MALI are proposed to enable a more uniform and controlled release of the active ingredient in the aqueous environment surrounding the seed, thereby preventing the formation of locally high concentrations that are responsible for phytotoxic responses. Overall, the present study demonstrates that polymorph and cocrystal engineering can be effectively applied to optimise the physicochemical and biological properties of acetamiprid.

Keywords: Acetamiprid, Insecticide, Solubility, Prevent Inhibition of growth

EH-059

Microplastic Contamination in Aquatic Systems: Origins, Detection Techniques and Polymer Membrane-Based Removal Methods

Magesh S, Kalaivizhi R*

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu-603203, Tamilnadu, India

***Corresponding author e-mail**: kalaivir@srmist.edu.in

ABSTRACT

Microplastic (MP) contamination has become a significant ecological issue in the aquatic environment due to the high use of plastic and inadequate management of plastic waste. MPs originating from the effluents of different industries, as well as wastewater and drinking water treatment plants. Their tiny size, chemical diversity, and ability to carry hazardous contaminants and microorganisms pose a potential risk to the entire aquatic environment. Conventional water treatment systems are highly ineffective for removing MPs from water, which has led to the development of advanced removal techniques for MP removal in water. Polymer membrane-based MP removal caught the attention of researchers due to the tunable pore size, high selectivity, mechanical strength, and ease of surface modification. Commercially available PVDF, PES, and PTFE-based polymer membranes showed over 90% MP removal efficiency in water. Recent research progress in biopolymer membranes, mixed-matrix membranes (MMMs), and electrospun nanofibrous membranes (ENMs) has further enhanced removal performance and also improved hydrophilicity and antifouling properties of the polymer membranes. This review summarises an overview of MP origins, detection methods, and advances in polymer-membrane-based removal strategies, highlighting current challenges and prospects for large-scale applications.

Keywords: Microplastic origin and detection, Microplastic removal, Mixed matrix membrane, Polymer membrane, Water treatment

References:

1. Gopakumar, A. N., Ccanccapa-Cartagena, A., Bell, K., & Salehi, M. (2024). Development of crosslinked polyvinyl alcohol nanofibrous membrane for microplastic removal from water. *Journal of Applied Polymer Science*, *141*(22). https://doi.org/10.1002/app.55428
2. Shim, W. J., Hong, S. H., & Eo, S. E. (2017). Identification methods in microplastic analysis: A review. In *Analytical Methods* (Vol. 9, Issue 9, pp. 1384–1391). Royal Society of Chemistry. https://doi.org/10.1039/c6ay02558g
3. Zhang, Y. Q., Lykaki, M., Alrajoula, M. T., Markiewicz, M., Kraas, C., Kolbe, S., Klinkhammer, K., Rabe, M., Klauer, R., Bendt, E., & Stolte, S. (2021). Microplastics from textile origin-emission and reduction measures. In *Green Chemistry* (Vol. 23, Issue 15, pp. 5247–5271). Royal Society of Chemistry. https://doi.org/10.1039/d1gc01589c

EH-060

Carbamodithioate- Modified Nanoscale Zerovalent Iron: Redox-Active Hybrid for Cr (VI) and p-Nitrophenol Remediation

Harrish Tony Praveen Antoni Raja[1] and K.K.R. Datta[*]

[1]*Functional Nanomaterials Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology,*

Kattankulathur, India

***Corresponding author e-mail:** kumarard@srmist.edu.in

ABSTRACT

The rise of redox-active nanoscale zerovalent iron materials toward the decontamination of heavy metals and nitroaromatics is witnessing upward trend toward sustainable water treatment technologies. Herein, we synthesize air-stable carbamodithioate- modified nanoscale zerovalent iron (NZVI-CD) via in situ route at room temperature conditions. The structure, wetting, and morphology of NZVI-CD were evaluated using various characterization techniques like XRD, FT-IR, XPS, SEM, TEM, and water contact angle (WCA) measurements. NZVI-CD showcases the excellent reduction of hexavalent chromium and p-nitrophenol under room temperature and optimal pH conditions. Kinetic studies revealed that removal of hexavalent chromium and p-nitrophenol using NZVI-CD follows pseudo second order kinetics, besides favoring Langmuir adsorption isotherm model with a maximum sorption capacity (Qmax) of 178.57 mg g−1 and 45.45 mg g−1 for Cr (VI) and p-nitrophenol, respectively.

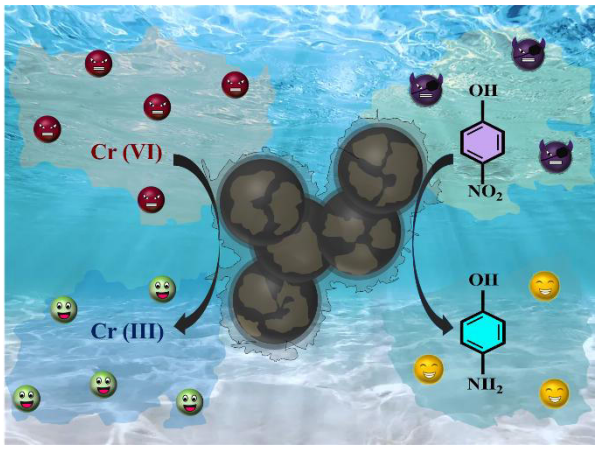


Fig 1. Reduction of Cr (VI) to Cr(III)

References:

1. L. Cancelada, J. M. Meichtry, H. Destaillats, and M. I. Litter, ACS Engineering Au 4 (2024) 464–473.

EH-061

Engineering Moisture-and Water-Resistant MOF-5 by Octaphenyl Polyhedral Oligomeric Silsesquioxane for Hydrophobic-Oleophilic Oil-Water Separation

Kanakarasu Dharmaraj[1], Mohandas Sanjay Kumar[2], Sankar Sathish[1], Muthuramalingam Prakash[2], Swaminathan Shanmugan[1]*

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India-603 203,*

[2]*Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India-603 203*

***Corresponding author e-mail:** shanmugs2@srmist.edu.in

ABSTRACT

The sustainable supply of clean water is one of the most important challenges for human societies. Because of the dramatic increase in the release of oil/water mixtures in the water bodies generated by domestic and industrial practices, water pollution has become a threat to all living environments, so the development of a non-toxic, eco-friendly hydrophobic/oleophilic material for oil-water separation is urgently needed. The polyhedral oligomeric silsesquioxane is an eco-friendly, non-toxic material with hydrophobic surfaces that will be a suitable material for oil/water separation applications, which offers effective functionalization and composition for the conversion of hydrophilic materials into hydrophobic materials, so we have prepared Ph-POSS@MOF-5 hybrid composite material via simple room temperature *in-situ* growth method for the conversion of hydrophilic and moisture sensitive MOF-5 to hydrophobic/oleophilic one for oil-water separation application. The synthesised Ph-POSS@MOF-5 hybrid composite material has been characterised through FT-IR, PXRD, BET, and Thermogravimetric analysis and it shows a contact angle of 140 ± 2° thus the synthesised material shows high selectivity and absorption capacity towards organic solvents and oils from water mixture. Concurrently, the Ph-POSS@MOF-5@PDA@Sponge has been effectively utilised for the separation of solvents and oils, showing more than 95% separation efficiency up to 20 cycles. More interestingly, the synthesised Ph-POSS@MOF-5 and Ph-POSS@MOF-5@PDA@Spinge show excellent stability towards harsh (acidic, alkaline) conditions, which is due to the presence of a mechanically and chemically stable inorganic-organic hybrid POSS nano cage. Based on the results obtained from this work, we suggest an eco-friendly, non-toxic hybrid composite material for efficient removal of solvents and oil pollution from water mixtures.

References

1. Shi, Z., Zhang, Z., Huang, W., Zeng, H., Mandic, V., Hu, X., Zhao, L. and Zhang, X., *Langmuir*, (2021), 37, 6728-6735.
2. Zhu, D., Shi, Z., Tan, X., Zhang, J., Zhang, S. and Zhang, X., *Applied Surface Science*, (2020), 527, 146741.
3. Zhang, W., Hu, Y., Ge, J., Jiang, H.L. and Yu, S.H., *Journal of the American Chemical Society*, (2014), *136*, 16978-16981.

EH-062

An Innovative Printed Device for Sensing of Exhaled Gas

Naveen Balaji[1,2], Dieu Linh Nguyen[1,3], Delli Babu[2] Thi Thu Vu[3], Jean-Christophe Lourme[4], Caroline Abreu[1], Sumangala T.P. [2], Benoît Piro*[1]

[1] *ITODYS, CNRS, Université Paris Cité, 75006 Paris, France*

[2] *Department of Physics, School of Advanced Sciences, Vellore Institute of Technology Vellore, Tamil Nadu, India - 632014*

[3] *University of Science and Technology of Hanoi, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, 100000 Hanoi, Vietnam.*

[4] *ValoTec, 1 mail du Professeur Georges Mathé, 94800 Villejuif, France*

***Corresponding author e-mail:** piro@u-paris.fr

ABSTRACT

Small Intestinal Bacterial Overgrowth (SIBO) and other food-related intolerances are increasingly diagnosed using breath tests that quantify hydrogen (H_2) and methane (CH_4) produced by bacterial fermentation. Although widely used in medical practice, current breath analysers exhibit significant limitations. Many systems cannot detect multiple gases simultaneously, some rely on reusable mouthpieces incorporating sensors that raise hygiene concerns, and others require large exhaled volumes due to remote sensor placement, making testing challenging for children and elderly patients. These constraints highlight the need for compact, low-cost, and highly sensitive sensing platforms suitable for point-of-care diagnostics.

In this work, we propose a fully printed gas sensor based on an original organic field-effect transistor (OFET) architecture functionalized with catalytic nanomaterials for hydrogen detection at room temperature. While conventional resistive gas sensors operate through changes in material resistivity upon gas exposure, transistor-based sensors offer intrinsic signal amplification via modulation of charge transport within the semiconducting channel. This architecture enables enhanced sensitivity while maintaining low power operation.

We demonstrate that the transistor configuration improves hydrogen sensitivity by approximately one order of magnitude compared to an equivalent resistive sensor fabricated from the same active material. Importantly, the device operates at room temperature, eliminating the need for integrated heaters and significantly reducing power consumption. The fully printed design further supports scalable and low-cost manufacturing, with the potential for disposable implementations to address hygiene requirements in clinical settings.

Overall, this work establishes organic transistor-based sensing as a promising strategy for next-generation breath analyzers, combining sensitivity, low power consumption, and patient-friendly design. The proposed approach opens new perspectives for reliable, non-invasive screening tools targeting SIBO and other gastrointestinal disorders.

Atomic-Scale Engineering of Sr-doped Bi_2MoO_6 for Ultrasensitive and Stable NO_2 Detection: Synergistic Enhancement via Catalytic Activation and Cloaking Effects

T. Ragavi [1], S. Harish S *[2], M. Navaneethan [2], M. Krishna Mohan *[1]

[1] *Center of Excellence in Materials for Advanced Technologies, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*Nanotechnology Research Centre, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** aravindharri@gmail.com

ABSTRACT

Nitrogen dioxide (NO_2) is a highly reactive atmospheric pollutant that causes significant health hazards when it is present beyond regulation thresholds. This study utilizes a Sr-doping method to alter the electronic structure of environmentally friendly Bi_2MoO_6 at the atomic scale, wherein substitutional Sr^{2+} generates defect-mediated sub-bandgap states that serve as efficient electronic intermediates. The emergence of these defect states results in bandgap narrowing and enhanced charge-carrier mobility, while the simultaneous development of bigger grains diminishes the density of grain borders, thereby lowering carrier scattering and promoting more efficient electron transport. The optimized 1 mol% Sr-Bi_2MoO_6 sensor, leveraging these synergistic effects, demonstrates an inherent selectivity for NO_2, achieving an experimentally validated detection limit of 83 ppb, along with rapid response and recovery times of 10 s and 60 s, respectively, at low operating temperatures. This study presents a flexible method for modifying band structure and microstructure to optimize charge-transfer energetics in oxide semiconductors, providing a reliable materials platform for selective and energy-efficient NO_2 sensing systems.

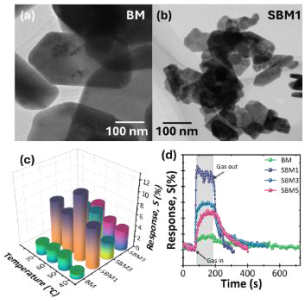


Fig. 1 (a,b) TEM analysis of pure Bi_2MoO_6 and 1% Sr doped Bi_2MoO_6 (c) Overall response and (d) Response and recovery time plot of all sensors.

Keywords: NO_2 sensing; fast kinetics; binary metal oxide; defect states.

EH-064

Binder-Free 3D CuO Nanowire Electrodes Decorated with Co and Ni Nanoparticles for Efficient Electrochemical Non-enzymatic Glucose Sensing

Sundararajan Karunakaran[1,2,3 *], Shinichi Mizuno[1,2], Abdul Kather Thameemul Ansari[1,2,4], J. Archana[3], M. Navaneethan[4], S. Harish[4], Hiroko Kominami[1], Atsushi Nakamura [1,2 *]

[1] *Graduate School of Science and Technology, Shizuoka University, Shizuoka, Japan,432-8011 Japan.*

[2] *Research Institute of Electronics, Shizuoka University, 3-5-1 Johoku, Naka-Ku, Hamamatsu, Shizuoka 432-8011, Japan.*

[3] *Centre of Excellence in Materials and Advanced Technologies (CeMAT), SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203.*

[4] *Nanotechnology Research Center, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203.*

***Corresponding author e-mail: nakamura.atsushi@shizuoka.ac.jp**

ABSTRACT

Glucose sensing technologies have garnered considerable attention due to their critical role in clinical diagnostics and personal healthcare, particularly in the monitoring and management of diabetes mellitus. Among the existing methodologies, electrochemical enzymatic sensors utilizing glucose oxidase are the most prevalently employed in commercial glucose monitoring systems. These sensors demonstrate high selectivity, exceptional sensitivity, and reliable performance under physiological pH conditions. Their sensing mechanism involves the enzymatic oxidation of glucose into gluconic acid, accompanied by the production of hydrogen peroxide, facilitating precise and selective detection. Despite these advantages, enzymatic glucose sensors have inherent limitations, including high fabrication costs, limited long-term stability, and susceptibility to environmental factors such as temperature and pH fluctuations. To address these limitations, non-enzymatic glucose sensors have emerged as a promising alternative, offering lower production costs, superior chemical stability, rapid response characteristics, and the potential for achieving lower detection limits. Unlike enzyme-based systems, non-enzymatic sensors rely on the direct electrochemical oxidation of glucose at the electrode surface, thereby circumventing enzyme degradation and extending operational lifespan. In this work, Hydrothermal and electrodeposition approach was used to grow CuO nanowire and Ni and Co nanoparticle deposition on the three-dimensional CuONW/Cu foam. It is anticipated that this technique will enhance the sensitivity and function as a binder free layer for charge transmission on Cu foam. The growth of CuO nanowire on the 3D-Cu foam is visible in the scanning electron microscopy image.

Keywords: CuO nanowire, Ni-Co nanoparticle, Electrodeposition, Glucose Sensing.

A Comprehensive Characterization of Oxygen and Sulfur-Doped Graphitic Carbon Nitride for Enhanced Functional Performance

Amarnath kumaran A[1], Vijaya Lakshmi V[2], Bakiya Lakshmi R[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*Department of Physics, Erode Sengunthar Engineering College, Erode - 638057, India*

***Corresponding author e-mail:** bakiyalr@srmist.edu.in

ABSTRACT

This study compares virgin graphitic carbon nitride (g-C_3N_4) to its O-doped (O- g-C_3N_4) and S-doped (S- g-C_3N_4) versions, all of which were made using a simple thermal polymerization method. Comprehensive characterization (XRD, FTIR, UV-Vis, PL, and SEM) confirmed the successful combination of both components, leading to significant functional alterations: The UV-Vis analysis showed that the band gap of both doped materials got smaller. S-g-C_3N_4 had the biggest red-shift and light absorption and PL spectroscopy showed that the emission intensity dropped a lot in both doped samples. Electron-hole pairs were better separated, SEM confirmed that O-g-C_3N_4 took on a shape that was very porous and foam-like, which was good for flat area. The results show that both oxygen and sulphur doping are good ways to change the properties of g-C_3N_4, which makes them good material for high-performance photo catalysis of non- metals.

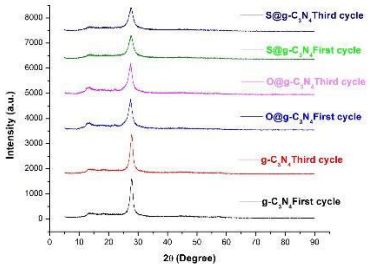


Fig. 1 - Reusability Analysis of pure and doped nanomaterials

References:

1. Cao S., Yang H., Zeng F., Lu Y., Chen H., Jiang F., ChemSusChem, 18 (2025) e202401570.
2. Jia X., Li Y., Liu X., Yu X., Wang C., Shi Z., Xing Y., Catalysis Science & Technology, 12 (2022) 5136–5146.
3. Mishra S. R., Gadore V., Ahmaruzzaman M., RSC Sustainability, 2 (2024) 91–100.
4. Hasija V., Singh P., Thakur S., et al., Chemosphere, 320 (2023) 138015.
5. Huang J., Wang H., Yu H., Zhang Q., Cao Y., Peng F., ChemSusChem, 13 (2020) 5041–5049.
6. You R., Dou H., Chen L., Zheng S., Zhang Y., RSC Advances, 7 (2017) 15842–15850.

EH-066

Facile Green Synthesis of ZnO/g-C_3N_4/Chitosan Ternary Nanocomposites for Photocatalytic Ciprofloxacin Degradation and Wastewater Disinfection

Oviya R, G Bakiyaraj*

Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603203, Tamil Nadu, India

***Corresponding author e-mail:** bakiyarg@srmist.edu.in

ABSTRACT

Wastewater contamination by pathogenic microorganisms and persistent pharmaceutical pollutants poses a serious global threat to public health. This highlights the urgent need for new nanomaterial approaches to inactivate pathogens and degrade pharmaceutical pollutants, thereby ensuring safe water reuse. The present study reports the facile and eco-friendly synthesis of ZnO-g-C_3N_4-Chitosan (ZGC) ternary nanocomposites, incorporating 10%, 20%, and 30% of g-C_3N_4, using *Sida acuta* leaf extract as capping agents. These ZGC nanocomposites were used to controlling the water pathogens and for *ciprofloxacin* (CIP) degradation. The ZGC nanocomposites were extensively characterized using techniques such as XRD, FTIR, UV–vis spectra, PL, zeta potential, SEM & EDS, TEM, XPS and BET surface area confirming their unique properties and structures. The photocatalytic activity of ZGC nanocomposites against CIP under sunlight degradation shows the highest activity for ZGC-20% was 76.8 % for the treatment of synthetic polluted water. This suggests a synergistic effect between the GCN and ZnO in enhancing the photocatalytic degradation of CIP. Moreover, the antibacterial activity against different types of bacteria shows that ZGC nanocomposites have maximum inhibition for *S. aureus* and *Escherichia coli, P. aeruginosa* highlighting their potential for controlling the bacterial population. This antibacterial activity is linked to ROS generation and membrane disruption Overall, the ZGC nanocomposite show promise as efficient photocatalysts for pollutant degradation in wastewater treatment and exhibit potential applications in pathogen removal due to their antibacterial properties. These findings contribute to the development of sustainable and multifunctional nanomaterials with diverse environmental and health-related applications.

Keywords: Zinc oxide, Sida acuta leaf, Chitosan, g-C_3N_4, Nanocomposite, Photocatalytic studies, antibacterial studies

Reference:

1. Aththanayaka, S., Thiripuranathar, G., & Ekanayake, S. (2025). Sustainable approach for fabrication of pineapple agro-waste mediated cellulose nanocrystals embedded with Ag/Ag2O/ZnO nanocomposites for efficient removal of waterborne pathogens in wastewater. *International Journal of Biological Macromolecules*, *310*, 143272.
2. Girish, Y. R., Byrappa, N. M., Alnaggar, G., Hezam, A., Nagaraju, G., Pramoda, K., & Byrappa, K. (2023). Rapid and facile synthesis of Z-scheme ZnO/g-C3N4 heterostructure as efficient visible light-driven photocatalysts for dye degradation and hydrogen evolution reaction. *Journal of Hazardous Materials Advances*, *9*, 100230.

Engineering Redox-Active MOFs for Field-Deployable Detection of Organophosphate Pesticides and Antibiotic Residues

Lakshya Sankhla[1] and Himmat Singh Kushwaha[2]*

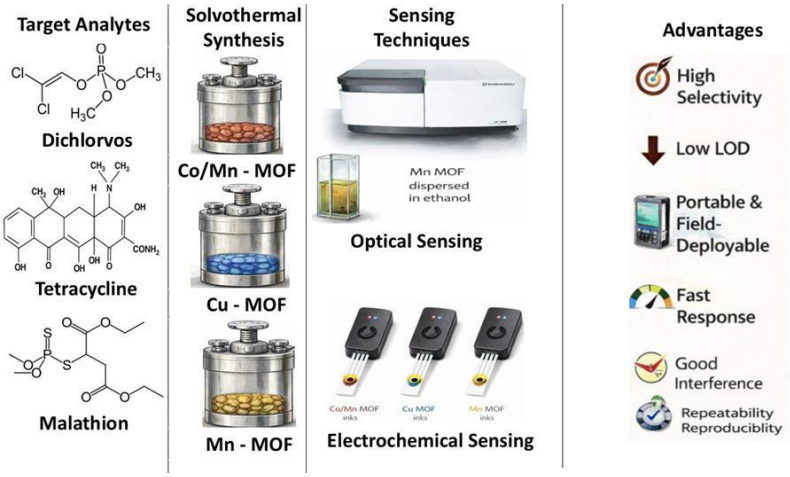
[1]*Undergraduate Department, Indian Institute of Science (IISc), Bengaluru, India- 560012*

[2]*Manipal University Jaipur, Jaipur, Rajasthan, India-303007*

***Corresponding author e-mail:** himmat.kushwah@jaipur.manipal.edu

ABSTRACT

Metal-Organic Frameworks (MOFs) are highly promising for environmental sensing because they possess a large surface area, flexible structures, controlled porosity, and numerous metal active sites that are readily accessible. In this research, mono- and bimetallic MOFs were systematically synthesised for electrochemical and fluorescence-based detection of hazardous contaminants. A Co/Mn bimetallic MOF was used for the electrochemical detection of dichlorvos, with synergistic redox interactions improving charge transfer kinetics and analytical sensitivity [1]. A Cu MOF was used to selectively detect tetracycline via strong metal-analyte coordination interactions [2]. Additionally, a Mn-MOF platform was developed for optoelectrochemical sensing of malathion, combining fluorescence spectroscopy with electrochemical signal transduction for dual-mode detection [3]. The constructed sensing platforms exhibited low detection limits, extensive linear ranges, elevated selectivity, and great reproducibility and repeatability, with little relative standard deviation over many cycles. These results show how useful MOF-based portable sensing devices may be for keeping surveillance on wastewater in real time and protecting the environment.



References:

1. L. Sankhla, M. Z. Abedeen, R. Gupta, and H. S. Kushwaha, J. Electrochem. Soc., 171, (2024)p. 066505.
2. L. Sankhla, A. Kumar, and H. S. Kushwah, Sci. Rep.,15(2025).
3. L. Sankhla and H. S. Kushwaha, Journal of Mat. Sci.: Mat. Eng., 19, (2024).

EH-068

Design and development of Ni MOF nanosheet-infused CA-modified PEI membrane for enhanced Congo red adsorption

Shanthi Kannivelan, Kalaivizhi Rajappan*

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu-603203, Tamil Nadu, India.

***Corresponding author E-mail:** kalaivir@srmist.edu.in

ABSTRACT

Adsorption by membrane technology has proven to be an effective solution for effluent purification in light of the increasing concern regarding dye-contaminated water, which can have long-term detrimental effects on biotic components. In this work, highly efficient membranes with excellent adsorptive characteristics were fabricated by incorporation of nickel metal-organic framework (Ni-MOF) in two different compositions (0.25 and 0.5%) into a citric acid (CA)-modified polyetherimide (PEI) membrane using a simple phase inversion technique with a focus to remove Congo red dye. Fourier-transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), field emission-scanning electron microscopy (FESEM), transmission electron microscopy (TEM), thermogravimetric analysis (TGA), and contact angle measurements revealed modifications in the crystalline structure, hydrophilicity, structural arrangement, and morphology of the pristine PEI membrane by the incorporation of the CA and metal-organic framework. UV-visible spectroscopic measurements were employed to assess the membrane's capacity to adsorb Congo Red (CR) dye from water. The Ni-MOF@CA/PEI polymer nanocomposite membrane, which contained 0.5 wt% Ni-MOF, exhibited an adsorption capacity of 23.3 mg/g and a superior dye removal efficiency of 93.4%. The adsorption process was characterized by pseudo-first-order kinetics, and the experimental data was in good agreement with the Langmuir adsorption isotherm. The membrane also exhibited excellent reusability, maintaining its efficacy over multiple cycles making it an effective adsorbent for the removal of congo red dye.

Keywords: Metal-organic framework, Nanocomposite membrane, Anionic dye, Interactions, Adsorption isotherm.

References:

1. Y. Kang, B. Zhang, J. Miao, Y. Yu, J. Fu, B. Jia, L. Li, Superparamagnetic Fe_3O_4@ Al-based metal-organic framework nanocomposites with high-performance removal of Congo red, J. Environ. Chem. Eng. 11 (2023) 109754.
2. M. Farooq, N. Rauf, S.A. Marwat, G. Shabbir, J. Ihsan, R.M. Mohamed, Facile synthesis and optimization of acacia senegal gum hydrogel for kinetically treated adsorptive removal of targeted industrial effluents, Int. J. Biol. Macromol. 279 (2024) 134879.

EH-069

Synthesis of But-2-yne-1,4-Diol Stabilized Gold Nanoparticles: An Efficient Catalyst for Methylene Blue and Rhodamine B Dye Degradation

Monika Senthilkumar and Anandhakumar Sukeri*

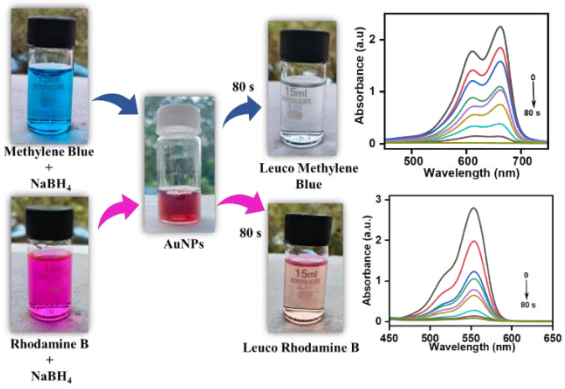
Nanoscale Materials Electrochemistry Laboratory, Department of Chemistry

SRM Institute of Science and Technology, Kattankulathur – 603203, Tamil Nadu, India.

***Corresponding author e-mail**: anandhas2@srmist.edu.in

ABSTRACT

A rapid and effective method for the synthesis of stable gold nanoparticles (AuNPs) from gold precursor and but-2-yne-1,4-diol, which serves as both reducing and stabilizing agent. The instantaneous colour change from yellow to wine-red indicates the formation of AuNPs at ambient temperature. UV-visible spectroscopy shows that the characteristic surface plasmon resonance peak at ~520 nm confirms the nanostructures of AuNPs. The XRD, HR-TEM, and XPS analysis confirms the face-centred cubic crystal structure, spherical particles with a size of ~5.0 nm ± 0.9 nm, and metallic nature of AuNPs, respectively. The catalytic activity of AuNPs was demonstrated for organic dye degradations using methylene blue (MB) and rhodamine B (RhB) as model compounds in the presence of sodium borohydride. The results indicate that MB and RhB dye degradation achieved ~99% and ~97%, respectively, within 80 sec. Such catalytic reactions follow the pseudo-first-order kinetics with the rate constants 0.059 s^{-1} and 0.045 s^{-1} for MB and Rh-B, respectively. Moreover, the high turnover frequencies (TOF) (MB = 223 h^{-1} and RhB = 146 h^{-1}) further confirm the excellent catalytic performance of the diol-stabilized AuNPs. Thus, the proposed simple methodology for the preparation of monodispersed AuNPs can be a potential candidate for clean water applications and environmental sustainability.



References:

1. Jeyabharathi, C., Karthik, P.E. and Phani, K.L.N, RSC Advances, 4(15), 2014, 7780-7785.
2. Shi, Y., Yang, Z., Xing, L., Zhang, X., Li, X. and Zhang, D., World Journal of Microbiology and Biotechnology, 37(8), 2021, 137.

EH-070

A Redox-Active Electron Acceptor Enabling Catalytic Oxygenation and Microgram-Scale Charge-Transfer Cocrystal Formation.

Logeshwari Seethapathy,[a] and Rajorshi Das[a]*

Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai - 603203, India.

***Corresponding author e-mail:** rajorshd@srmist.edu.in, rajorika@gmail.com.

ABSTRACT

2,4,6-Tri(4-pyridyl)-1,3,5-triazine (TPT) is a tripodal ligand widely used in the field of supramolecular chemistry due to its divergent applications in material science, catalysis and also in charge-transfer complexes.[1,2] With a triazine core and three pyridyl arms, TPT exhibits rigid planarity and high electron accepting ability, making it an excellent candidate for supramolecular assembly.[3] In this study, The trialkylated TPT shows remarkable electron accepting ability allowing us to perform metal-free supra catalytic oxygenation reactions of sulphur based derivatives such as tetrathiafulavalene and dibenzothiophene are otherwise readily inaccessible. It can also easily oxidize electron-rich metal complexes such as ferrocene and decamethyl ferrocene, upon simple co-crystallization. Cooperative π-π interactions that stabilize charge-transfer donor-acceptor interactions promote high-throughput crystallization with electron-rich donors, affording noncovalent cocrystals in microgram-scale quantities.

Keywords: supramolecular chemistry, trialkylated TPT, donor-acceptor interactions, metal-free oxygenation, high-throughput.

References:

1. Fujita, M.; Tominaga, M.; Hori, A.; Therrien, B. Coordination Assemblies from a Pd(II)-Cornered Square Complex. Acc. Chem. Res. 2005, 38 (4), 369–378. https://doi.org/10.1021/ar040153h.
2. Chakrabarty, R.; Mukherjee, P. S.; Stang, P. J. Supramolecular Coordination: Self-Assembly of Finite Two- and Three-Dimensional Ensembles. Chem. Rev. 2011, 111 (11), 6810–6918. https://doi.org/10.1021/cr200077m.
3. Cook, T. R.; Stang, P. J. Recent Developments in the Preparation and Chemistry of Metallacycles and Metallacages via Coordination. Chem. Rev. 2015, 115 (15), 7001–7045. https://doi.org/10.1021/cr5005666.

Development of $NaTaO_3/Co_3O_4$ Based Photocatalyst for Berberine Chloride Degradation

John Alphin Joseph [1], Aruljothy John Bosco[1*]

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603 203, Tamil Nadu, India.*

***Corresponding author e-mail:** johnbosa@srmist.edu.in,

ABSTRACT

Antibiotic pollutant released from pharma industries; animal sources pose severe threat to the water ecosystem. Physical, biological, chemical process of removing antibiotic pollutants suffer from few drawbacks such as requirement of secondary treatment, time consuming, release of toxic byproducts respectively. Photocatalysis is an alternating green and sustainable technology has known to be an effective strategy to degrade the pollutants. Herein, we synthesized the $NaTaO_3$, Co_3O_4 and $NaTaO_3/Co_3O_4$ composite through hydrothermal and calcination methods. XRD reveals the crystalline nature of $NaTaO_3$ and Co_3O_4. UV-DRS shows $NaTaO_3$, Co_3O_4 and $NaTaO_3/Co_3O_4$ has band gap of 4.12eV, 1.74eV and 3.79eV respectively. The bandgap of the composite decreased on the addition of different weight percentage of Co_3O_4. SEM analysis showed that $NaTaO_3$ exhibits cubic morphology and Co_3O_4 resembles nanosheets. The photocatalytic degradation of the berberine chloride showed that maximum degradation of 61% was achieved under visible light irradiation using $NaTaO_3/Co_3O_4$ nanocomposite.

Keywords: berberine chloride, degradation, perovskites, photocatalyst

References:

1. Rabé, K., Liu, L., Nahyoon, N. A., Zhang, Y., & Idris, A. M. (2019). Visible-light photocatalytic fuel cell with Z-scheme g-C3N4/Fe0/TiO2 anode and WO3 cathode efficiently degrades berberine chloride and stably generates electricity. Separation and Purification Technology, **212**, 774-782.
2. Yan, Z., & Shigang, S. (2011). Kinetics study on photocatalytic degradation of berberine hydrochloride in Nano-TiO2 suspension system. Journal of Hebei Medical College for Continuing Education, **28**(1), 12.

EH-072

Bimetallic Ce-Co-MOF with Enhanced Peroxidase-like Activity for the Highly Sensitive Colorimetric Detection of Amoxicillin

Surendhar Sasikumar, Panneerselvam Perumal*

Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, 603203 Tamil Nadu, India.

ABSTRACT

Antibiotic contamination in aquatic ecosystems represents a critical global threat to environmental stability and public health. Developing rapid, cost-effective, and highly sensitive analytical tools for the onsite monitoring of these pharmaceuticals remains a significant challenge. In this study, a bimetallic Ce-Co-MOF (Cerium-Cobalt Metal-Organic Framework) was synthesized and evaluated as a high-performance colorimetric sensing platform for the detection of amoxicillin. Comprehensive characterization using various analytical techniques confirmed the successful formation of the bimetallic framework, revealing high surface area, excellent structural stability, and a uniform distribution of redox-active metal centers. The peroxidase-like activity of the Ce-Co-MOF toward the chromogenic substrate 3,3',5,5'-tetramethylbenzidine (TMB) was systematically investigated. The catalytic mechanism is driven by the synergistic interaction between Ce and Co sites, which facilitates the decomposition of H_2O_2 to generate reactive oxygen species (ROS). These radicals efficiently oxidize colorless TMB into its blue-colored form (oxTMB), with a distinct absorbance peak at 652 nm. In the presence of amoxicillin, the catalytic oxidation is significantly modulated, allowing for precise quantification. The optimized colorimetric sensor exhibited a rapid response toward amoxicillin, delivering a wide linear detection range and a remarkably low detection limit is 0.24 µM. These results underscore the importance of bimetallic coordination and electronic tuning in MOF-based nanozymes, positioning Ce-Co-MOF as a promising candidate for rapid, visual, and low-cost antibiotic detection in environmental and clinical monitoring.

Keywords: Nanozyme activity, Peroxidase-mimetic catalysis, Amoxicillin detection, Bimetallic Ce-Co-MOF, Redox synergy.

EH-073

Porous N-Doped Carbon from Musa Acuminata Stem for Adsorptive Removal of Toxic Dyes and Pharmaceutical Drugs from Wastewater

Alibasha Akbar , M. Bhavani Lakshmi , Mihir Ghosh *

Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203, India.

***Corresponding author e-mail:** mihirg@srmist.edu.in

ABSTRACT

The persistent discharge of synthetic cationic dyes and pharmaceutical residues into aquatic environments necessitates the development of sustainable, high-performance sorbents for wastewater treatment. This study presents the design and synthesis of porous nitrogen-doped activated carbon (PNAC) derived from banana plant stems, demonstrating its excellent potential as a bio-based adsorbent for wastewater purification. PNAC exhibits a remarkably high surface area of 1978.8 m2 g−1 and abundant nitrogen functionalities that collectively enhance adsorption capacity, selectivity, and kinetics. It achieves over 95% removal of methylene blue, brilliant green, and crystal violet within 20 minutes, outperforming commercial activated carbon (84%, 54%, and 76% removal, respectively). The adsorption process follows the Langmuir isotherm model, confirming monolayer coverage, and proceeds through hybrid pseudo-second-order and intraparticle diffusion mechanisms. Thermodynamic analysis reveals a spontaneous and endothermic adsorption nature, indicating strong interactions between PNAC and the pollutant molecules. Beyond synthetic dye removal, PNAC also exhibits efficient uptake of pharmaceutical contaminants, 79.8% for ciprofloxacin and 81.1% for cefixime, within 30 minutes and achieves 97% dye removal from real textile effluents within 15 minutes. The material demonstrates excellent recyclability, retaining approximately 80% efficiency after five adsorption–desorption cycles and 85% after eight cycles of acid-assisted regenerations. These findings highlight PNAC as a scalable, eco-friendly, and high-performance sorbent derived from agricultural waste, offering a promising platform for next-generation wastewater treatment and sustainable environmental remediation.

References:

1. Z. M. Yunus, A. Al-Gheethi, N. Othman, R. Hamdan and N. N. Ruslan, Advanced methods for activated carbon from agriculture wastes; a comprehensive review, Int. J. Environ. Anal. Chem., 2022, 102, 134–158.
2. V. I. Isaeva, M. D. Vedenyapina, A. Y. Kurmysheva, D. Weichgrebe, R. R. Nair, N. P. T. Nguyen and L. M. Kustov, Modern carbon–based materials for adsorptive removal of organic and inorganic pollutants from water and wastewater, Molecules, 2021, 26, 6628.

EH-074

Pyrene-Based Fluorescent Probes for Selective Detection of Ciprofloxacin in Food and Environmental Samples

Amutha Selvaganesan[1], Venkatramaiah Nutalapati [1, 2*], Gopal Chandru Senadi[1*]

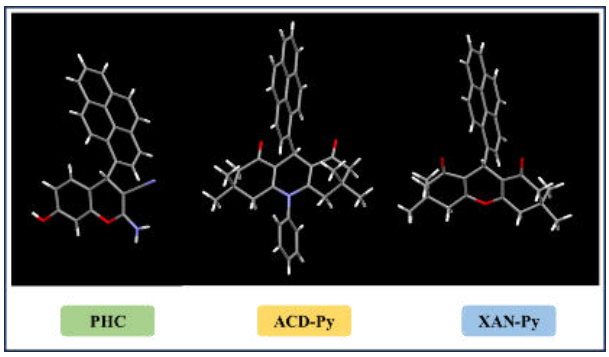
[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur, 603203, India.*

[2]*Centre for Interdisciplinary Research (CIDR), SRM University AP, Amaravati, Andhra Pradesh 522 240, India*

***Corresponding author e-mail:** chandrug@srmist.edu.in, Venkatramaiah.n@srmap.edu.in

ABSTRACT

Development of efficient fluorescent probes for antibiotic detection is of growing importance in environmental and food safety monitoring. In this study, we synthesized and evaluated three pyrene-based derivatives, PHC, ACD-Py, and XAN-Py, with various acceptors such as chromene, acridine, and xanthene using single crystal XRD, NMR, HR-MS, and other spectroscopic techniques. Detailed photophysical properties and the formation of excimer emission motivated to develop the *turn-on* fluorescence chemosensors towards the detection of antibiotics. Among all, XAN-Py emerged as the most effective probe, showing outstanding sensitivity and selectivity towards the detection of ciprofloxacin (CIP) with an exceptionally low detection limit of ~0.413 nM. The fluorescence response was rapid, stable, and consistent across a wide pH range, indicating robustness under complex environmental and biological conditions. The fluorescence enhancement mechanism was attributed to the inner filter effect (IFE) mediated by hydrogen-bond interactions. Selectivity is further confirmed through competitive studies involving structurally similar antibiotics. To complement experimental findings, density functional theory (DFT) calculations were employed to elucidate the electronic and photophysical properties of the derivatives. The practical applicability of XAN-Py was validated through successful detection of CIP in real-world samples, including water, milk, and fish. Additionally, a smartphone-assisted fluorometric platform is established, demonstrating the feasibility of portable and on-site analysis. Collectively, these results identify XAN-Py as a promising candidate for rapid ciprofloxacin detection in complex matrices.



References:

1. Mageshwari, N. Venkatramaiah, N. Sohrab, *Organic Electronics*, 136 (2025) 107162.
2. D. Van Dien, G. Akhilesh Babu, and D. Ruey-an, *ACS Appl. Mater. Interface,* 12 (2020) 32247–32258.
3. Y. Yingwang, C. Jinxuan*, and S. Yizhong*, *ACS Appl. Mater. Interfaces,* 12 (2020) 14552−14562.

EH-075

Biocatalytic Transformation of Benzil Using Endophytic Fungus Isolated from Tarlmounia Elliptica

Dheepthy Fabius S[1], Munuswamy-Ramanujam Ganesh*[1,2]

[1]*Department of Chemistry, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*IIISM, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** ganeshm1@srmist.edu.in

ABSTRACT

In the current study fungus mediated biotransformation, involves transforming the substrate using endophytic fungus. This type of transformation typically results in selective reaction by the fungus, which act as the biocatalyst. Endophyte is the microorganism that colonize with the plant, which enhance the resistivity to insects and helps the growth of the host plant. Applying these endophytes for chemical transformation process adds value to these microorganisms. In this study an endophytic fungus isolated from Tarlmounia elliptica successfully transformed aromatic compound benzil into benzoin. Characterisation of the product was carried out using UV, H^1 & C^{13} NMR. This indicates ability of the endophytic fungus to produce keto reductase. This type of selective reduction of one keto functionality in the presence of another keto group will be a valuable option in synthetic derivatization of molecules.

References:

1. P. Singh et al., *Biocatal. Biotransform.*, 2019, **37**, 304–309.
2. H. Tian et al., *Phytochemistry*, 2021, **185**, 112682.
3. Y. M. Ying et al., *Fitoterapia*, 2019, **138**, 104341.
4. L. Niu et al., *Int. J. Mol. Sci.*, 2022, **23**, 11935.
5. Z. Xu et al., *Appl. Biochem. Microbiol.*, 2020, **56**, 313–320.

EH-076

Heterostructured Co-MOF derived Co_3O_4/WS_2 Nanocomposites for Portable Electrochemical Detection of Allura Red

Jeevanantham Arumugam, Ganesan Shanmugam

Energy Conversion and Energy Storage Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu-603203, India.

***Corresponding author e-mail:** sakthi_ganesan@rediffmail.com, ganesans2@srmist.edu.in

ABSTRACT

Allura Red (ARD) is a synthetic dye widely used for food colouring, whose toxicity poses potential health risks. Herein, a disposable electrochemical sensor was fabricated with a MOF derived Co_3O_4 integrated WS_2 for ARD detection. Co_3O_4/WS_2 (MOS-10) heterostructure was synthesized hydrothermally which efficiently facilitated the electrochemical conversion of azo-enol form to keto-hydrazone form of ARD under optimized conditions (PBS of pH 7.0). The elevated electron transfer during ARD oxidation enabled by Co^{2+}/Co^{3+} redox couple, leads to the better electrocatalytic performance. The fabricated sensor exhibited a linear response from 0.33-6.7 µM, with a detection limit of 0.0058 µM, quantification limit of 0.0193 mM, and sensitivity of 20.65 µA μM^{-1} cm^{-2}. Overall, the sensing platform demonstrated good selectivity, stability, reproducibility, and successful quantified ARD in beverage samples, achieving satisfactory recoveries, demonstrating its potential for portable food dye monitoring.

EH-077

Mechanistic Understanding of c-CNF/CA/KGM SAPs Through Swelling Kinetics, DFT Calculations, and Molecular Docking for Sustainable Personal Hygiene Application

Cheera Prasad, Hyeong Yeol Choi*

Department of Fashion Design, Dong-A University, Busan 49315, Republic of Korea

***Corresponding authors:** spaachoi@dau.ac.kr

ABSTRACT

Superabsorbent polymers (SAPs) are hydrophilic, crosslinked materials capable of absorbing large amounts of water. However, most commercial SAPs are acrylic acid–based and exhibit poor biodegradability. In this study, environmentally friendly SAPs were developed using carboxymethylated cellulose nanofibrils (c-CNF), konjac glucomannan (KGM), and citric acid (CA) as a natural crosslinker. Characterization results confirmed that ester linkages formed between the carboxyl groups of CA and the hydroxyl groups of c-CNF and KGM, creating a stable hybrid polymeric network. Swelling performance decreased with increasing CA content due to higher crosslink density. The KGK2 sample showed the highest swelling in distilled water (88.43 g/g), while KGK4 exhibited the greatest swelling in 0.9 wt% NaCl solution (71.56 g/g). Swelling kinetics were well described by both the Fickian diffusion model and Schott's pseudo-second-order model, indicating diffusion-controlled absorption combined with polymer relaxation. Molecular docking studies revealed strong binding between KGK-based SAP and DNA gyrase, mainly due to carboxyl, carbonyl, ester, and hydroxyl groups. Density Functional Theory results supported these findings, showing high softness (0.3682 eV^{-1}) and electrophilicity, which enhance charge transfer and reactivity. Overall, the developed hydrogels demonstrate strong potential as biodegradable, sustainable materials for eco-friendly hygiene applications.

EH-078

Interfacial Engineering of Bi_2S_3 Thin Films Using an rGO Seed Layer for Enhanced Room Temperature H_2S Sensor

P. Priyadharsini[1], R. Abimaheshwari[1], E. Vinoth[1], S. Harish*[1], J. Archana[2], M. Navaneethan[1]

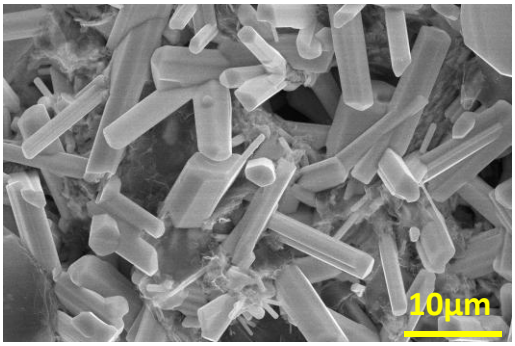
[1]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603 203.*

[2]*Center of Excellence in Materials for Advanced Technologies, Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203.*

***Corresponding author:** harishs@srmsit.edu.in

ABSTRACT

Hydrogen sulfide (H_2S) is a highly toxic and flammable gas widely released from petroleum refining, natural gas processing, and mining activities, posing serious risks to human health and the environment. Therefore, the development of sensitive and reliable H_2S sensors operating at room temperature is critically important. In this work, we report an interfacial engineering strategy to enhance the room-temperature H_2S sensing performance of Bi_2S_3 thin films using a reduced graphene oxide (rGO) seed layer. The rGO interlayer significantly influences the nucleation and growth behavior of Bi_2S_3 during chemical vapor deposition, leading to the formation of longer, denser microrods with improved crystallinity. In addition to structural improvement, rGO provides a highly conductive pathway and forms a heterojunction interface with Bi_2S_3 facilitating efficient charge carrier transport and reducing the overall resistance of the sensing layer. As a result, the rGO-assisted Bi_2S_3 sensor exhibits a higher sensing response of 44.3% for 8 ppm H_2S, good selectivity, reversibility and long term stability at room temperature.



References:

1. Yu, Meiling, Jiayu Li, Dongmin Yin, Zhenze Zhou, Chenda Wei, You Wang, and Juanyuan Hao." *Journal of Hazardous Materials* 476 (2024): 134932.
2. Rosolina, Samuel M., Thomas S. Carpenter, and Zi-Ling Xue. *Analytical chemistry* 88, no. 3 (2016): 1553-1558.

EH-079

Room-Temperature Ammonia Detection Using 2H-Phase MoS_2 for Sustainable Environmental and Health Monitoring

Hiritika[1], Aman Mahajan*[1]

[1]*Guru Nanak Dev University, Amritsar, Punjab, India, 143005*

***Corresponding author e-mail:** aman.phy@gndu.ac.in

ABSTRACT

Ammonia (NH_3) is a toxic environmental pollutant and an important biomarker associated with various human health conditions, making its rapid detection crucial for environmental safety and medical monitoring. However, conventional metal-oxide gas sensors typically require high operating temperatures (200-400 °C), leading to high energy consumption and limiting their application in portable sensing systems. In this work, hexagonal (2H) phase molybdenum disulfide (MoS_2) was synthesized via a hydrothermal method and employed to fabricate a chemiresistive gas sensor capable of operating at room temperature. Structural analysis using X-ray diffraction and Raman spectroscopy confirmed the formation of the 2H-MoS_2 phase. The fabricated sensor exhibited excellent selectivity towards NH_3 over interfering gases such as ethanol, methanol, and hydrogen peroxide. A sensing response of 22.13% was obtained for 20 ppm NH_3 with response and recovery times of 175.64 s and 120 s, respectively. Furthermore, the response increased from 25.2% at 40 ppm to 50.9% at 100 ppm NH_3. These results demonstrate the potential of 2H-MoS_2 as a promising material for low-power, sustainable environmental and health monitoring applications.

References:

1. B. Chen, X. Liu, S. Wu, J. Hou, P. Shang, Y. Chamba, K. Mehmood, D. Fouad, Y. Li AND H. Zhang. Science of The Total Environment 912, (2024), 169036.
2. R. J. Rath, S. Farajikhah, F. Oveissi, Z. Shahrbabaki, F. Dehghani, S. Naficy and J. Yun. Advanced Sensor Research 3, (2024), 2300125.
3. J. Cao, J. Zhou, J. Chen, W. Wang, Y. Zhang and X. Liu. ACS Omega 5, (2020), 28823–28830.

EH-080

Sustainable Sequential Precipitation Strategy for Selective Recovery of Gold and Copper from E-Waste

Madhumitha Manickasundaram[1], Sajith Babu M K[2], and Srinivasarao Kancharla*

Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India.

***Corresponding author e-mail:** srinivak5@srmist.edu.in

ABSTRACT

The sustainable recovery of noble metals from electronic waste is closely linked to environmental protection and public health monitoring [1]. In this study, we report a sequential, precipitation-assisted extraction strategy for the selective recovery of gold and copper from aqua regia leachates of discarded CPU pins. Gold was selectively precipitated as tetraphenylphosphonium tetrachloroaurate ($TPPAuCl_4$) via a double displacement reaction, achieving 99% recovery even at trace concentrations (0.5 ppm) and exhibiting a high precipitation capacity of 466 mg g^{-1}. Subsequently, copper was efficiently recovered as $Cu(DDTC)_2$ (98%) through a pH-controlled coordination precipitation process. The recovered complexes were systematically characterized using XPS, HR-MS, and UV–Vis spectroscopy, and chemical reduction of $TPPAuCl_4$ yielded metallic gold with 99.8% purity (23.94 karats). Importantly, this method eliminates the need for conventional liquid–liquid extraction involving volatile organic solvents, thereby reducing secondary pollution and associated health risks. The use of a commercially available and recyclable reagent (TPPBr) further enhances process sustainability and operational feasibility. By integrating high selectivity, trace-level recovery, and environmentally benign processing, this approach provides a practical framework for multi-metal recovery from e-waste. It contributes to environmental monitoring efforts by mitigating toxic metal discharge and supports safer resource recycling practices aligned with public health and sustainable industrial development [2].

Keywords: E-waste, sustainable metal recovery, gold and copper recovery, tetraphenylphosphonium bromide, sodium diethyldithiocarbamate, sequential precipitation to minimize secondary pollution.

References:

1. Işıldar, E.R. Rene, E.D. van Hullebusch, P.N.L. Lens, Electronic waste as a secondary source of critical metals: Management and recovery technologies, Resour. Conserv. Recycl. 135 (2018) 296–312.
2. M. Manickasundaram, S. Babu M K, J. Wen, E. Byeon, K. Sekar, H. Kim, S. Kancharla, Sequential Precipitation-Assisted Selective Recovery of Gold and Copper from E-Waste, Ind. Eng. Chem. Res. 64 (2025) 24884–24894.

EH-081

Mxene-Integrated $CuWO_4$ Nanocomposite by Hydrothermal Synthesis and its Characterization for Photocatalytic and Biological Application

Sherin Celshia S[a], Jency Sebatine P[c], K. Arul varman[b], Muthamizh S*[a]

[b]*Department of Physiology, Saveetha Dental College & Hospitals, Saveetha Institute of Medical & Technical Sciences, Saveetha University, Chennai - 600077, Tamil Nadu, India.*

[b]*Department of Physics & Nanotechnology, SRM Institute of Science & Technology, Kattankulathur-603203, Tamil Nadu, India.*

[c]*Department of Physics, Presidency College Chennai 600005, Tamil Nadu, India.*

***Corresponding authors e-mail:** muthamizh23@ymail.com.

ABSTRACT

Copper tungstate ($CuWO_4$) nanoparticles and their composite with titanium carbide (TiC) were synthesized and investigated for structural, optical, and antibacterial properties. $CuWO_4$ was prepared by a hydrothermal route followed by calcination, while TiC was obtained from titanium aluminium carbide through selective etching. The $CuWO_4$/TiC composite was fabricated via ultrasonication. X-ray diffraction (XRD) confirmed the triclinic phase of $CuWO_4$. The composite displayed additional diffraction peaks at 8.2°, 19.0°, and 22.0° corresponding to TiC planes, confirming successful incorporation. FT-IR spectra of $CuWO_4$ exhibited characteristic bands at 909 cm^{-1} (W–O stretching), 726 cm^{-1} (Cu–O stretching), and 468 cm^{-1} (CuO vibrations), with noticeable band narrowing upon TiC addition, indicating lattice modification. UV–Visible diffuse reflectance spectroscopy (DRS-UV) revealed strong absorption of $CuWO_4$ between 350–650 nm, with band gap narrowing compared to WO_3. The composite showed additional absorption near 645 nm due to TiC, enhancing visible-light activity and utilized for the photocatalytic degradtion of industrial dye. Antibacterial activity was assessed using the well diffusion method against Staphylococcus aureus and Enterococcus. Overall, the $CuWO_4$/TiC nanocomposite showed improved crystallinity, optical absorption, and antibacterial efficiency, highlighting its potential in antimicrobial and photocatalytic applications.

Keywords: $CuWO_4$, $CuWO_4$/TiC, Hydrothermal, Photocatalysis, Antibacterial activity.

Bimetallic MOF for Wearable Electrochemical Glucose Sensor

Parkkavi K[1], Ajay Rakkesh R[1*]

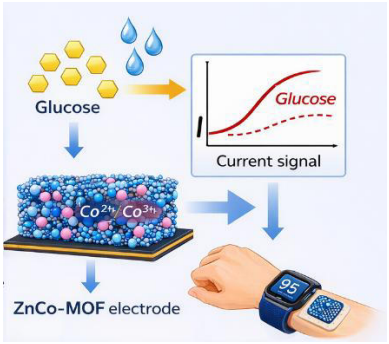
[1]*Funtional Nano-Material (FuN) Laboratory, Department of Physics*

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail:** ajayr1@srmist.edu.in, ajayrakkesh@gmail.com

ABSTRACT

Wearable glucose sensing technologies are gaining significant attention for continuous and non-invasive monitoring in personalized healthcare. In this work, a bimetallic metal–organic framework based on a ZnCo-imidazole framework (ZnCo-Im MOF) was developed as an electrocatalytically active material for a nonenzymatic wearable glucose sensor. The synergistic interaction between Zn and Co metal centers within the porous imidazole-linked structure enhances catalytic activity and structural stability. The high surface area and interconnected pores facilitate rapid glucose diffusion and provide abundant active sites for glucose oxidation. Electrochemical studies using cyclic voltammetry and amperometry demonstrated strong catalytic activity in alkaline medium, driven by the reversible Co^{2+}/Co^{3+} redox transition. The sensor exhibited high sensitivity, rapid response, low detection limit, and improved electron transfer compared with single-metal MOF systems.



Keywords: Bimetallic MOF, synergistic effect, charge transfer kinetics

References

1. Liu, J., Shi, L., Shi, Y., Zeng, Q., & Yang, Y. (2024). Glucose sensing performance of bimetallic MOFs CoFe-ZIF/CC for enzyme-free saliva sensor applications. *Journal of Alloys and Compounds*, *999*, 174733.
2. Zhang, Y., Yu, X., Hou, Y., Liu, C., Xie, G., & Chen, X. (2024). Current research status of MOF materials for catalysis applications. *Molecular Catalysis*, *555*, 11385.

EH-083

Real-Time Gastrointestinal Transit Tracking Using Intelligent Textile-Based Wearable Devices

Jayaram Alais Jaii A[1], Dr. Bhargavi Haripriya A[1*]

[1] *Department of Biomedical Engineering, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, India – 603203*

***Corresponding author e-mail:** bhargava@srmist.edu.in

ABSTRACT

Gastrointestinal disorders are often linked to abnormalities in stomach motility, which affect the normal movement of food through the digestive system. Monitoring stomach activity is important for diagnosing and managing these conditions, but current diagnostic methods are usually hospital-based, invasive, and performed only for short periods. This makes continuous monitoring and early detection difficult. The proposed study focuses on developing a wearable, non-invasive device for real-time monitoring of gastrointestinal activity. The device records the electrical signals of stomach muscles through the abdominal skin using electrogastrogram (EGG) signals. These signals reflect gastric slow-wave activity, which represents normal or abnormal stomach rhythms. With real-time data processing and analysis, the system can help interpret gastric patterns more easily. Due to its low cost, portability, and lightweight design, the device can support long-term monitoring outside hospital environments.



Fig. 1a) Wearable Gastrointestinal Monitoring T-Shirt Prototype 1 b) Real-Time EGG Monitoring Mobile Application

Keywords: Gastrointestinal Motility, Electrogastrography (EGG), Wearable Devices, Real-Time Monitoring, Non-Invasive Healthcare, Gastric Electrical Activity.

References

1. S. Reddy, P. Chawla, J. Med. Devices Digit. Health, 12 (2025) 45–58
2. S. Parama Sivam, K. Kamal Anand, Biomed. Signal Process. Control, 60 (2020) 101987.

Enhanced Sensing properties of Y-doped Bi_2S_3 Nanostructures for NO_2 Detection

Aashna Sharin M[1], Vinoth E[2] Archana J[3], Navaneethan M[2*], Karthigeyan A[1*]

[1]*Hydrogen Storage Materials and Nanosensors Laboratory, Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science & Technology, Kattankulathur-603203, Tamil Nadu, India.*

[2]*Nanotechnology Research Centre, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India.*

[3]*Centre of Excellence in Materials and Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603 **203, India.***

***Corresponding author's e-mail**: karthiga@srmist.edu.in, navaneem@srmist.edu.in

ABSTRACT

Rapid industrialization and the expansion of transportation systems have resulted in the continuous release of harmful gases into the atmosphere, posing serious environmental and health risks. Among these pollutants, nitrogen dioxide (NO_2) is particularly dangerous, as long-term exposure can cause severe respiratory disorders and other health complications. Consequently, there is a strong need for affordable, highly sensitive gas sensors capable of detecting low concentrations of NO_2. Bismuth sulfide (Bi_2S_3) is a narrow band gap semiconductor (1.3–1.7 eV) that has attracted considerable interest due to its potential applications in solar cells, gas sensors, electronic and optoelectronic devices, and hydrogen storage systems. Its high surface reactivity and large surface area make it especially promising for NO_2 sensing applications. The incorporation of suitable dopants into Bi_2S_3 can further enhance gas adsorption–desorption dynamics by increasing the number of active sites and improving charge transfer processes. In this work, pure Bi_2S_3 and yttrium (Y)-doped Bi_2S_3 were synthesized using a hydrothermal method, and their structural, morphological, and gas-sensing properties were systematically investigated. The results demonstrated that dopant incorporation significantly enhanced the sensing performance compared to pristine Bi_2S_3. Notably, the 1% Y-doped Bi_2S_3 sample exhibited an exceptional response of 3419% toward 5 ppm NO_2 at 50 °C, highlighting its strong potential for low-temperature NO_2 detection.

References:

1. Hesterberg TW, Bunn WB, McClellan RO, Hamade AK, Long CM, Valberg PA. Critical reviews in toxicology. 2009 Oct 1;39(9):743-81.
2. Yang Y, Zhu M, Zhang H, Wang B, Chen C, Li J, Wang Y, Hao J. Chemical Engineering Journal. 2024 Jun 15; 490:151872.
3. Chen X, Wang T, Shi J, Lv W, Han Y, Zeng M, Yang J, Hu N, Su Y, Wei H, Zhou Z. Nano-micro letters. 2022 Dec;14(1):8.

EH-085

Optimizing the Influence of Bimetallic Oxides $NiMoO_4$ for Ultra-Sensitive NO_2 Detection at Room Temperature

Shubalakshmi T [1], Vinoth E [2], Sathiyamoorthy K[2], Navaneethan M [1,2], Kirshna Mohan M [1*]

[1] *Centre of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

[2]*Nanotechnology Research Centre (NRC), SRM Institute of Science and Technology (SRMIST),Kattankulathur 603203, India*

***Corresponding author e-mail:** krishnam1@srmist.edu.in

ABSTRACT

The growing demand for low-temperature metal oxide sensors has stimulated the development of a continuous, interdigitated chemical sensor for the detection of NO_2 gas. Hydrothermally grown nanorods with monoclinic crystal structure $NiMoO_4$ (NMO) were coated on the active surface of the substrate by the physician-blade method. Active cation centers in the form of a multiple oxidation-state of the catalytic centre of the alpha-$NiMoO_4$ (Ni^{2+} or Mo^{6+}) and the formation of the beta-$NiMoO_4$, leading to a highly sensitive NO_2 detection. However, in order to increase the effective NO_2 detection, isovalent tungsten is substituted for $NiMoO_4$ in the assay. Impact of tungsten-doped α-$NiMoO_4$ on enhanced sensory properties. The kinetics of response and recovery of $NiMoO_4$ in pristine and tungsten-treated samples were examined. Among samples of 1%, 3%, 5% and 7%, the sample of W-doped NMO1 shows a high response of 40% to NO_2 gas, which is higher than the pristine NMO. The remarkable sensing performance of the sample of 1% is due to the enhanced charge transfer kinetics, lattice defects and surface oxygen vacancy reactions, which affect the environmental monitoring sensing performance. The detection limit is tested at 1 ppm and shows a different selectivity for NO_2 compared to other interfering gases such as H_2S, SO_2, NH_3 and volatile organic compounds such as ethanol and IPA, with a stability of approximately 70 days. Thus, bimetallic oxide $NiMoO_4$ provides a starting material for gas detection applications at room temperature and with low energy consumption.

References:

1. Xuelan Cheng, Yizheng Liu, Wei Zhong, Shuai Li, Yan Li, Zixi Zhao, Chunlei Zhang, Jidong Shi, Hui Liu, Zonglong Zhu, and Fang Xu
2. N. Padmanathan a,b , Han Shao a , Kafil M. Razeeb
3. Yao Zhang,ab Haoran Guo,a Xinpan Li,c Wenlu Rena and Rui Song

Acoustic Feature Dynamics of Bowel Sounds Prior to Defecation

Lavanya Maruthachalam*[1], Shota Miyagawa[2], Shobana Devi A[1], Kazushi Ikeda[2]

[1] *Department of Data Science and Business Systems, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India – 603203*

[2] *Nara Institute of Science and Technology (NAIST) Ikoma, Nara, Japan*

***Corresponding author e-mail:** lm9435@srmist.edu.in

ABSTRACT

Bowel sounds provide important, non-invasive way to observe gastrointestinal activity. Although earlier research has reported that number of bowel sounds often increases before a bowel movement, it still needs study whether the acoustic properties of individual bowel sound events themselves change as defecation approaches.

This study, examines acoustic characteristics of bowel sounds evolve over time prior to defecation using signal-processing techniques. A dataset containing 6,316 segmented bowel sound events extracted from long-duration abdominal recordings was analysed. Events were identified using WebRTC Voice Activity Detection algorithm and linked with metadata indicating remaining time until next defecation event. Each audio segment was then processed using a hybrid feature extraction framework and Teager–Kaiser Energy Operator energy.

To investigate how these features evolve over time, extracted parameters were analysed relative to time remaining until defecation. Two complementary approaches were applied: Spearman rank correlation to examine monotonic trends and non-parametric near-versus-far comparisons ($\leq$ 60 mins vs $\geq$ 8 hours before defecation) to identify distributional differences. Spectral characteristics and measures of signal irregularity show consistent differences between sounds recorded close to defecation and those occurring much earlier.

Overall, findings suggest that bowel sound acoustics tend to change gradually rather than abruptly as defecation approaches. Results highlight potential of bowel sound analysis as a complementary tool for studying digestive physiology and for developing future biomedical monitoring systems.

Keywords: bowel sounds, acoustic feature analysis, temporal analysis, signal processing, spectral analysis, gastrointestinal acoustics, time-to-event modelling, biomedical acoustic sensing

References:

1. S. Miyagawa, T. Yamakawa, M. Tanabe, and K. Ikeda, “Detecting Defecation Premonition from the Acoustic Activity of Bowel Sounds,” in *Proc. Asia Pacific Signal and Information Processing Association Annual Summit and Conference (APSIPA ASC)*, 2025, pp. 1663–1668.
2. S. Marumoto, T. Kubo, M. Tada, and K. Ikeda, “Defecation prediction system using bowel sound,” *IPSJ Transactions on Bioinformatics*, vol. 15, pp. 17–21, 2022.
3. T. Haraguchi, T. Emoto, K. Kozuka, and H. Kobara, “Bowel sound feature-based stimulus/response plots to differentiate healthy controls from functional constipation and functional diarrhea,” *IEEE Access*, vol. 13, pp. 148396–148404, 2025.

EH-087

Accelerating Carbon Capture Materials Discovery: A Machine Learning Framework for Predicting CO_2 Adsorption and Structure-Property Relationships in MOFs

Tanishka Pal[1,2], Xavier Mulet[2], Sarbani Ghosh[*1]

[1]*Department of Chemical Engineering, Birla Institute of Technology and Science (BITS), Pilani Campus, Vidya Vihar, Pilani, 333031, Rajasthan, India*

[2]*School of Science, RMIT University, Melbourne, VIC, 3000 Australia*

***Corresponding author e-mail**: sarbani.ghosh@pilani.bits-pilani.ac.in

ABSTRACT

Metal-organic frameworks (MOFs) are promising candidates for carbon capture due to the ease with which the material properties can be tailored. MOFs can offer lower regeneration energy requirements and higher CO_2 capture selectivity compared to the other materials and techniques that are currently used for CO_2 capture. Rational design of effective materials for carbon capture applications demands a fundamental understanding of the CO_2 adsorption phenomenon occurring in the MOFs. Calculation of the CO_2 adsorption capacity of the MOFs by conventional trial-and-error experiments demands sophisticated experimental techniques and costly equipment. Additionally, calculating the CO_2 adsorption capacity of MOFs using molecular simulation techniques also incurs high computational costs. To overcome the above issues, a machine learning (ML) technique was applied to the prediction and understanding of the CO_2 adsorption phenomenon. A comprehensive dataset of the MOFs with diverse physical, structural, and chemical properties was used to train the ML model to effectively capture the CO_2 capture phenomenon. Benchmarking of the machine learning model's performance with respect to the CO_2 adsorption phenomenon was carried out by the application of effective statistical measures. These machine learning frameworks successfully reconstructed CO_2 adsorption isotherms across a diverse range of operating pressure regimes, with excellent agreement with simulated or experimental results. Apart from the prediction accuracy of the machine learning model with respect to the CO_2 capture phenomenon, another important aim of the research investigation was to obtain a deeper understanding of the physical chemistry phenomenon from the dataset. The SHAP (SHapley Additive exPlanations) analysis technique was applied to the dataset to effectively understand the driving forces behind the CO_2 adsorption phenomenon. This analysis showed the existence of a hierarchy of structural properties with respect to the CO_2 capture phenomenon. Additionally, the analysis revealed that, in addition to the thermodynamic operating pressure and the physical properties of the MOFs, the chemical properties also play a dominant role in the CO_2 capture phenomenon.

References:

1. Meduri, S.; Nandanavanam, J. Energy and AI 2023, 12, 100230.
2. Xin, R.; Wang, C.; Zhang, Y.; Peng, R.; Li, R.; Wang, J.; Mao, Y.; Zhu, X.; Zhu, W.; Kim, M.; Nam, H. N.; Yamauchi, Y. ACS Nano 2024.
3. Orhan, I. B.; Le, T. C.; Babarao, R.; Thornton, A. W. 2023, 6, 214.

EH-088

Portable LED-Photodiode Based Colorimetric Sensor for PFAS detection Integrated Pith Mobile App

Parikshit Adhikari[1], Dr. Jaligam Murali Mohan[1*]

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** jaliagmm@srmist.edu.in

ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are a large group of synthetic chemicals containing strong carbon–fluorine (C–F) bonds. They found in nonstick cookware, water-repellent fabrics, firefighting foams, food packaging, and industrial applications. As known as "Forever chemicals", they are extremely resistant to degradation in the environment and in the human body and are subsequently highly carcinogenic. They accumulate in water, soil, and living organisms, leading to worldwide human exposure and hence the detection of PFAS is crucial.

Traditional detection techniques, such as liquid chromatography–mass spectrometry (LC-MS) and gas chromatography–mass spectrometry (GC-MS), provide a high level of precision but are expensive, labour-intensive, and reliant are on the advanced laboratory facilities.

This initiative seeks to create a cost effective, portable, and field-ready colorimetric sensing method for the swift detection of PFAS in water samples. In the present work, a photodiode-based colorimetric platform is developed with methylene blue as a reagent that yields a visible colour change in the solvent after a reaction occurs with the PFAS molecule (PFOA). The degree of colour intensity change is proportional to the PFAS concentration, allowing for semi-quantitative assessment.

To improve accessibility and user-friendliness, the system is designed to work with a mobile application that can capture the colour response and translate it into concentration data using data processing and calibration algorithms. This method offers an effective, cost-efficient substitute for conventional analytical techniques, enabling on-site PFAS contamination monitoring and aiding in early detection and environmental management initiatives.



Fig. 1 (a) Visual level of detection at 25 parts per billion (b) Linearity of colour intensity increase of the solvent from 1 to 50 parts per million as seen on an absorbent pape

Keywords: Colorimetric Sensor, Point of Care Device, PFAS Detector.

EH-089

Defect-Induced Charge Separation in Ca-Doped $BiVO_4/AgFeO_2$ Heterostructures for Enhanced Photocatalysis of Ciprofloxacin

Nandana Sadanandan[1], G Bakiyaraj*[2], J Archana[1], M Navaneethan[1,3]

[1]*Center of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603 203, India*

[2]*Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603 203, India*

[3]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail**: bakiyarg@srmist.edu.in

ABSTRACT

The development of efficient visible-light-driven photocatalysts for the removal of emerging pharmaceutical pollutants is of significant environmental importance. In this work, calcium-doped $BiVO_4/AgFeO_2$ heterostructures were successfully synthesised via hydrothermal and precipitation techniques for the photocatalytic degradation of ciprofloxacin and antibacterial applications. Monoclinic $BiVO_4$, possessing a suitable band gap (~2.4 eV), was modified by Ca^{2+} doping to induce lattice distortion and oxygen vacancies, thereby enhancing charge carrier separation. The doped semiconductor was further coupled with $AgFeO_2$ to construct an effective heterojunction for improved interfacial charge transfer. Among different Ca-doped $BiVO_4$ samples, 1 wt.% (C1BVO) is showing superior activity. So that sample is taken to couple with $AgFeO_2$ to form heterostructures - Ca-doped $BiVO_4$/5 wt.% $AgFeO_2$ (C1BA5), and Ca-doped $BiVO_4$/10 wt.% $AgFeO_2$ (C1BA10). Among them, C1BA5 exhibited superior photocatalytic performance in degrading ciprofloxacin under visible light irradiation. The enhanced activity is attributed to the synergistic effects of Ca-induced defect states and the formation of an efficient heterojunction. The reactive oxygen species, such as superoxide and hydroxyl radicals, facilitate the mineralisation of ciprofloxacin molecules.Structural, optical, and morphological properties were characterised using X-ray diffraction (XRD), UV–visible spectroscopy, photoluminescence (PL) spectroscopy, and electron microscopy analyses. Additionally, the optimised heterostructure (C1BA5) demonstrated significant antibacterial activity, indicating its dual-functional potential for environmental remediation. The results reveal that Ca doping combined with heterojunction engineering is an effective strategy to enhance photocatalytic efficiency and antimicrobial performance for wastewater treatment applications.

References:

1. X. Zhong, Y. Li, H. Wu, and R. Xie, Mar. 01, 2023, Elsevier Ltd. doi: 10.1016/j.mseb.2023.116278.
2. J. Ahmed, N. Alhokbany, A. Husain, T. Ahmad, M. A. M. Khan, and S. M. AlshehriJ Solgel Sci Technol, vol. 94, no. 2, pp. 493–503, May 2020, doi: 10.1007/s10971-020-05274-3.

EH-090

Fabrication of Mothership Capsules using Polymers for Lipase Enzymes Delivery to Treat Pancreatic Insufficiency

Johnson Thinakaran[1], Anandhakumar Sundaramurthy[2*]

[1] *Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2] *Department of Chemical Engineering, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** anandhas@srmist.edu.in

ABSTRACT

Pancreatic lipase deficiency leads to impaired lipid digestion and malabsorption, resulting in significant gastrointestinal and nutritional complications. Although oral lipase supplementation is a promising therapeutic strategy, its efficacy is limited by degradation in the acidic gastric environment. To overcome this challenge, stimuli-responsive mothership capsules (MCs) have been developed as an advanced platform for the encapsulation and controlled release of enzymes. In this study, we fabricated MCs using a simple extrusion method using an anionic polymer, gellan gum (GG), and a cationic polymer, poly (allylamine hydrochloride) (PAH), through electrotactic charge interactions, as result forming the MCs. The pH-responsive MCs exhibited enhanced stability in a 1% PAH solution at pH 5. The formed capsules exhibited smooth, spherical structures with a diameter ranging from 2 to 3 mm. The MCs served as compartments for carrying and releasing the lipase in the small intestine. To assess lipase release, the MCs were exposed to simulated gastric fluid (SGF) for 2 hours. While the MCs remained stable, only a small amount of lipase was released. The MCs were then incubated in simulated intestinal fluid (SIF) at pH 6.8 for 8 hours, which triggered the breakdown of the polymeric capsules and facilitated the release of lipase. The release of lipase was quantified spectrophotometrically, revealing minimal leakage under acidic conditions and enhanced release in SIF due to pH-induced destabilisation of the polyelectrolyte network. The preserved enzymatic functionality of the released lipase highlights the protective capability of the mothership capsule system. Overall, this study demonstrates that pH-responsive GG/PAH mothership capsules represent a promising strategy for targeted intestinal enzyme delivery and offer significant potential for improving oral enzyme replacement therapy in pancreatic lipase deficiency.

References:

1. Sharma, Varsha, Maarten Vergaelen, Sangamithra Nehru, Richard Hoogenboom, and Anandhakumar Sundaramurthy. "Poly (2-n-propyl-2-oxazoline)/tannic acid nanocapsules with in-situ synthesized gold nanorods for cancer theranostics." *European Polymer Journal* 198 (2023): 112409.
2. Sharma, Varsha, Gokul Paramasivam, Maarten Vergaelen, Richard Hoogenboom, and Anandhakumar Sundaramurthy. "Tannic acid-stabilized self-degrading temperature-sensitive poly (2-n-propyl-2-oxazoline)/gellan gum capsules for lipase delivery." *ACS Applied Bio Materials* 4, no. 9 (2021): 7134-7146.

EH-091

Catalytic Innovations and Transesterification Approaches for Sustainable Biodiesel Production from Diverse Lipid Feedstocks

Kamalraj Venkatesan [1, 2], Ayyadurai Saravanakumar[2, *]

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603 203, Chengalpattu District, Tamil Nadu, India*

[2]*Centre for Research in Environment, Sustainability Advocacy and Climate Change (REACH), Directorate of Research and Virtual Education, SRM Institute of Science and Technology, Kattankulathur – 603 203, Chengalpattu District, Tamil Nadu, India*

*** Corresponding author email:** sara_mnes@yahoo.co.in & saravana7@srmist.edu.in

ABSTRACT

Biodiesel's renewable nature, biodegradability, and lower environmental effect have made it a viable substitute for fossil fuel-based diesel. This page gives a thorough examination of biodiesel production methods, with an emphasis on various feedstock types such as animal fats, used cooking oil, plant edible and non-edible oils, and algal lipid sources. The primary production technique is transesterification. It is studied in conjunction with improved catalytic systems such as homogeneous, heterogeneous, enzyme-based, and nano-catalysts, emphasising their contributions to greater efficiency and sustainability. Furthermore, the study evaluates technological improvements such as enzymatic, ultrasound-assisted, and supercritical methanol procedures, which improve reaction rates while using less energy. Challenges such as feedstock availability, process scalability, and economic feasibility are eventually assessed. The study investigates possible pathways for sustainable biodiesel production, such as integrated biorefinery technology, algal genetic manipulation, and policy-driven incentives. This article seeks to provide a fundamental resource for researchers, businesses, and governments interested in investigating greener energy alternatives based on biodiesel.

Keywords: Biodiesel; Transesterification; Renewable Energy; Non-edible Oils; Catalysts; Emerging Methods

PVP-Capped Flower-like Bi_2WO_6 Nanostructures for Highly Selective H_2S Gas Sensing

K Anbarasan [1], D Kanchan Kumar [2], E Vinoth[1], M Navaneethan[1], S Harish *

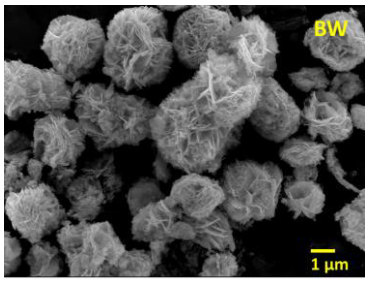
[1] *Nanotechnology Research Centre, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2] *Centre of Excellence in Materials for Advanced Technologies, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author email:** aravindharri@gmail.com

ABSTRACT

Hydrogen Sulfide (H_2S) poses severe health risks at low concentrations, necessitating advanced gas sensors with high sensitivity and selectivity. We developed PVP-capped bismuth tungstate (Bi_2WO_6) nanostructures via a one-pot hydrothermal synthesis at 180°C for 12 h, where polyvinylpyrrolidone (PVP) acts as a capping agent to direct flower-like morphology for enhanced H_2S detection. X-ray diffraction (XRD) patterns exhibit well-defined peaks matching the orthorhombic Bi_2WO_6 phase (JCPDS No. 39-0256), with prominent reflections at $2\theta = 28.3°$ (131), 30.7° (002), and 32.8° (060), confirming high crystallinity and phase purity without secondary phases. The sharp, intense peaks indicate successful PVP mediation, preventing aggregation and promoting ordered crystal growth.Field-emission scanning electron microscopy (FESEM) reveals distinctive hierarchical flower-like microstructures (1µm diameter) assembled from ultrathin nanosheets (~20-50 nm thick), the material demonstrates exceptional H_2S sensing at 200°C: response/recovery times of 8 s/12 s and selectivity over NO_2, CO, CH_4, and NH_3. The enhanced performance arises from the flower morphology's facilitated oxygen ion adsorption, electron depletion upon H_2S interaction, and rapid diffusion pathways.



References:

1. Nanostructure Bi_2WO_6: Surfactant-assisted hydrothermal synthesis for high sensitive and selective sensing of H_2S Wencheng Liu et al. Sensors and Actuators B: Chemical
2. Room temperature WO_3-Bi_2WO_6 sensors based on hierarchical microflowers for ppb-level H2S detection Zhang et al. Chemical Engineering Journal

EH-093

Low dimensional Bi_2S_3 nanorod network for highly sensitive and selective NO_2 sensor at room temperature

Deepalakshmi S[1], R. Aysha Parveen[1], E. Vinoth[1]*, M. Navaneethan[1]

[1]*Nanotechnology Research Center (NRC), Faculty of Engineering and Technology, SRM Institute of science and Technology (SRMIST), Kattankulathur 603203, India*

***Corresponding author e-mail:** vinothe1@srmist.edu.in

ABSTRACT

The demand for effective monitoring of nitrogen dioxide (NO_2) is increasing day by day owing to its abundancy and high toxicity. The NO_2 being prevalent in the atmosphere from various sources such as automobiles, industrial emissions, power plants, deforestation, etc., requires a precise monitoring device to detect its presence at trace concentrations of less than 1 ppm, i.e., the exposure limit of NO_2 prescribed by WHO. Among various class of materials explored for NO_2 detection, the 2D layered transition metal di-chalcogenides (TMDs) hold prominence because of its high surface area, tuneable electrical properties, and surface reactivity. Among various TMDs, bismuth sulphide (Bi_2S_3) is a promising candidate for NO_2 detection ascribed to its narrow band gap, large surface area and high carrier mobility However, the pristine Bi_2S_3 is usually inert for effective detection of ppb-level NO_2 at room temperature (RT) owing to the lack of active sites. In this study Ag-doped Bi_2S_3 nanorods were successfully synthesized by one step hydrothermal method to improve their response and recovery time. The structural properties and phase of Bi_2S_3 nanorods were confirmed by X-ray diffraction (XRD), which exhibited a notable shift in diffraction pattern confirming the successful incorporation of Ag in Bi_2S_3.

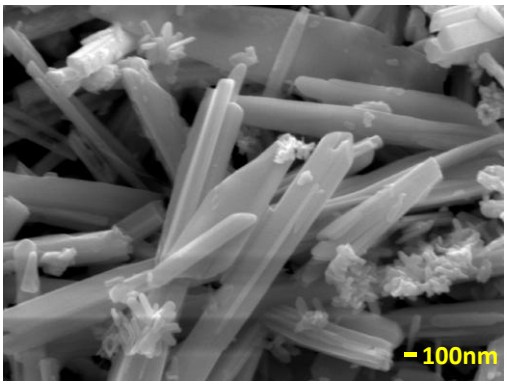


Fig. 1) FE-SEM analysis of nanorod Bi_2S_3

Keywords: Nitrogen dioxide (NO_2), Bismuth Sulfide (Bi_2S_3), Sensor

References:

1. R. Aysha Parveen. et al. small methods, 2024.
2. Tingting Wang.et al. Journal of Materials Chemistry A, 2022.

Nano-Engineered α-MoO_3 for Environmentally Sustainable NO_2 Detection

Aysha Parveen R[1], Vinoth E[1], Navaneethan M[1]*

[1]*Nanotechnology Research Centre (NRC), SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** m.navaneethan@gmail.com

ABSTRACT

Environmental toxic and highly abundant nitrogen dioxide (NO_2) possess serious threats to health, biodiversity, and sustainability. The low threshold limit of 1 ppm demands a precise NO_2 monitoring device at various manufacturing & mining industries to ensure human safety. Among various materials explored so far, the layered metal oxides hold prominence owing to its graphene analogous though tunable band gap & electrical properties. Among them, is the layered molybdenum oxide (**α**-MoO_3) that possesses singly, doubly and triple coordinated oxygen atoms. The modification of surface activation energy of **α**-MoO_3 can be modified via nano-engineering (i.e., nano-insertion of metal atoms), serves as a viable technique for reducing the operating temperature of the sensor without compromising the response, stability and other characteristics. Here, the escape of singly coordinated oxygen in **α**-MoO_3 is the direct consequence of nano-insertion that induces defects mediated NO_2 interactions. Various transition metals such as copper (Cu), iron (Fe) and alkaline earth metals such as magnesium (Mg) were resulted in reduced operating temperature, high response **α**-MoO_3 based NO_2 sensors. However, the defect chemistry of nano-engineering in **α**-MoO_3 requires more exploration.

Keywords: Layered metal oxides; graphene analogous; nano-engineering; sensor.

References:

1. Parveen, R. Aysha, et al. Sensors and Actuators B: Chemical 389 (2023): 133810.
2. Parveen, R. Aysha, et al. Small Methods 9.4 (2025): 2401214.
3. Parveen, R. Aysha, et al. Sensors and Actuators B: Chemical 417 (2024): 136017

Fabrication and Application of a CuNi-MOF-Modified Electrochemical Sensor for Ultrasensitive Vitamin K Quantification.

G. Diviyasri[1], R. Aysha Parveen[2], E. Vinoth[2], M. Navaneethan*[1, 2], J. Archana*[1]

[1]*Centre of Excellence in Materials for Advanced Technologies, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, India.*

[2]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, India.*

*__Corresponding author email__: archanaj@srmist.edu.in

ABSTRACT

Precise tracking of vitamin levels is crucial, since vitamins govern key biochemical processes like metabolism, enzyme activation, immune regulation, and cellular balance. Vitamin K is essential for hemostasis, bone mineralization, and cardiovascular function, with deficienciesprecipitating hemorrhagic diatheses and associated pathophysiological disturbances. Therefore, developing sensitive, rapid, and reliable Vitamin K detection methods is critical for clinical and pharmaceutical applications. Electrochemical sensing offers high analytical sensitivity, rapid response, and compatibility with advanced diagnostic platforms through controlled interfacial electron-transfer kinetics. Metal-organic frameworks (MOFs) have emerged as promising electroactive materials due to their structural tunability, high surface area, and porous crystalline edifice that promotes efficient analyte diffusion and mass transport. To enhance electrochemical performance, a bimetallic Copper-Nickel MOF (CuNi-MOF) was rationally engineered, where synergistic Cu^{2+}/Cu^{3+} and Ni^{2+}/Ni^{3+} redox transitions enhance faradaic activity and catalytic efficiency. The CuNi-MOF, synthesized via a one-pot solvothermal method, exhibits a broad linear response range, high sensitivity, and low detection limits for Vitamin K using differential pulse voltammetry. The superior performance is attributed to improved electron transport, increased electroactive surface area, and synergistic redox interactions within the bimetallic framework.

Keywords: Electrochemical sensing, Detection of vitamins, MOF based Vitamins detection, Bimetallic CuNi-MOF, Synergistic redox catalysis.

Reference:

1. Draz, Muhammad Umar, et.al RSC advances 14, no. 15 (2024): 10331-10347.
2. Sá, Éder S., et.al Sensors and Actuators B: Chemical 209 (2015): 423-430.
3. Bindu, Konda, et.al Chemical Physics Letters 865 (2025): 141936.

Charge Transport Dynamics in LiOH-Intercalated $Ti_3C_2T_x$ MXene: Highly Sensitive and Rapid NO_2 Sensor

A. Jasmine Christilla[1], R. Aysha Parveen[2], E. Vinoth[2], J. Archana[1]*, M. Navaneethan[2]

[1]*Centre of Excellence in Materials for Advanced Technologies*

[2]*Nanotechnology Research Centre*

SRM Institute of Science and Technology, Kattankulathur – 603203

***Corresponding author e-mail**: archanaj@srmist.edu.in

ABSTRACT

Long term exposure to high concentrations of nitrogen dioxide (NO_2) severely affects the human respiratory system. Nitrogen dioxide (NO_2) is an extremely dangerous gas mainly produced by factory combustion, automobile exhaust, and coal mining. According to occupational safety guidelines, nitrogen dioxide (NO_2) exposure limits are set to protect human health, with organisations such as OSHA recommending a PEL of up to 5 ppm and NIOSH suggesting a lower REL of 1 ppm, while environmental agencies like WHO and EPA recommend even stricter ambient limits in the ppb range. Therefore, the development of efficient and sensitive gas sensors for NO_2 detection is essential. For gas sensing materials, the larger the specific surface area, better gas adsorption/desorption performance, leading to improved sensitivity. Since two-dimensional MXene possesses a layered structure with a high specific surface area and abundant active surface sites, it was employed as the sensing material for NO_2 detection in this work. Additionally, MXene sheets contain surface functional groups such as –O, –OH and –F. These groups help in the adsorption of NO_2 gas molecules and improve charge transfer, which increases the sensor response**.** Mxene has been successfully synthesised by the wet chemical etching method. The synthesised samples were subjected to XRD and SEM characterisation to investigate their structural and morphological properties. The gas sensing performance was evaluated towards different concentrations (10 to 40 ppm) of NO_2 and the sensor exhibited a measurable change in resistance. However, slow and partial recovery behavior was observed after gas exposure, which may be attributed to strong adsorption of NO_2 molecules and restacking of MXene layers. To enhance the recovery characteristics, LiOH intercalation is adopted. Intercalation can expand the interlayer spacing and reduce restacking between MXene sheets, thereby facilitating improved charge transport and faster desorption of gas molecules. This helps gas molecules to diffuse easily between the layers and improves the sensitivity and recovery behaviour of the sensor. This strategy is expected to enhance the overall sensing performance and stability of the MXene-based gas sensor.

Keywords: MXene, surface functional groups, NO_2 sensing

References:

1. Guo, Fuqiang, Cheng Feng, Zheng Zhang, Lili Zhang, Chang Xu, Congting Zhang, Shuang Lin et al. "A room-temperature NO2 sensor based on Ti3C2TX MXene modified with sphere-like CuO." *Sensors and Actuators B: Chemical* 375 (2023): 132885.
2. Gasso, Sahil, Manreet Kaur Sohal, and Aman Mahajan. "MXene modulated SnO2 gas sensor for ultra-responsive room-temperature detection of NO2." *Sensors and Actuators B: Chemical* 357 (2022): 131427.

EH-097

A Glutathione-Stabilized Copper Nanocluster-Molybdenum Disulfide Composite for Electrochemical Non-Enzymatic Detection of Dopamine and Uric acid

Lisa Maria Malhiers[1], Haritha Kuttoth[1], Dr. N. Sandhyarani[1]*

[1]*National Institute of Technology Calicut, Kozhikode, Kerala, India, 673601*

***Corresponding author e-mail:** sandhya@nitc.ac.in

ABSTRACT

Accurate detection of dopamine (DA) and uric acid (UA) is crucial for early diagnosis of some common diseases like Alzheimer's and Gout [1]. The current methods are often slow, complex, and costly [2]. In this study, a novel electrochemical biosensor using Glutathione-stabilized Copper nanoclusters (GSH-CuNCs) integrated with Polyacrylic acid exfoliated Molybdenum disulfide (MoS_2-PAA) nanosheets was developed for simultaneous DA and UA detection [3][4]. The composite was synthesized by sonicating MoS2-PAA with the freshly made GSH-CuNCs and then characterized using Scanning Electron Microscopy (SEM), High-Resolution Transmission Electron Microscopy (HRTEM), Fourier Transform Infrared (FT-IR) Spectroscopy, Raman Spectroscopy (Raman) and X-ray Diffraction (XRD). The electrochemical performance of the sensor material GSH-CuNCs/MoS2-PAA was analysed by Differential Pulse Voltammetry (DPV), Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS). The sensor demonstrated high sensitivity, with detection limits of 0.20 µM for DA and 14 µM for UA, along with excellent selectivity and stability. The real time detection of DA and UA was carried out in synthetic urine with good sensitivity and recovery rates. This suggests its potential for clinical diagnostics and point-of-care applications. This biosensor offers a simple, scalable, and efficient platform for biomolecule detection in biomedical settings [5].

References:

1. Cheng, R., Fang, X., Wang, Y., Gu, C., Zheng, X., Yang, M., Microchem. J., 212 (2025).
2. Vadivelu, Y., Sendrayal Raj, A., Muniyandi, R., S. R., S., Ramachandran, B., Talanta Open, 12 (2025).
3. Rehman, A. U., et al., Microchem. J., 209 (2025).
4. Zhang, L. L. M., Wong, W. Y., Aggregate, 4 (2023).
5. Sai Iswarya Bakavaty, T., Gurunathan, K., Mater. Sci. Eng. B, 299 (2025).

EH-098

Ultrasound-Enhanced Adsorption of Fluoride using Thermally Activated Al/Si-Rich Industrial Sludge: Performance, Mechanism and Safety Assessment

Supriya Jena*, Sankha Chakrabortty, Suraj Kumar Tripathy

School of Chemical Engineering, KIIT Deemed to be University, Bhubaneswar, India

***Corresponding author e-mail:** jena.supriya99@gmail.com

ABSTRACT

This study demonstrates an efficient and sustainable strategy for fluoride removal from contaminated water using ultrasound-assisted batch adsorption with thermally activated Al/Si-rich industrial sludge (ASIS). Calcination at 550 °C significantly improved the physicochemical properties of the adsorbent, while ultrasonication enhanced particle dispersion and surface area, resulting in improved adsorption performance (Fig.1). The high silica and alumina content facilitated effective fluoride binding through surface complexation mechanisms1. Key operational parameters, including contact time, solution pH, adsorbent dosage, and initial fluoride concentration, were systematically optimized, achieving fluoride removal efficiencies exceeding 90% under optimal conditions. Process optimisation using Response Surface Methodology–Central Composite Design was further refined through Artificial Neural Network–Genetic Algorithm modelling, which exhibited superior predictive accuracy compared to conventional statistical models2. Adsorption followed the Langmuir isotherm and pseudo-second-order kinetics, was spontaneous and endothermic, while MTT assay on 3T3 fibroblasts confirmed high cell viability and environmental safety of treated water.

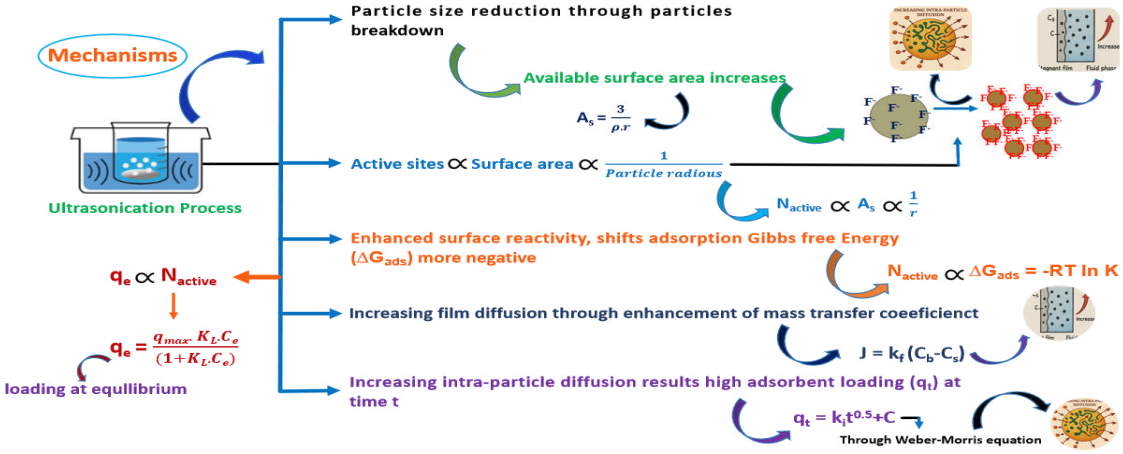


Fig.1. Proposed mechanisms involved in ultrasound-assisted fluoride adsorption using Al/Si-rich industrial sludge (ASIS).

References:

1. R. Zaidi, S. U. Khan, I. H. Farooqi, and A. Azam, RSC Adv., 11 (2021) 28744–28760.
2. M. Fan, T. Li, J. Hu, R. Cao, X. Wei, X. Shi, and W. Ruan, Materials, 10 (2017) 544.

EH-099

Sunlight-Driven Photocatalytic Inactivation of E. coli and Staphylococcus aureus using Iron-doped ZnO Nanoparticles

Gobinda Chandra Mahapatra*, Suraj Kumar Tripathy, Amrita Mishra, Sankha Chakrabortty

School of Chemical Engineering, KIIT Deemed to be University, Bhubaneswar, India

***Corresponding author e-mail:** mahapatragobinda143@gmail.com

ABSTRACT

Solar-active functional materials that enable efficient water disinfection under natural irradiation are essential for sustainable purification technologies and decentralized treatment devices (Chong et al., 2010; Ikehata et al., 2006). In this study, iron-doped zinc oxide (Fe/ZnO) nanoparticles were investigated as a sunlight-responsive photocatalytic material for simultaneous organic contaminant degradation and microbial inactivation in water. The photocatalytic performance of Fe/ZnO was systematically optimized by varying catalyst dosage, solution pH, temperature, and irradiation time under natural sunlight conditions. Iron incorporation significantly enhanced visible-light absorption and reduced electron–hole recombination, leading to an increased formation of reactive oxygen species responsible for oxidative reactions at the catalyst surface (Das et al., 2017; Misra et al., 2022). Under optimized operating conditions, complete degradation of the target organic compound was achieved within 210 minutes of solar exposure. The water disinfection capability of the system was confirmed through microbiological assays, demonstrating complete inactivation of Staphylococcus aureus and Escherichia coli within short irradiation periods (Sturini et al., 2012). The results highlight the strong oxidative and antimicrobial activity of Fe/ZnO without the need for external energy input or chemical disinfectants. Owing to its low-cost synthesis, solar operability, and high disinfection efficiency, Fe/ZnO shows strong potential for integration into solar-driven water disinfection modules, photocatalytic reactors, and functional purification devices. This work underscores the applicability of doped metal oxide nanomaterials in advanced functional materials and devices for sustainable water treatment applications.

References:

1. M. N. Chong, B. Jin, C. W. K. Chow, and C. Saint, Water Res., 44 (2010) 2997–3027.
2. S. Das, S. Sinha, B. Das, R. Jayabalan, M. Suar, A. Mishra, A. J. Tamhankar, C. S. Lundborg, and S. K. Tripathy, Sci. Rep., 7 (2017) 104.

EH-100

Toxicity of PET Microplastic and Nanoplastic in Human Lung Alveolar Epithelial Cells

Aditya Bagkar[1] , Sharine Priscilla[1], Meenakshi Podwal[1], Sanjeshri Patil [1], Sushilkumar Ningthoucha[1], Sahabudeen Sheik Mohideen*[1]

[1] *Department of Biotechnology School of Bioengineering, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu District, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** sahabuds@srmist.edu.in

ABSTRACT

Airborne Microplastics and Nano plastics are increasingly identified as emerging environmental pollutants with potential implication for human respiratory health. Polyethylene terephthalate (PET) Microplastics and Nano plastics is Commonly released from consumer product and textiles forms a major fraction of inhalable particles in both indoor and outdoor environments. Despite of rising exposure levels, the cellular effects of PET Microplastic and Nano plastics on lung tissue remains underexplored. This study aims to investigate the acute toxicological response caused by PET Microplastic and Nano plastics in human alveolar epithelial cell. This study examines how short-term exposure to different concentrations and heterogeneous sizes and shapes of PET Microplastic and Nano plastics particles influences cell viability, cellular stress and gene expression. It intends to examine if the lung cells are capable of internalizing Microplastics and Nano plastics by monitoring rapid changes in physiological and molecular response, the study seeks to identify early indicators of Microplastic and Nano plastics induced toxicity during acute exposure.

References:

1. Biswas, A., Saini, N., Darbha, G. K., Environ. Int., 205 (2025) 109897.
2. Jenner, L. C., Rotchell, J. M., Sadofsky, L. R., Sci. Total Environ., 831 (2022) 154907.
3. Traversa, A., Romano, E., Ceccarelli, S., Int. J. Mol. Sci., 25 (2024) 10168.
4. Michelini, S., Fenoglio, I., Drobne, D., J. Nanobiotechnol., 23 (2025) 388.
5. Annangi, B., Villacorta, A., Hernández, A., Environ. Toxicol. Pharmacol., 100 (2023) 104140.

EH-101

Hierarchical HOF-Templated Ru-Borophene Hybrid: Synergistic Interface Engineering Toward Efficient OER in Alkaline and Marine Media

S. Sarmila, Sethumathavan Vadive*, P. Sujita, Manabu Fujii, Takahiro Kondo

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu 603203, India.

ABSTRACT

The oxygen evolution reaction (OER) is a sluggish half-reaction, which makes water electrolysis much less efficient. To achieve a more sustainable approach to H_2 and O_2 production, it is necessary to develop highly effective and stable electrocatalysts. In this work, a ternary hydrogen-bonded organic framework (HOF)-templated Ru-modified borophene (HOF-BB-Ru) electrocatalyst is synthesized, which involves the construction of an HOF–borophene heterostructure and subsequent integration of Ru species. This novel ternary structure increases the accessibility of the active site, enhancing charge-transfer properties and improving the structure's stability. XRD, SEM, TEM, and XPS analysis revealed that the ternary framework was successfully formed and chemically integrated. Electrochemical analysis, including linear sweep voltammetry (LSV), Tafel plots, and electrochemical impedance spectroscopy (EIS), reveals significantly improved OER kinetics for HOF-BB-Ru. The HOF-BB-Ru catalyst exhibited low overpotentials of 349 mV in an alkaline solution, 420 mV in alkaline seawater (simulated), and 473 mV in natural seawater at the current density of 50 mA cm^{-2}. These findings concluded that the HOF-BB-Ru catalyst's capability to work effectively across a wide range of electrolytic conditions demonstrates its strength and flexibility. This study introduces a novel heterostructure that exhibits high efficiency in HER and OER applications in real marine water environments.

Keywords: Hydrogen-bonded organic framework, Ru, Borophene, Electrocatalyst, OER

EH-102

Enhanced Sunlight-Assisted Wastewater Treatment via SnO2-Coated Jute Fibers

Pawan Chetri[1]* and Rituraj Mahanta[2]

[1]*Department of Physics, North Eastern Regional Institute of Science and Technology, (NERIST) Nirjuli, Arunachal Pradesh, India, 791109.*

[2]*Department of Physics, Thong Nokbe College, Dokmoka, 782441, Karbi-Anglong, Assam, India.*

***Corresponding author e-mail:** chetripawan2009@gmail.com & pcr@nerist.ac.in

ABSTRACT

In this study, we introduce a novel fabrication method for a sunlight-responsive photocatalyst designed for wastewater treatment. A biocompatible photocatalyst, "SnO_2-coated jute fiber," is synthesized using a simple, cost-effective sol-gel process followed by a hydrothermal method. The structural and optical properties of this composite photocatalyst are thoroughly investigated and compared with those of pure SnO_2. The photocatalytic performance is evaluated by degrading methyl orange, used as a model pollutant, under natural sunlight exposure. Results demonstrate that the SnO_2-coated jute fiber exhibits significantly enhanced photocatalytic activity compared to pure SnO_2. Moreover, recyclability tests reveal that the photocatalyst remains stable and effective, successfully degrading methyl orange over more than two cycles. This work highlights the potential of this biocompatible photocatalyst for sustainable wastewater treatment and its ability to address water pollution challenges.

Keywords: SnO_2, Photocatalysis, Dye, 2,4-D, Levofloxacin, Sunlight.

EL-001

Revealing the Non-Linear Optical Properties in Lead-Free Potassium Sodium Niobate ($K_{0.5}Na_{0.5}NbO_3$) Thin Films Through Two-Wave Mixing Interactions

Denny Singh Thokchom[1], Reema Gupta[2], Monika Tomar[3]*, Arijit Chowdhuri[4], H. Basantakumar Sharma[1]*

[1]*Department of Physics, Manipur University, Canchipur-795003, Manipur, INDIA*

[2]*Department of Physics, Hindu College, University of Delhi, Delhi-110007, INDIA*

[3]*Department of Physics, Miranda House, University of Delhi, Delhi-110007, INDIA*

[4]*Department of Physics, Acharya Narendra Dev College, University of Delhi, Delhi-110019, INDIA*

***Corresponding author e-mail:** hbslab.18@gmail.com, monika.tomar@mirandahouse.ac.in

ABSTRACT

Non-linear optics (NLO) is a rapidly advancing scientific field that directly influences modern day technologies including high-speed telecommunications, laser systems, medical imaging, environmental sensing, precision manufacturing, defence photonics besides scientific instrumentation. The NLO response of a medium arises from the non-linear variation of its polarization post application of an externally applied electric field. Lead-based ferroelectric materials including Lead Zirconate Titanate (PZT) have traditionally dominated NLO applications due to their large non-linear coefficients, high electro-optic (EO) efficiency together with excellent photorefractive behaviour. However, the environmental hazards associated with lead have prompted the scientific community to look for sustainable, lead-free alternatives. Lead-free perovskites have emerged as strong candidates, with Potassium Sodium Niobate ($KxNa_{1-x}NbO_3$, KNN) showing particular promise owing to its inherent high dielectric permittivity and favourable non-linear, acousto-optic and EO characteristics[1]. Despite envisioned potential, limited work exists on the NLO behaviour of KNN thin films mainly due to its multicomponent nature. In the current study, KNN-50 ($K_{0.50}Na_{0.50}NbO_3$) thin films were deposited using RF magnetron sputtering. X-ray diffraction confirmed phase formation and crystallinity, while UV–Visible spectroscopy was employed to determine the optical transmittance and band gap. The refractive index was determined using Swanepoel's envelope method. NLO properties were examined through two-wave mixing in a pump–probe configuration using KNN-50 films integrated with gold micro-discs. Periodic modulation in the transmitted probe signal clearly demonstrated a strong NLO response. The obtained results highlight KNN thin films as a highly promising lead-free material system for next-generation non-linear optical and electro-optic device applications.

Keywords: Non-linear Optics; KNN thin films; RF magnetron sputtering; Two-wave mixing.

References:

1. S. Sharma, R. Gupta, V. Gupta, and M. Tomar, Phys. Status Solidi A 215 (2018) 1700452

Tuning the Photoconductivity of SnSe Thin Films Through Investigating the Impact of Deposition Pressure.

Satyam Garg[1,2], Kajal Jindal[3], Monika Tomar[2]*

[1]*Department of Physics and Astrophysics, University of Delhi, Delhi – 110 007, INDIA*

[2]*Department of Physics, Miranda House (University of Delhi), Delhi – 110 007, INDIA*

[3]*Department of Physics, Kirori Mal College (University of Delhi), Delhi – 110 007, INDIA*

***Corresponding author e-mail:** Monika.tomar@mirandahouse.ac.in

ABSTRACT

Photodetectors are the optoelectronic devices that detect light signals of specific wavelengths by converting them into electrical signals. These photodetectors are used in many applications such as spectroscopy, communication systems, and defense. Wide band gap semiconductor such as Zinc Oxide (ZnO), Gallium Oxide (Ga_2O_3), and Tantalum Oxide (Ta_2O_3) etc. have sensitivity in the ultraviolet region of the electromagnetic spectrum. Group IV-VI layered semiconductors such as Tin Selenide (SnSe), Tin Sulfide (SnS), Lead Selenide (PbSe), and Lead Sulfide (PbS) are the emerging materials that can be used to fabricate wide spectrum photodetectors. In this study, Tin Selenide (SnSe) thin films were grown over the SiO_2/Si substrate at different Ar gas pressures of 5, 7.5, 10, and 12 mTorr in the sputtering chamber using RF magnetron sputtering technique to study their photodetection properties from the UV (254 nm) to NIR (1064 nm) region of the EM spectrum. The deposited films were characterized by X-ray diffraction, field emission scanning electron microscopy (FESEM), energy dispersive X-ray analysis (EDAX), atomic force microscopy (AFM), Raman, and UV-Vis-NIR spectroscopy. X-ray diffraction studies confirm the formation of orthorhombic phase of SnSe in thin films with the lowest indirect and direct band gap energy of 0.9 and 1.38 eV at an Ar gas pressure of 7.5 mT. Gold (Au) metal electrodes were deposited to study the current-voltage characteristics of SnSe thin films. Current-voltage characteristics of SnSe thin films deposited at different Ar gas pressures of 5, 7.5, 10, and 12 mT show the ohmic nature of electrical contacts. Photodetection measurements were carried out at wavelengths of 254, 296, 365, 405, 632, 840, 950, and 1064 nm. The Fabricated photodetector shows the highest responsivity of 0.53 mA/W, a current on/off ratio of 2.734 × 101, rise time of 79 ms, and a fall time of 80 ms, for 840 nm wavelength incident radiation with an intensity of 50 μW/cm^2 for SnSe thin films deposited at 12 mT pressure of Ar gas. The photocurrent for SnSe thin films deposited at 12 mT Ar gas pressure increases with the rise in intensity of incident radiation, following a power law of $I_p = aP^{0.29}$. This study shows that Tin Selenide is a promising material for photodetector applications in the wavelength range from UV (254 nm) to IR (1064 nm) region of the electromagnetic spectrum.

Keywords: SnSe thin films, RF magnetron sputtering, UV-Visible to near infrared photodetector.

EL-003

Energy harvesting technologies: A robust technology for self-powered systems

Sugato Hajra[1]*

[1]*Daegu Gyeongbuk Institute of Science and Technology, South Korea*

***Corresponding author e-mail:** sjc@gmail.com

ABSTRACT

The growing demand for autonomous, maintenance-free electronic systems has driven rapid advancements in energy harvesting technologies. This talk introduces a novel class of self-powered systems integrating piezoelectric nanogenerators (PENG), triboelectric nanogenerators (TENG), and mechanoluminescent (ML) materials. By synergizing these mechanisms, hybrid devices can simultaneously convert biomechanical, vibrational, and ambient mechanical stimuli into electrical and optical signals, enabling real-time sensing and energy generation without external power. PENGs and TENGs exploit mechanical deformation and contact electrification, respectively, while ML materials provide visual feedback through stress-induced light emission. These hybrid platforms not only enhance energy conversion efficiency but also open pathways for interactive, low-cost, and robust systems for applications in wearable electronics, smart healthcare, and infrastructure monitoring. The talk will cover the fundamental mechanisms, materials design, and integration strategies for hybrid PENG–TENG–ML devices, emphasizing their transformative potential in sustainable, battery-free technologies.

References:

1. S. Hajra, K. K. Ruthvik, S. Panda, S. Song, S. M. Jeong, Y. K. Mishra, T. H. Oh, G. Das, S. Divya, and H. J. Kim, Nano Energy (2025) 111418.
2. S. Hajra, S. Panda, K. R. Kaja, S. Song, Y. Ryu, B. K. Panigrahi, N. Vittayakorn, J.-H. Lee, S. M. Jeong, and H. J. Kim, J. Mater. Chem. C 13 (2025) 19297–19307.
3. A. Babu, L. Bochu, S. Potu, R. Kaja, N. Madathil, M. Velpula, A. Kulandaivel, U. K. Khanapuram, R. K. Rajaboina, H. Divi, P. Kodali, B. Ketharachapalli, and R. Ammanabrolu, ACS Sustainable Chem. Eng. 11 (2023) 16806–16817.

Real-Time Hazardous Gas Detection Using a Hybrid Nano-Material Assisted SPR Sensor

Akash Srivastava*

Indian Institute of Information Technology, Ranchi, India, 835217

***Corresponding author e-mail:** akashsrivastava@iiitranchi.ac.in

ABSTRACT

Continuous monitoring of hazardous gases is essential in safety-critical environments where gas concentrations may exceed from permissible range. In this work, a cost-effective and real time surface plasmon resonance (SPR) sensor shown that operates in the Kretschmann configuration and is numerically investigated using the Transfer Matrix Method (TMM). The proposed multilayer architecture incorporates a silicon interlayer along with heterostructured two-dimensional (2D) and transition-metal dichalcogenide (TMD) materials, such as MXene and WS_2, to strengthen electromagnetic field confinement at the sensing interface. This hybrid integration significantly enhances light–matter interaction, leading to improved resonance characteristics and sensing performance. The sensor response is evaluated for gaseous analytes with refractive indices ranging from 1.00 to 1.001380 at an operating wavelength of 633 nm. Key performance parameters, including sensitivity, figure of merit (FoM), and detection accuracy, are systematically analyzed. A maximum angular sensitivity of 85°/RIU is achieved, representing an enhanced sensitivity compared to conventional SPR sensors in the visible regime and able to distinguish very small change in refractive index. the proposed sensor is well suited for applications in coal mines, sewer line operations, chemical industries, and other hazardous environments requiring reliable gas monitoring.

Keywords: Silicon interlayer, Electromagnetic field confinement, Gas detection, Visible wavelength, High-resolution sensing

Reference:

1. M. Jangid and V. Janyani, Diamond Relat. Mater., 155 (2025) 112357
2. J. Wekalao and O. Elamri, Plasmonics, (2025).
3. L. Han and C. Wu, Plasmonics, 14 (2018) 901–906.

Investigation of Structural, Intramolecular Charge Transfer, and Nonlinear Optical Characteristics of the Push-Pull Chromophore 1-[{2-Methyl-4-[(2-methylphenyl) diazenyl] phenyl} diazenyl] naphthalen-2-ol – Lipid Crimson: A Vibrational Analysis

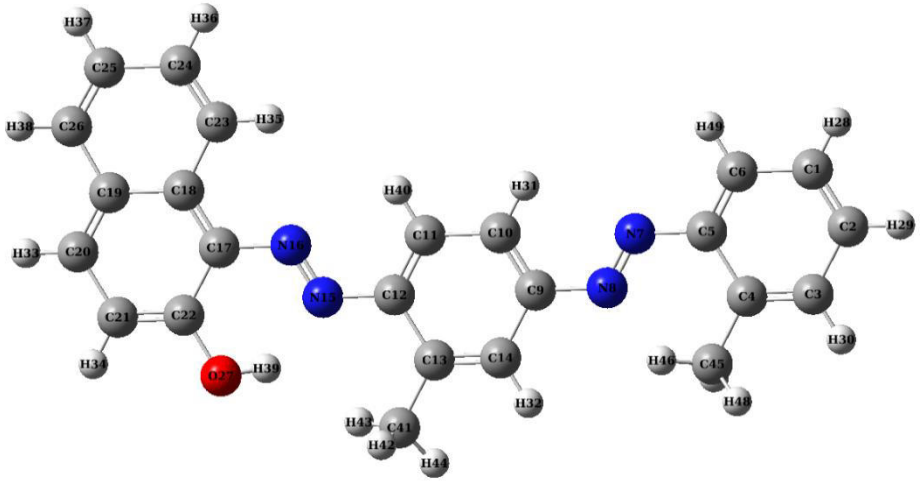
S. Manvizhi[1], M. R. Kannan[1], T. Vijayakumar[1]*

[1]*Futuristic Materials Research Centre for Planetary Exploration, Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603 203, Kancheepuram, Tamilnadu, India*

***Corresponding Author E-mail id:** vijayakt1@srmist.edu.in

ABSTRACT

Non-linear optical (NLO) features of 1-[{2-Methyl-4-[(2-methylphenyl) diazenyl] phenyl} diazenyl] naphthalen-2-ol (SUDAN IV) chromophore are investigated by FT-IR, FT-Raman, and UV-visible spectra aided by Density Functional Theory (DFT) using the B3LYP/6-311++G(d,p) basis set of Gaussian 16W package. The optimized geometry and structural features of the most prospective electro-optic crystal 1-[{2-Methyl-4-[(2-methylphenyl) diazenyl] phenyl} diazenyl] naphthalen-2-ol (SUDAN IV), and the vibrational spectral investigations have been comprehensively described with the Fourier transform (FT-Raman) Raman and Fourier transform infrared (FT-IR) spectra supported by the density functional theoretical (DFT) computations to elucidate the contribution of vibrational modes to the linear electro-optic (LEO) effect. Mulliken population analysis and natural bond orbital (NBO) analysis have also been carried out to analyze the effects of intramolecular charge transfer (ICT), hyperconjugative interactions on the geometries. The influence of CT interaction between the phenyl ring and the dimethyl amino group of the nonlinear optical (NLO) chromophore on the endocyclic and exocyclic angles have been examined. The effects of frontier orbitals, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), transition of electron density (ED) transfer and the influence of planarity in the stilbazolium ring on the first hyperpolarizability are also discussed. The third order nonlinear optical properties of the SUDAN IV also measured.



EL-006

Nanohybrid Functionalized MEMS Cantilever: Chitosan/Graphene QDs for Mercury (II) Monitoring in Water

Hari Amirtharaj G[1*], T. Shanmuganantham[1], D. Sindhanaiselvi[2]

[1]*Pondicherry University, Kalapet, Puducherry, India, 605014*

[2]*Puducherry Technological University Puducherry, India.605014*

Corresponding author e-mail: hariamirthraj17@pondiuni.ac.in

ABSTRACT

"Water mercury pollution can pose a serious threat to public health and the environment because of the toxicity of mercury. Although other methods such as atomic absorption spectroscopy provide very high sensitivity, they can be expensive and time-consuming in laboratories. To address this challenge, a new microelectromechanical systems cantilever sensor with a chitosan-graphene quantum dot nanohybrid is proposed in this research for ultrasensitive mercury ion analysis in water samples. With numerous amino and hydroxyl functional groups in chitosan, this macromolecule can form a highly selective mercury-binding interaction with mercury ions in water," offer outstanding surface area, fluorescence quenching, and excellent charge transfer capabilities for enhanced signal transduction. With Hg^{2+} ion adsorption, the nanohybrid produces accurate mass loading and surface stress effects on the cantilever's resonance frequency and deflection, effectively transducing femtogram-level signals into an available electrical output. Such a combination amassed record-breaking sensitivity to ppb levels, selectivity among interferents, and fast responsiveness. Through an integration of biodegradable nanomaterials with miniaturized MEMS technology, this work presents a compact, low-power sensor head suitable for in situ water analysis without being bound by lab requirements. Groundbreaking in this "smart skin" application with chitosan/GQD-modified cantilevers will initiate a new age of eco-conscious sensors for heavy metal surveillance in support of public health protection.

Reference:

1. H. Zhang and T. Nguyen, J. Mater. Chem. A, 9 (2021) 4567–4576.
2. E. Thompson and F. Rodriguez, Anal. Chem., 93 (2021) 2345–2353.
3. D. Hernandez and J. Wu, Nano Lett., 21 (2021) 3123–3130.
4. C. Morales and H. Tanaka, Appl. Surf. Sci., 542 (2021) 148678.
5. N. Verma and G. Santos, J. Hazard. Mater., 412 (2021) 125234.

Thickness Dependent Properties of ZnO Thin Films for Enhanced UV Photodetector Performance

Satyam Garg[1,2], Amritanshu¬ Chaudhary[1,3], Anjali Sharma[1], Mallika Verma[2], Arijit Chowdhuri[3], Jitender Kumar[4], Upendra Mittal[4], Archibald Theodore Nimal[4], Monika Tomar[2]*

[1]*Department of Physics and Astrophysics, University of Delhi, Delhi – 110 007, INDIA*

[2]*Department of Physics, Miranda House (University of Delhi), Delhi – 110 007, INDIA*

[3]*Acharya Narendra Dev College (University of Delhi), Kalkaji, New Delhi – 110 019, INDIA*

[4]*Solid State Physics Laboratory, Timarpur, Delhi – 110 054, INDIA*

***Corresponding author e-mail:** monika.tomar@mirandahouse.ac.in

ABSTRACT

Photodetectors designed for ultraviolet (UV) detection find myriad applications including ozone layer monitoring, defense and the biomedical field. Literature reports indicate preferential usage of semiconducting metal oxides like Zinc Oxide (ZnO), Gallium Oxide (Ga2O3), Iridium Dioxide (IrO2) and Tantalum Oxide (Ta2O3) for UV detection applications. In the present study, rf sputtered ZnO thin films (10 – 70 nm) were grown on SiO_2/Si substrates having underlying interdigitated electrodes (IDE) followed by their structural, optical and electrical characterizations. Structural characterization using X-ray diffraction (XRD) confirmed the formation of polycrystalline ZnO with a hexagonal wurtzite structure corresponding to the P63mc space group, consistent with JCPDS card No. 00-230-0450. Optical properties studied using UV–Visible spectroscopy in transmission mode indicated more than 85% transparency for wavelengths greater than 400 nm, thereby justifying ZnO films' suitability for UV light detection applications. Thereafter photodetection performance of ZnO films (10 – 70 nm) configured as photodetector were systematically investigated at different UV wavelengths – 220, 256, 296, 320 and 365 nm under applied bias voltages of 5 V and 30 V. It is interesting to note that 60 nm thick ZnO film based photodetector demonstrated a strong photoresponse exhibiting a high photocurrent-to-dark-current ratio (Iph/ID) of 4.02 × 102 at 365 nm, confirming its high sensitivity towards UV-A radiation. Additionally, it exhibited a rise time of 83 ms and a fall time of 155 ms, indicating fast and efficient charge transport within the ZnO thin film. The obtained results unequivocally demonstrate that optimized ZnO thin films integrated with interdigital electrode (IDE) architectures are promising and efficient candidates for realizing high-performance UV photodetectors.

Keywords: ZnO thin films, X-ray diffraction, UV-Visible spectroscopy, UV photodetector.

High Performance Multifunction Integrated Optical Chip with Emergent Materials for Fiber Optic Gyroscope Applications – An Analysis

Bhuvaneswari M S[1], Shanthi Prince[1]*

[1]*Department of Electronics and Communication Engineering, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India -603203*

*** Corresponding author e-mail:** shanthip@srmist.edu.in

ABSTRACT

Multifunction Integrated Optical Chip (MIOC) integrating the polarization maintenance, phase modulation and beam splitting functions on to a single chip play a vital role in the performance of Fiber Optic Gyroscopes (FOG) for linear sensitive response and for compactness. So far, Lithium Niobate electro optic modulators have been identified as the optimal performance choice for fiber optic gyroscopes due to their electro-optic properties yielding efficient phase modulation. However, several emerging materials such as organic polymers, perovskites, silica and III-V semiconductors show potential hybrid integration with silicon photonics for high performance integrated optics. Hence this research work focusses on the analysis of hybrid integration of Silicon with emerging materials for MIOC for the possible use in FOGs. A mathematical simulation model of MIOC with different materials has been analyzed for fast phase compensation time in a feedback configuration of fiber optic gyroscope and the results show potential high speed phase nulling closed loop performance with polymer and III-V semiconductor materials.

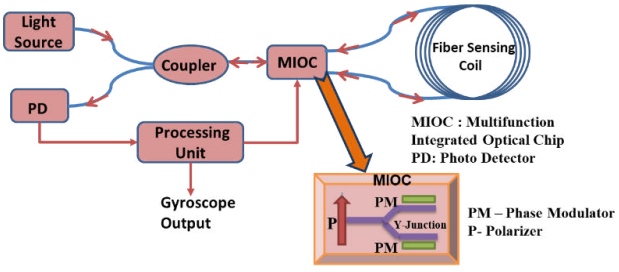


Fig.1 Block Diagram of Fiber Optic Gyroscope with MIOC components

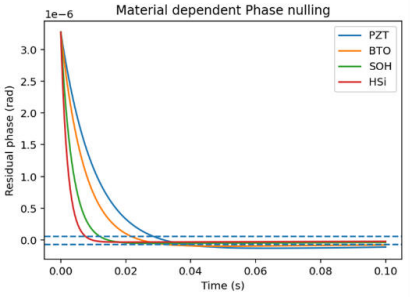


Fig.2 Material dependent Phase Nulling Plot

References:

1. H. C. Lefevre, Artech House, (2022).
2. W. Freude, A. Kotz, H. Kholeif, A. Schwarzenberger, A. Kuzmin, C. Eschenbaum, A. Mertens, S. Sarwar, P. Erk, S. Bräse, and C. Koos, IEEE J. Sel. Top. Quantum Electron., 30 (2024) 1.
3. L. R. Dalton, Opt. Mater. Express, 15 (2025) 2037.
4. C. Zhang, P. A. Morton, J. B. Khurgin, J. D. Peters, and J. E. Bowers, Opt. Express, 24 (2016) 19040.
5. S. M. McKiel, M.Sc. Thesis, Univ. Toronto, (2021).

EL-009

Performance Comparison of Five different Cs-Bi-I Perovskite Compositions for Solar Cells: A SCAPS-1D Study

*Vinitha B.Elza[1,4,5], Nelsa Abraham[2,5], V. Suresh Babu[3,5], Sahaya Dennish Babu George[6], Aseena S[7]

[1]*Department of Electronics and Communication Engineering, Government Engineering College Barton Hill, Thiruvananthapuram, Kerala, 695035, India.*

[2]*Department of Electronics and Communication Engineering, RIT, Kottayam*

[3]*Principal, Mohandas College of Engineering and Technology, Anad*

[4]*Department of Electronics and Communication Engineering, Marian Engineering College, Thiruvananthapuram, Kerala, 695582, India.*

[5]*APJ Abdul Kalam Technological University, Thiruvananthapuram, Kerala, 695016, India.*

[6]*Associate Professor, Dept. of Physics, Chettinad College of Engineering and Technology, Karur, India*

[7]*Engineer, Keltron, Kerala.*

***Corresponding author e-mail:** vinithaelza484@gmail.com

ABSTRACT

This study explores the potential of Caesium Bismuth Iodide (CBI) perovskites as an environmentally friendly solar cells, focusing on optimizing their composition for enhanced efficiency and stability. Through simulation studies, the comparison of five CBI compositions (CsBi3I10, CsBi2I7, Cs2BiI6, Cs2BiAgI6, and Cs3Bi2I9) have been done and CsBi3I10 is identified as the most promising formulation. When paired with ZnO as the Electron transport material (ETM) and CuSCN as the Hole transport material (HTM), CsBi3I10 achieves a Power Conversion Efficiency (PCE) of 19.72%, Fill Factor (FF) of 83%, Short Circuit Current (Jsc) of 19.3 mA/cm², and Open Circuit Voltage (Voc) of 1.22V. The material's non-toxicity, suitable bandgap, and broad absorption spectrum make it an attractive candidate for solar cells and photo-enhanced triboelectric Nano generators. Our findings suggest that CsBi3I10 is a promising lead-free perovskite for commercial applications, offering efficient charge collection and conversion, low charge transport resistance, and broad absorption spectrum. This work highlights the potential of CBI perovskites for sustainable and efficient solar energy harvesting.

References:

1. Mahapatra, P. Kumar, S. Kumar, and B. Pradhan, Sci. Adv., 23 (2022) 100686.
2. Yang, P. Song, R. M. El-Shishtawy, F. Mia, and Y. Li, Phys. Chem. Chem. Phys., 47 (2021).
3. N. Singh, A. Agarwal, and M. Agarwal, Sol. Energy, 208 (2020) 399.

Growth, Structural, Linear and Non-Linear Optical Limiting Properties of a Novel Barium (II) Bis benzo (15-Crown-5 ether) Manganese (II) Thiocyanate (BBCMT) Single Crystal

S. Sengottaiyan[1], B. Gunasekaran[1]*

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603 203.*

***Corresponding author e-mail:** gunasekb@srmist.edu.in

ABSTRACT

A novel Barium (II) Bis 15-Crown-5 ether Manganese (II) Thiocyanate single crystal were grown at ambient temperature, synthesized via the slow evaporation method. The single crystal X-ray diffraction confirms that the grown crystal system is Tetragonal with a centrosymmetric space group I41/a. Additionally, the cell parameters a = 28.13 Å, b = 28.13 Å, c = 9.73 Å and V = 7697(4) Å^3 were observed and well matched with both powder and single crystal X-ray diffraction. The UV-Vis optical transmission spectrum shows that the grown crystal cut-off wavelength of 281nm, using Tauc's plot a band gap value of 3.45eV. The CN stretching vibrations of NH4(SCN) functional group were found to be in FTIR and micro-Raman spectroscopy studies. The reverse growth rates and rectangular shape layered etch pattern of the grown crystal were investigated using etching studies. The thermogravimetric curve showed the decomposition temperature was found at 100 °C, differential thermal analysis curve revealed two endothermic peaks at 150-200°C and 250-300°C, respectively. The mechanical stability of grown crystal confirmed as hard material (n = 1.4) was tested by Vickers micro hardness studies. The Z-scan measurement operate at 532nm Q-switched Nd: YAG laser, revealing the reverse saturable absorption, the calculated nonlinear absorption coefficient (β) is 0.68 × 10^{-10} m/W and optical limiting threshold value is 2.42 × 10^{12} W/m^2. The above-mentioned results suggest that the grown crystal has favorable optical transmittance, moderate thermal and mechanical stability, excellent optical limiting property, therefore the grown crystal is suitable for non-linear and optical limiting applications.

Keywords: Slow evaporation method, Single crystal X-ray diffraction, TG-DTA and Optical limiting studies.

References:

1. T. A. Hegde, A. Dutta, T. C. S. Girisun, M. Abith, and G. Vinitha, J. Mater. Sci. Mater. Electron., 30 (2019) 18885.
2. T. Kamalesh, P. Karuppasamy, M. S. Pandian, P. Ramasamy, and S. Verma, J. Mater. Sci. Mater. Electron., 32 (2021) 6141.

EL-011

Unravelling Piezoelectricity in Surface Charge Tuned Two-Dimensional Poly (L-Lactide) for Self-Powered Sensors

Swadesh Paul[1], Chandreyee Banerjee[1], Anuja Datta[2,3]* and Anindita Das[1]*

[1]*School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, 2A and 2B Raja S. C. Mullick Road, Kolkata, India-700032*

[2]*Technical Research Center, Indian Association for the Cultivation of Science, 2A and 2B Raja S. C. Mullick Road, Kolkata, India-700032*

[3]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai, 603203, India*

***Corresponding author's e-mail:** anujad@srmist.edu.in , psuad2@iacs.res.in

ABSTRACT

Precision two-dimensional (2D) architectures derived from π-conjugated systems offer unique opportunities for advanced electronic, optoelectronic, and biomedical applications due to their directional anisotropy, large surface areas, and tunable surface functionality. Among various fabrication strategies, crystallization-driven self-assembly (CDSA) of semicrystalline polymers has emerged as a powerful bottom-up approach to generate anisotropic nanostructures with molecular-level precision. In particular, poly (L-lactic acid) (PLLA), a biocompatible and biodegradable polymer1, has attracted increasing attention owing to its intrinsic piezoelectric properties arising from the non-centrosymmetric alignment of carbonyl dipoles in its crystalline β-phase. However, harvesting piezoelectricity from precisely controlled 2D PLLA nanostructures via CDSA remains unexplored. Herein, we report a versatile CDSA-based strategy to construct surface-functionalized crystalline 2D PLLA platelets using chromophore-end-capped PLLA homopolymers. Two naphthalene diimide (NDI)-functionalized PLLA systems neutral NDI-1-PLLA and cationic NDI-2-PLLA were self-assembled in isopropanol to yield well-defined diamond-shaped 2D platelets with surface-exposed NDI chromophores. The electron-accepting NDI units enabled programmable supramolecular donor-acceptor (D-A) charge-transfer (CT) interactions with complementary electron-rich donors, including neutral and anionic 1,5-dihydroxynaphthalene derivatives. Systematic modulation of the surface chemistry revealed a strong correlation between end-group functionality, supramolecular CT interactions, and the resulting piezoelectric performanceNotably, the introduction of cationic NDI-2 significantly enhanced the piezoelectric output, which was further amplified through electrostatically driven CT complexation with an anionic donor. The optimized NDI-2-PLLA/D-A system demonstrated superior piezoelectric response and was successfully employed as a self-powered, flexible sensor capable of detecting physiological signals such as arterial pulse waves with high sensitivity2, 3. This work establishes CDSA as a powerful platform for engineering functional 2D piezoelectric polymer assemblies and highlights the synergistic role of surface supramolecular interactions in amplifying piezoelectric performance for biomedical sensing applications.

Keywords: PLLA, 2D nanostructures, Piezoelectricity, Charge-transfer interactions

Pulsed Laser Ablation Derived Plasmonic Nanoparticles with Enhanced Antibacterial Efficacy and SERS Sensitivity

Jyotsna Patra, Govind Chouhan, Pratyush Dash, Manika Dandapat, Satyaranjan Satyajit, Umakanta Tripathy, Sheeja Jagadevan and Amitava Adak*

IIT (ISM) Dhanbad, Jharkhand-826004, India

***Corresponding author e-mail:** amitavaadak@iitism.ac.in

ABSTRACT

The environment pollution causes major threat to the public health globally. The untreated industrial waste such as toxic dyes and human waste releases infectious bacteria and cancerous elements into the water bodies and atmosphere. Over the time, these bacteria have become antibiotic-resistant, causing millions of disease and hospitalization. Also, the detection and degradation of toxic dyes is very crucial for human health. Plasmonic nanoparticles have proven significant promise in nanoparticle-based therapeutic medicines used against antibiotic-resistant bacteria. These plasmonic nanoparticles have also shown its excellency in the detection and degradation of toxic dyes through surface enhanced Raman scattering (SERS) sensing applications. In the present study, the aim is was fabricate biocompatible plasmonic nanomaterial by a novel and green fabrication approach that functions as antibacterial agent and possess SERS features. Plasmonic Cu nanoparticles are fabricated by Pulsed laser ablation(PLA) in liquid method. Particles are characterized by XRD, TEM and UV-Vis spectroscopy. The antibacterial efficacy of the prepared plasmonic nanoparticle samples were tested against E.coli bacteria by spread-plate method. The cytotoxicity of the prepared nanoparticles was tested on normal Human cell lines by performing MTT assay. Bioimaging of the live cells was also performed. The SERS performance of the prepared samples on a toxic dye (Congo red dye) molecule was tested by using Raman spectroscopy. The cytotoxicity results on HEK cells showed viability of about 80% which indicates biocompatible nature of our sample. The antibacterial test results showed 90 % killing of E.coli bacteria. The Raman spectroscopy results showed an enhancement intensity of 103 in the toxic dye molecule spectra indicating satisfactory SERS performance of our sample. Our work provides an insight of a novel and green approach of plasmonic nanoparticle fabrication. These nanoparticles have excellent antibacterial efficacy and possess SERS characteristics for sensing applications.

EL-013

Synergistic Exciton–Plasmon Coupling in Noble metal nanoparticle - Rhodamine system: A combined DFT and experimental Study

Aarti Diwan[1], Vijay Vel Rajankumar[1], Anaswara BP[1] , Shailendra K. Saxena[1]*

[1] *Optics and Nanoelectronics Laboratory (ONE), Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** shailens@srmist.edu.in

ABSTRACT

The rational design of hybrid nanostructures with tailored optoelectronic properties hinges on a precise understanding of exciton-plasmon coupling (EPC)1. Herein, we present a comprehensive, synergistic investigation of the interactions between rhodamine dye and plasmonic gold nanoparticle (AuNP), combining first-principles density functional theory (DFT) calculations with detailed experimental studies2. The charge transfer between them was mapped by charge density difference calculations and quantitatively analysed with Loudin charge analysis. Experimentally, we validate these predictions through controlled synthesis and advanced spectroscopic characterization, observing enhanced photoluminescence and modified emission lifetimes that correlate directly with nanoparticle composition. The system reveals, synergistic enhancement in coupling efficiency, mediated by tunable localized surface plasmon resonance (LSPR) energy and interfacial electronic structure, which DFT attributes to optimized orbital overlap and suppressed non-radiative pathways. This integrated study establishes a definitive structure-property relationship for exciton-plasmon hybrids, providing a predictive blueprint for their application in nanophotonic devices.

Keywords: exciton–plasmon coupling, photoluminescence, charge transfer, density functional theory, Loudin charge transfer analysis.

References:

1. M. Achermann, J. Phys. Chem. Lett., 1 (2010) 2837.
2. T. Sen and A. Patra, Int. J. Nanosci., 10 (2011).

EL-014

Thermoelectric Properties of Chalcogenide Perovskite Exhibiting Ultra-Low Thermal Conductivity

Sanjukta Mukherjee, Tanmoy Maiti*

Department of Materials Science & Engineering, Plasmonics and Perovskite Laboratory, Indian Institute of Technology Kanpur, India 208016

***Corresponding author e-mail:** tmaiti@iitk.ac.in

ABSTRACT

Chalcogenide perovskites are novel class of perovskites with rich tunability in functionalities, owing to its promising optical, electrical properties as well as thermal and aqueous stability, which make them a potential candidate for applications in electronic, photonic, and energy technologies. They have a general chemical formula of ABX_3, where A is an alkaline earth metal, B is a transition metal and X is a chalcogen (S or Se). Though these materials have been explored for optoelectronic and photonic applications, their thermoelectric properties remain poorly investigated. Although chalcogenides like tellurides and selenides have shown reasonably good thermoelectric performance determined by their figure of merit ($ZT= \alpha^2\sigma T/\kappa$), these materials suffer from high cost, toxicity, high temperature instability etc. The sulphide-based perovskites being cost effective and environmentally benign can emerge as an alternative solution for novel low cost thermoelectrics. Furthermore, the rich tunability with respect to their structural diversity and defect tolerance offers an opportunity to innovate desired functionalities for thermoelectric applications. In this work, we have explored several perovskite compositions that have been synthesized by solid state reaction route and densification has been carried out using spark plasma sintering technique. Electrical and thermal transport properties have been studied for the samples that revealed exciting properties for the same. For instance, BaTiS3 depicted ultralow lattice thermal conductivity (0.4 W m^{-1} K^{-1}) owing to its low Debey temperature and lattice anharmonicity arising from weak chemical bonding due to rattling nature of barium in TiS6 octahedron. This value is lower than most of the state-of-the-art thermoelectric materials.

Keywords: Chalcogenide perovskites, Figure of merit, thermoelectrics, characterization, thermal conductivity.

References:

1. T. Ishihara, in Springer Handbook of Electronic and Photonic Materials, Springer, Cham, (2017).
2. Y.-Y. Sun, M. L. Agiorgousis, P. Zhang, and S. Zhang, Nano Lett., 15 (2015) 581.

Lead-Free Halide Double Perovskite $Cs_2Ag_{0.4}Na_{0.6}In_{0.9}Bi_{0.1}Cl_6$ as a Cold White Emitter for Indoor Application

Prakash Kanapathi, Nalini Ravi, Tamilselvan Appadurai*

LEEP Device Research Group, Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India - 603 203.

***Corresponding author e-mail:** tamilsea3@srmist.edu.in

ABSTRACT

Single-component white light-emitting materials are potential candidates in solid-state lighting systems due to the rising demand in display technology and energy-efficient lighting. In this context, halide double perovskites with the flexible structural composition ($Cs_2B'B''Cl_6$) have emerged with the groundbreaking potential, such as high stability, high absorption coefficient, large Stokes shift, and tunable band gap, which favor precise color tuning to meet the specified applications. For this, the researchers employed various substitution and doping strategies on the compound $Cs_2AgInCl_6$ to achieve efficient emission from the material through the alkali (Na^+), post-transition metals (Bi^{3+}) and transition metals (Mn^{2+}, Cr^{3+}, Ni^{2+}, Cu^{2+}) ions. As a consequence, warm white light has been accomplished, demonstrating potential for outdoor lighting applications. However, for an indoor lighting system, the development of cold white light-emitting materials remains a significant challenge in this field. In this work, we have chosen the double site-substituted halide double perovskite $Cs_2Ag_{0.4}Na_{0.6}In_{0.9}Bi_{0.1}Cl_6$ (CANIBC), establishing 98% photoluminescence quantum yield (PLQY), to tune its emission from the warm white to the cold white region. Thus, the rare earth ions such as Ce^{3+}, Er^{3+}, Yb^{3+}, and Pr^{3+} have been incorporated into CANIBC at a concentration of 5%, to introduce the distinct d→f and f→f localized states within the forbidden energy level of the material. Such a transition enables the new emission centers, which will effectively tailor the emission towards the cold white region as well as encourage the radiative recombination rate to intensify the emission. We have utilised the hydrothermal method to prepare all the compounds. All the synthesized compounds have been crystallised in a cubic crystal structure with $Fm\bar{3}m$ space group confirmed by structural analysis. In addition, we have also performed UV-visible and photoluminescence spectroscopy to confirm our findings, and their results will be discussed in detail.

Keywords: Solid state light, halide double perovskite, cold white light, single component

References:

1. Wang, H., Chen, J., Sun, Y. et al, Sci Rep 14, 14740 (2024).
2. Sun, R., Zhou, D., Ding, Y. et al., Light Sci Appl 11, 340 (2022).

Site-Occupation Engineering of Sm^{3+} in $NaLaInNbO_6$ Double Perovskite toward Enhanced Efficient Red-Emitting Phosphors for pc-WLEDs

M. Nitesh Kumar, P. Samuel*

Department of Physics, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu, India, 632014

***Corresponding author e-mail:** samuel.p@vit.ac.in

ABSTRACT

Phosphors play a crucial role in the development of high-performance phosphor-converted white light-emitting diodes (pc-WLEDs). In this study, Sm^{3+} activated $NaLaInNbO_6$ double perovskite phosphors were synthesized using a conventional solid-state reaction method. Sm^{3+} ions were systematically doped into both the La^{3+} and In^{3+} crystallographic sites. The phase purity and structural stability of the samples were confirmed through X-ray diffraction analysis, which indicated the successful incorporation of Sm3+ without altering the host lattice with tetragonal phase. Photoluminescence excitation and emission studies revealed intense characteristic emissions from Sm^{3+} ions, specifically arising from the $^4G^{5/2} \rightarrow {}^6HJ$ (where J = 5/2, 7/2, and 9/2) transitions. This produces dominant orange-red and red emissions within the 600-650 nm range under near-ultraviolet (UV) excitation. The site-dependent luminescence behavior shows that Sm3+ ions located at the La^{3+} and In^{3+} sites experience different local crystal field environments. This leads to variations in emission intensity and spectral distribution. The red emission effectively complements blue and green components, making it suitable for spectral compensation in pc-WLEDs to enhance color rendering performance. These findings suggest that Sm^{3+} doped $NaLaInNbO_6$ is a promising candidate for red-emitting phosphors in near-UV-excited pc-WLED applications.

Keywords: Red Phosphor; Double Perovskite; Luminescence

References:

1. Chun Che Lin, Andries Meijerink, and Ru-Shi Liu, J. Phys. Chem. Lett. 7 (2016).
2. Govind B. Nair, H.C. Swart, S.J. Dhoble, Prog. Mater. Sci. 109 (2020).

EL-017

AWaV: Adaptive Wavelength-Multiplexed Optical Emulation Framework for Semantic Feature Extraction and Vision Classification in Photonic AI Systems

G. Annapoorani[1], Ms. Lathaselvi G[2], Dr. Gopikha S[2]*

[1]*University College of Engineering, BIT Campus,Anna University, Tiruchirappalli, Tamil Nadu, India*

[2]*St. Joseph's College of Engineering,Chennai, Tamil Nadu, India*

***Corresponding author e-mail:** gopikha.re@gmail.com

ABSTRACT

The rapid expansion of artificial intelligence and vision-centric applications has increased the demand for computing architectures capable of overcoming the speed, bandwidth, and energy limitations of conventional electronic processors. All-optical and photonic computing paradigms provide inherent parallelism and high-throughput signal processing; however, existing photonic vision approaches typically rely on static wavelength allocation, hardware-specific implementations, and fixed optical configurations, which limit adaptability, scalability, and systematic evaluation.AWaV is introduced as an adaptive wavelength-multiplexed optical emulation framework designed for semantic feature extraction and vision classification. The framework enables software-defined exploration of photonic intelligence by numerically emulating key optical computing mechanisms without requiring physical device fabrication. Optical encoding of visual inputs, phase modulation, wavelength-division multiplexing, and optical interference are modeled using complex-valued representations. An adaptive wavelength allocation strategy dynamically prioritizes spectral resources according to semantic feature relevance, supporting efficient wavelength-parallel computation. Photodetection-inspired nonlinear responses are incorporated to enhance feature discrimination and semantic synthesis. The proposed framework offers dynamic adaptability, spectral parallelism, hardware independence, and scalability for large-scale experimentation. These characteristics facilitate flexible evaluation of photonic vision concepts while reducing computational redundancy and latency. Validation using benchmark vision datasets and classical texture datasets demonstrates effective semantic feature extraction and competitive vision classification performance compared with conventional static photonic architectures. Overall, AWaV provides a scalable and reproducible platform for investigating adaptive photonic computing strategies and supports the advancement of next-generation optical intelligence systems.

Keywords: Wavelength Multiplexing, Optical Emulation, Semantic Feature Extraction, Photonic Artificial Intelligence, Vision Classification

pH-Controlled Synthesis and Optical Limiting Behavior of Phase Change Materials

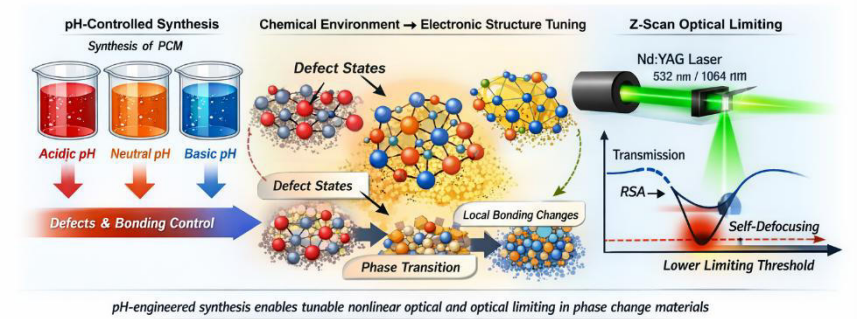
Ida Florence Sharon E[1], Annie Sujatha R[1]*

[1]*Nano Photonics Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** anniesur@srmist.edu.in

ABSTRACT

Phase change materials (PCMs) synthesized via solution-based routes offer significant advantages for nonlinear optical and optical limiting applications due to their tunable chemistry, defect landscape, and phase stability. In this work, we demonstrate pH-controlled synthesis as an effective strategy to engineer the nonlinear optical response and optical limiting performance of phase change materials. Systematic modulation of pH during synthesis alters nucleation kinetics, local coordination environment, and defect density, leading to pronounced changes in electronic structure and excited-state dynamics. Structural and optical characterizations reveal that pH-induced protonation–deprotonation processes modify bonding heterogeneity and defect-assisted absorption pathways. Open- and closed-aperture Z-scan measurements using nanosecond laser excitation show enhanced reverse saturable absorption and self-defocusing behavior under optimized pH conditions, resulting in reduced optical limiting thresholds and improved limiting efficiency. The observed nonlinear response is attributed to synthesis-driven modification of defect states, carrier trapping centers, and phase transition energetics. These findings establish chemical environment control during synthesis as a powerful tool for tailoring optical limiting characteristics in phase change materials. The study provides a synthesis–structure–property framework for the rational design of adaptive optical limiters and laser protection devices based on chemically engineered phase change systems.



pH-engineered synthesis enables tunable nonlinear optical and optical limiting in phase change materials

Keywords: Phase change materials; solution synthesis; optical limiting; Z-scan; nonlinear optics

References

1. Zhang et al., Journal of Materials Chemistry C, 9, 14862–14871 (2021).
2. Kalcheim et al., Chemistry of Materials, 32, 944–954 (2020).

EL-019

Fabrication and Characterization of PEDOT: PSS and Activated Charcoal Based Two Terminal Devices

Raja Vipul Gautam[1], Meenakshi Sundereswaran U[2], Deepjyoti Deb[3], Soumyaranjan Routray[2], Rupam Goswami[1]*

[1]*Tezpur University, Napaam, Tezpur, Assam, India 784028*

[2]*SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603203*

[3]*SRM Institute of Science and Technology, Vadapalani, Tamil Nadu, India 600026*

***Corresponding author e-mail:** rupam21@tezu.ac.in

ABSTRACT

This work proposes the fabrication of two-terminal devices using carbon (activated charcoal) as the active material and copper electrodes, as shown in Fig. 1(a), with the dimensions illustrated in Fig. 1(b). The deposition methodology adopted in this study is the doctor-blade technique. Activated charcoal is extensively used due to its high adsorption capacity and large surface area, and it has found applications in purification systems, sensors, and memory devices [1-2]. In the field of electronics, charcoal is selected as the base material because of its ready availability, low cost, and favorable absorbent and adhesive properties. The electrical characteristics of copper-coated substrates with activated charcoal were systematically investigated, and the results demonstrate a significant improvement in electrical conductivity after coating [2]. Comprehensive morphological characterization was performed to analyze the samples, targeting potential applications in sensing devices and physical unclonable functions (PUFs). Furthermore, the observed repeatability of the electrical characteristics, with only minor deviations, confirms that the doctor-blade deposition technique is an efficient and reliable method for fabricating such carbon-based devices. This work also aims to explore the properties of activated charcoal with organic polymer binders. In Fig. 1(c) and (d), the sample device shows better conductivity, and the current reaches up to the range of 0.1-1 mA as the voltage ranges from -10 V to 10 V.

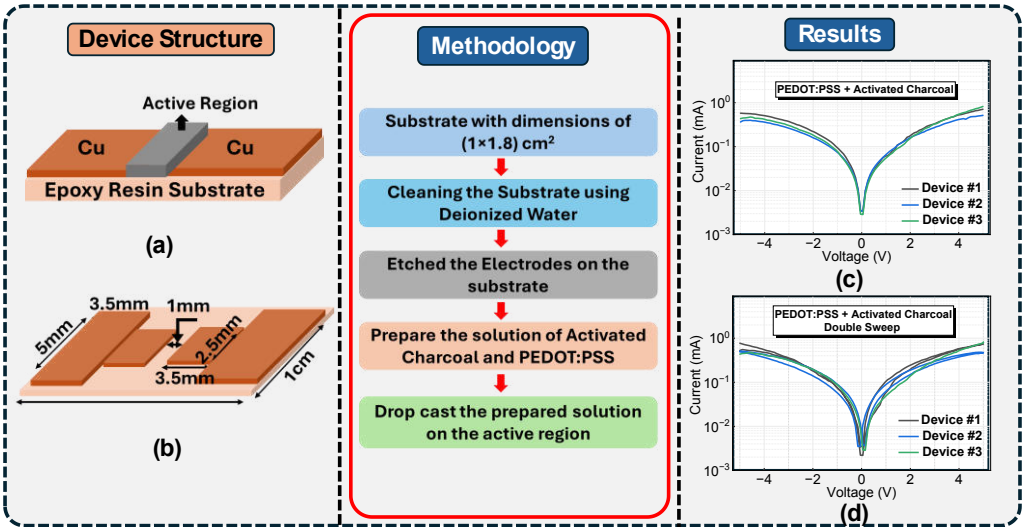


Fig. Flow Chart for the Methodology; (a) Dimensions, (b) Schematic Diagram, (c) Linear, (d) Dual

Keywords: Activated Charcoal, PEDOT: PSS, Crystalline, Carbon nanotubes (CNTs)

EL-020

Theoretical investigation of Dark Current and Responsivity of AlGaN/GaN HEMT-based High-Performance UV-Detection Photodetector

Lakhan Yadav, Shubham Kumar, Samarendra Samal, Ashish Kumar

Department of Electronics and Communication Engineering, National Institute of Technology Raipur, C.G., India

***Corresponding author e-mail:** lyadav023.mtech2024@ece.nitrr.ac.in

ABSTRACT

In this work, we report an AlGaN/GaN HEMT device used as an ultraviolet photodetector. The excellent material and heterostructure properties of the GaN-based device make it a suitable FET sensor. In addition, using indium tin oxide (ITO) as a gate electrode enhances device efficiency due to its high optical transparency and electrical conductivity. SiO_2 is employed as the gate dielectric, reducing interface traps and suppressing dark current, thereby improving the device's signal-to-noise ratio and response. The proposed MOSHEMT device offers a reduction in dark current to $4.98x10^{-11}$ A using SiO_2 as the gate dielectric and ITO as the controlled electrode. The device also boosts Iphoto at an optical incident intensity of 3 mW/cm^2 to $8.75x10^{-5}$ A with an enhanced responsivity of the order of 108 A/W. These results suggest a significant improvement in the phototransistor's performance using HEMT and demonstrate the application of ITO as an alternative transparent electrode.

Keywords: AlGaN/GaN, HEMT, 2-DEG, UV, Photodetector.

References:

1. Q. Cai et al., Light Sci. Appl., 10 (2021).
2. R. K. Mondal et al., ACS Appl. Mater. Interfaces, 17 (2025).
3. C. H. Chen et al., IEEE Photon. Technol. Lett., 13 (2001) 848–850.
4. D. Kim et al., J. Sensors, 2025 (2025) 4284783.

EL-021

High-Sensitivity BK7–Ag–BN–BlueP/WSe_2–BP SPR Biosensor for Label-Free Detection of A549 Lung Cancer Cells

Gundala Vasanthi [1], Balaji Ramachandran[1],*, Yesudasu Vasimalla[1], Santosh Kumar[1]

[1]*Centre of Excellence for Nanotechnology, Department of Electronics and Communication Engineering, KL University, Vaddeswaram, Andhra Pradesh, India, 522302*

***Corresponding author e-mail:** rbalaji@kluniversity.in

ABSTRACT

Early and precise diagnosis of lung cancer plays a vital role in enhancing patient survival rates. The multilayer structure of BK7–Ag–BN–BlueP/WSe_2–BP is considered to be a highly sensitive surface plasmon resonance (SPR) biosensor for label-free detection of A549 lung cancer cells. The two-dimensional (2D) materials hexagonal boron nitride (BN), blue phosphorene/tungsten diselenide (BlueP/WSe_2) heterostructure, and black phosphorene (BP) confine plasmonic fields better than the individual materials and decrease the energy loss at the metal-dielectric interface. The transfer matrix method (TMM) was used to simulate a wavelength of 633 nm. The sensing medium, which had a refractive index (RI) ranging between 1.370 and 1.388, was used to simulate the optical response of A549 cells. The proposed sensor has a high resonance angle change with a peak sensitivity (S) of 366.58°/RIU, quality factor (QF) of 148.60 RIU^{-1}, and detection accuracy (DA) of 2.6749 Deg^{-1}, which is a good sensing performance compared to traditional Ag-based SPR structures. This improvement is due to the large plasmon-exciton coupling and high carrier mobility of the 2D hybrid materials. The findings demonstrate that the proposed BK7AgBNBlueP/WSe_2 BP system is a promising system for the real-time and label-free detection of lung cancer (A549) cells, and could serve as a promising option for the future of plasmonic biosensors in medical diagnostics.

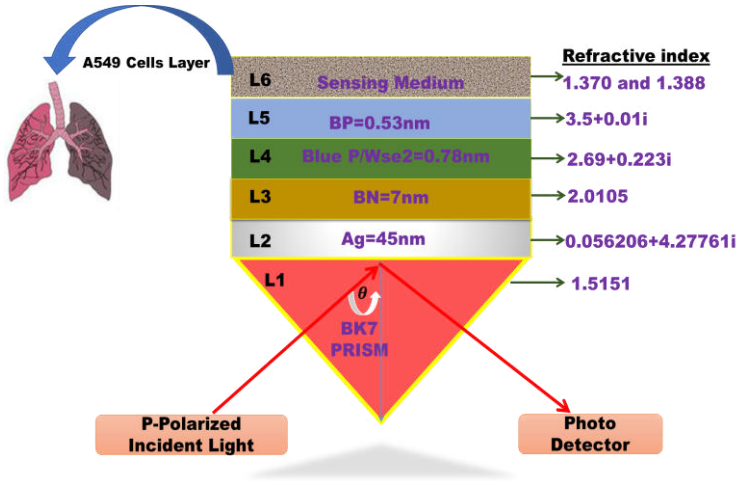


Fig: 1. Schematic design of the proposed BK7–Ag -BN -BlueP/WSe_2 -BP prism-based SPR biosensor, where the layer stack, thickness of the various layers, and refractive index of each layer used to detect A549 lung cancer are indicated.

References:

1. B. Rodenak-Kladniew et al., J. Drug Deliv. Sci. Technol., 2023, 80, 104159.
2. M. Elumalai, G. Nagaraj, J. Kasthuri, E. Vellaichamy and N. Rajendiran, Inorg. Chem. Commun., 2023, 153, 110834.

Plant-Mediated Synthesis of Cu–ZnO Nanocomposites with Multifunctional Environmental Applications

Ruchi Bharti[1]*

[1]*Department of Chemistry, University Institute of Sciences, Chandigarh University, Mohali, Punjab (140413), India.*

***Corresponding author e-mail:** ruchi.uis@cumail.in

ABSTRACT

An environmentally benign strategy was employed for the biosynthesis of bimetallic Cu–ZnO nanocomposites using Athyrium filix-femina leaf extract as a natural reducing and stabilizing agent. Phytochemical constituents in the extract enabled a one-pot synthesis under mild conditions without hazardous reagents. Formation of the Cu–ZnO nanocomposites was indicated by a characteristic color change and confirmed by UV–Vis spectroscopy, FTIR, XRD, SEM, TEM, DLS, and EDX analyses, revealing nanoscale, predominantly amorphous to nanocrystalline structures with bio-organic surface capping and high elemental purity. The multifunctional performance of the material was evaluated. The Cu–ZnO nanocomposites exhibited photocatalytic activity toward bromophenol blue and amaranth dyes, achieving degradation efficiencies exceeding 80% under optimized conditions. Enhanced performance is attributed to charge separation and synergistic interactions at the CuO–ZnO heterojunction, promoting reactive oxygen species generation. Electrochemical measurements demonstrated corrosion protection of mild steel in acidic media, with inhibition efficiencies up to 85%, consistent with formation of a protective film. Additionally, the nanocomposites displayed antioxidant activity in DPPH and ABTS assays, outperforming individual metal oxides due to combined effects of metal oxides and retained plant-derived phytochemicals. Overall, this work establishes a sustainable route to Cu–ZnO nanocomposites with integrated photocatalytic, anticorrosive, and antioxidant functionalities, highlighting potential for remediation and protection.

EL-023

Formalin Detection Using a Multilayer Surface Plasmon Resonance Sensor Incorporating Blue Phosphorus/Tungsten Disulfide Heterostructure, Aluminum Oxide, and Barium Borate Functional Layers

Jyothsna Vaadaala[1], Ragini Singh[2,1], Yesudasu Vasimalla[1], Santosh Kumar[1*]

[1] *Centre of Excellence for Nanotechnology, Department of Electronics and Communication Engineering, Koneru Lakshmaiah Education Foundation, Vaddeswaram, Andhra Pradesh 522302, India*

[2] *Department of Biotechnology, Koneru Lakshmaiah Education Foundation, Vaddeswaram, Andhra Pradesh 522302, India*

***Corresponding author e-mail:** santosh@kluniversity.in

ABSTRACT

Formalin is a highly toxic and commonly abused chemical preservative that has potentially hazardous effects on human health following illegal use in foods, as well as for drinking purposes. In the present work, we propose a highly sensitive surface plasmon resonance (SPR) biosensor to detect formalin using an optimized multilayer heterostructure. This SPR sensor structure is designed based on the conventional Kretschmann configuration, in which a silver (Ag) metal layer is employed to excite surface plasmons. Next, various BlueP-based heterostructures are explored as the constituent layers of the proposed BlueP/TMDC architecture. The performance of our sensor at a wavelength of 633 nm is evaluated using the transfer matrix method (TMM) and the angular interrogation technique. First, the thickness of the Ag layer is optimized to achieve maximum sensitivity while maintaining minimum reflectance loss. Next, the influence of integrating the proposed functional layers is examined by comparing the sensing performance with other layer-specific configurations that exhibit lower detection capability. Furthermore, the sensor response is investigated for different formalin concentrations by analyzing the resonance angle shift and reflectance variation. The designed SPR biosensor demonstrates excellent sensing performance with a sensitivity of 233.83 °/RIU, a quality factor (QF) of 49.8359 RIU^{-1}, and detection accuracy (DA) of 0.9968. These results reveal a remarkable improvement compared to previously reported SPR-based formalin sensing designs.

Keywords: Formalin, SPR biosensor, Kretschmann configuration, Transfer matrix method (TMM), BlueP/TMDC.

TPE-Based Donor-π-Acceptor AIE-Luminophores for Sensing and Solid-State Lighting Applications

Manjit Dehury, Snigdhamayee Rana, Sabita Patel*

National Institute of Technology Rourkela, Odisha, India, 769008

***Corresponding author e-mail:** sabitap@nitrkl.ac.in

ABSTRACT

Organic fluorophores featuring donor-π-acceptor (D-π-A) push–pull architectures have attracted significant attention due to the push-pull D-π-A systems exhibit strong visible-light absorption and photoluminescence, enabling applications in organic electronics such as OFETs, OLEDs, OPVs, and DSSCs. Their π-conjugated D-A architecture promote efficient intramolecular charge transfer, producing highly dipolar molecules applicable for sensing, fingerprint detection, bioimaging and related applications. However, many conjugated organic fluorophores suffer from aggregation-caused quenching (ACQ) in the solid state due to the intermolecular π-π stacking interaction, limiting their practical utility. This drawback can be mitigated by employing aggregation-induced emission (AIE) luminogens. Aggregation-induced emission (AIE)-based pH sensors incorporating pH-responsive functional groups (such as phenol, hydrazone, benzimidazole, or pyridine) offer enhanced stability, high sensitivity, and good performance in water-rich environments, enabling precise detection of small pH variations. Efforts have been made to synthesize and utilize D-π-A based AIEgens as rare-earth free yellow phosphor TPESCNPy with a weaker electron-donating TPE moiety. This work reports two D-π-A push-pull blue fluorophores PI-Fl-*p*-CH_3-TPE and PI-2Ph-*p*-CH_3-TPE with different spacer units to develop latent fingerprints and white solid-state lighting featuring energy efficiency, low cost, simple fabrication and environmentally friendly. PI-Fl-*p*-CH_3-TPE with fluorene conjugation have a rigid structure and shows red shift emission in solid state than twisted biphenyl ones. PI-2Ph-*p*-CH_3-TPE been utilized to develop latent fingerprints using the powder dusting method. Due to their tunable emissions across visible range and high photoluminescence quantum yield (PLQY) in thin film state both the flluorophores PI-Fl-*p*-CH_3-TPE and PI-2Ph-*p*-CH_3-TPE were used to fabricate white LEDs (WLEDs) with a CRI of 81 and 83 and CIE values of 0.34, 0.29 and 0.34, 0.30 respectively.

References:

1. S. Rana, S. R. Nayak, A. Saenubol, V. Promarak, S. Patel, S. Vaidyanathan, Adv. Funct. Mater. 35 (2025) 2507011.
2. S. Rana, S. Vaidyanathan, S. Patel, J. Mater. Chem. C 12 (2024) 14148–14164.
3. S. Rana, S. R. Nayak, S. Patel, S. Vaidyanathan, J. Mater. Chem. C 12 (2024) 765–818.

Oxygen Vacancy–Engineered Optical, Luminescent and Dielectric Response in $BaPO_4$& Re^{3+}Modified $BaPO_4$ Nanophosphors (Where Re = Dy^{3+}, Tb^{3+}, Eb^{3+})

Anitaa, SunitaDahiya[1] and Sunil Kumar[2]*

[1]*Department of Physics, Baba Mastnath University, Asthal Bohar, Rohtak, Harayna, India-124021*

[2]*Department of Applied Physics, Sardar Beant Singh State University, Gurdaspur, Punjab, India-143521*

***Corresponding author e-mail:** sunil_nano@yahoo.com

ABSTRACT

Rare-earth activated barium phosphate ($BaPO_4$) nanophosphors exhibit multifunctional properties governed by defect chemistry and lattice distortion. In the present study, we systematically investigate the influence of oxygen vacancy engineeringon theoptical band structure, photoluminescence behavior, and dielectric responseinBaPO4 andRe^{3+}Modified $BaPO_4$ Nanophosphors (Where Re = Dy^{3+}, Tb^{3+}, Eb^{3+}) nanophosphors, combining experimental characterization. Structural refinement confirms the successful substitution of Eu^{3+} at the Ba^{2+} lattice sites, inducing charge compensation through the formation of oxygen vacancies (V_o••). UV–Vis diffuse reflectance spectroscopy reveals a reduction in optical band gap with increasing Eu^{3+} content, attributed to defect-induced intermediate energy states near the conduction band edge. Photoluminescence studies demonstrate intense characteristic Eu^{3+} emissions dominated by the $^5D_0 \rightarrow {}^7F_2$ transition, with emission enhancement arising from vacancy-assisted energy transfer and symmetry distortion around Eu^{3+} ions. Dielectric measurements exhibit strong frequency dispersion in permittivity and loss, governed by space-charge polarization associated with oxygen vacancy clusters and defect dipoles. The strong correlation between theoretical defect states and experimentally observed optical–dielectric responses highlights oxygen vacancies as key tuning parameters. These results establish Re^{3+}-modified $BaPO_4$ nanophosphors as promising candidates for defect-driven optoelectronic, phosphor, and dielectric device applications.

Color Modulation in Samarium-Doped Borotellurite Glass Embedded with Eu: Y_2O_3 Nanophosphor Composites

Rohit Sharma[1], Y. Dwivedi[1]*

[1]*Department of Physics, National Institute of Technology Kurukshetra, Haryana, 136119, India*

***Corresponding author e-mail:** yashjidwivedi@nitkkr.ac.in

ABSTRACT

In this article, we present the synthesis of a series of composite materials (glass with nanophosphor) incorporating samarium-doped borotellurite glass (Sm:BT) and Eu:Y_2O_3 nanophosphor using a co-sintering technique. Structural analysis reveals the coexistence of glassy and nanocrystalline phases within the material. Comprehensive spectroscopic investigations were conducted through methods such as UV-visible-infrared absorption, and laser spectroscopy in addition to estimation of optical parameters, including Urbach energy, refractive index, and bandgap. The photoluminescence spectra show a combination of sharp, red-dominant emissions from Eu^{3+} ions and broader emission bands from Sm^{3+} ions, spanning wavelengths from 509 nm to 1410 nm. Laser spectroscopy confirms effective interactions between Eu^{3+} and Sm^{3+} ions, even though these active species are encapsulated in different matrices via radiative energy transfer. Notably, the sharp emission from Eu^{3+} in the nanophosphor broadens when integrated into the glass matrix. The addition of nanophosphor to the glass not only extends the emission spectrum into the infrared range but also improves control over color modulation and allows for higher concentrations within the lattice. Color analysis was performed by estimating the CIE and CCT coordinates, indicating precise tuning of the overall emission color hue.

References:

1. S. Ghosh, S. Jana, J. Lumin. 263, (2023)119980.
2. V. Dimitrov, S. Sakka, J. Appl. Phys. 79(3), (1996) 1741–1745.
3. Y. Dwivedi, S.B. Rai, J. Lumin. 194, (2018) 401–406.
4. K. Kalkal, Y. Dwivedi, Mater. Res. Bull. 182(1), (2024) 113154.
5. A.S. Asyikin, A.A. Latif, M.K. Halimah, M.H.M. Zaid, M.A. Kamarudin, M.F. Faznny, I. Zaitizila, Opt. Laser Technol. 168, (2024) 109857.
6. M.M. Naaim, M.F. Malek, Ceram. Int. 49(7), (2023) 10342–10353.
7. R.Y. Dwivedi, J. Appl. Phys. A 125, (2019) 1-10.
8. M.E. Alvarez-Ramos, R.C. Carrillo-Torres, R. SánchezZeferino, J. Non-Crystall. Solids 521, (2019) 119462.
9. I. Jlassi, H. Elhouichet, M. Ferid, J. Mater. Sci. 46, (2011) 806–812.

EL-027

Chiral Perovskite Device Stacks: Multifunctional Platforms for Energy, Sensing and Neuromorphic Computing

Parthiban T, Gopi N, Raja R*

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** rajar@srmist.edu.in

ABSTRACT

Chiral perovskites are new and interesting materials that combine the best features of metal–halide perovskites with the unique properties of chiral molecules. These materials not only absorb light well, but they can also tell which way the light is going and regulate the spin of electrons. This makes them better than regular perovskites. In this article, we talk about how chirality is added to perovskite structures, how it modifies their electrical and optical properties, and how it opens new possibilities for solar energy, sensing and neuromorphic (Brain-like) computing. Then we also talk about chiral perovskite how it used to find circularly polarized light, recognize biomolecules, store information like synapses and operates in a multifunctional device's stacks. Finaly, we highlight the main problem that need to be solved, such as stability, standardization, and the requirement for lead-free materials. And how to commercialize these promising materials into useful next-generation technologies in future.

References:

1. Z. Li, Y. Zhai, Y. Han, J. Appl. Physics, 126 (2019) 230902.
2. Y. Zhai, J. Ma, Z. Li, ChemComm, 56 (2020) 5611–5614.
3. J. Ma, D. N. Beratan, J. Appl. Physics, 128 (2020) 130901.
4. H. Wang, Q. Xu, Y. Liu, ChemComm, 58 (2022) 1845–1848.
5. Q. Xu, H. Wang, Z. Liu, J. Appl. Physics, 131 (2022) 050901.
6. X. Liu, R. Zhang, M. Gao, ChemComm, 59 (2023) 1123–1126.
7. Y. Han, Z. Li, J. Ma, J. Appl. Physics, 129 (2021) 040902.

Design and Investigation of Nanoscaled GaN-Based Truncated-FinFET for High-Sensitivity Hydrogen Gas Sensing

Ajay Kumar[1]*, Neha Gupta[2], Aditya Jain[3], Kaushal Kumar[4], and Amit Kumar Goyal[5]

[1]*ECE Department, Jaypee Institute of Information Technology, Noida, India, 201309.*

[2]*Department of Applied Sciences, GNIOT Group of Institutions, Uttar Pradesh, India, 201306.*

[3]*ECE Department, SIT, Symbiosis International (Deemed University), Pune, Maharashtra, India, 412115.*

[4]*ECE Department, Graphic Era Deemed to be University, Dehradun, Uttarakhand, India.*

[5]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104.*

***Corresponding author e-mail:** ajay.kumar@jiit.ac.in

ABSTRACT

Gallium Nitride (GaN) has emerged as a promising wide bandgap semiconductor material owing to its excellent electronic, chemical, and thermal stability, making it suitable for harsh environment sensing applications. In this work, a GaN-based FinFET structure is proposed and investigated for hydrogen (H_2) gas sensing. The FinFET geometry provides enhanced electrostatic control over the channel and increased surface-to-volume ratio, which are crucial for improving gas adsorption sensitivity. The interaction of hydrogen molecules with the catalytic gate metal modifies the surface potential, thereby modulating the drain current and threshold voltage of the device. The study demonstrates that GaN FinFET exhibits high sensitivity, fast response, and good selectivity towards hydrogen due to its strong affinity and stable chemical interface. Furthermore, the wide bandgap of GaN ensures low leakage current and reliable operation at elevated temperatures, offering a significant advantage over conventional MOSFET-based sensors. The proposed device holds strong potential for next-generation hydrogen sensing applications in energy, safety, and industrial monitoring systems.

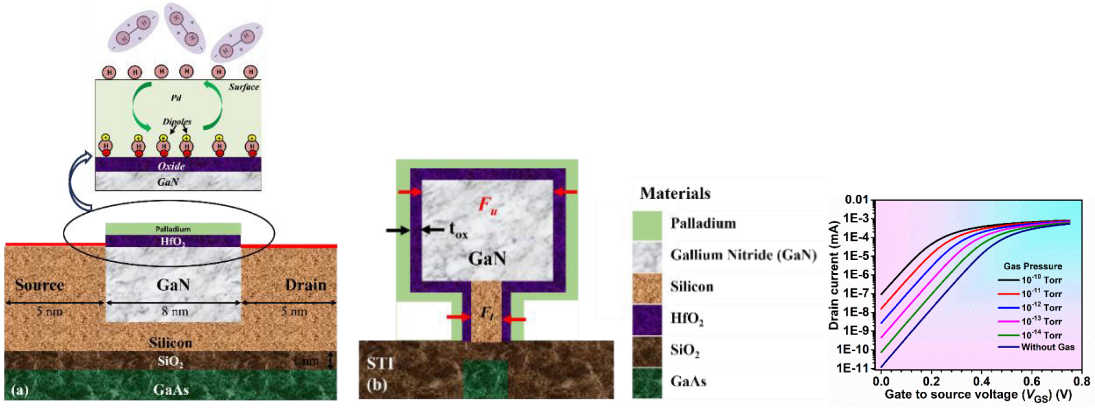


Fig. 1. (a) Device structure, (b) Cross-sectional view of GaN-based Truncated-FinFET Hydrogen gas sensor at 8 nm node. (c) ID-VG characteristics of GaN-based Truncated-FinFET Hydrogen gas sensor at 8 nm node.

EL-029

Interface Mode Excitation Optimization in Nanophotonic Structures using Machine Learning Approaches

Shruti Jha[1], Ajay Kumar[2], Amit Rathi[3], and Adarsh Nigam[1], Amit Kumar Goyal[1]*

[1]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India*

[2]*ECE Department, Jaypee Institute of Information Technology, Noida, U.P., India*

[3]*ECE Department, Manipal University Jaipur, Jaipur, Rajasthan, India*

***Corresponding author e-mail:** amit.goyal@manipal.edu

ABSTRACT

In the field of nanophotonics, precise control of Bloch Surface Waves (BSWs) stands as a pivotal challenge to develop miniaturized optical devices with enhanced performance characteristics. This study delves into the optimization of the incidence angle that influences BSW excitation by employing machine learning (ML) models as a novel solution to traditionally complex and computationally intensive problems. We utilized a multi-faceted ML approach, utilizing Neural Networks, Support Vector Regression, Random Forest, and XGBoost algorithms to model the relationship between induced porosity within nanophotonic structures and the optimal incidence angle for BSW excitation. Through extensive data collection and preprocessing, the study evaluates the efficacy of these algorithms to predict BSW excitation angle. The results indicate that ML models significantly outperform traditional optimization methods, offering rapid and accurate predictions that facilitate a more efficient design process. These models have shown strong predictive accuracy and provided insights into the physical phenomena of BSW excitation, potentially revealing new design principles. Numerical evaluation revealed that the XGBoost model achieved the highest prediction accuracy with a mean absolute error of 0.02778° and a mean squared error of 0.00147°, outperforming the other models. Finally, the obtained results are cross-verified with the conventional FEM method, which confirms its validity. This study paves the way for future explorations of the synergy between machine learning and nanophotonics, opening the door to sophisticated optimization strategies that could redefine our interaction with light at the nanoscale.

References:

1. S. Yadav, S. Senapati, S. Kumar, S. K. Gahlaut, J. P. Singh, Biosensors, 12(12), (2022) 1115.
2. A. K. Goyal, J. Saini, Y. Massoud, Optical and Quantum Electronics, 55(6), (2023) 563.
3. F. Michelotti, B. Sciacca, L. Dominici, M. Quaglio, E. Descrovi, F. Giorgis, F. Geobaldo, Physical Chemistry Chemical Physics, 12(2), (2010), 502–506.
4. M. Chen, D. Pang, X. Chen, H. Yan, P. Zhou, Plasmonics, 16 (2021), 653–659.
5. C. C. Nadell, B. Huang, J. M. Malof, W. J. Padilla, Optics Express, 27(20) (2019), 27523–27535.

EL-030

Growth, Structural, and Optical Characterization of Malachite Green (MG) Doped Triglycine Sulphate (TGS) Single Crystals

Badrinarayan V R, Praveen Joshwa Ramesh, Rajesh Paulraj*

Centre for Crystal Growth, Department of Physics, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai – 603110

***Corresponding author e-mail:** rajeshp@ssn.edu.in

ABSTRACT

Triglycine sulphate (TGS) single crystals doped with malachite green were grown using the slow evaporation solution growth technique with two different dopant concentrations. The influence of malachite green incorporation on the structural and optical properties of TGS was systematically investigated. Powder X-ray diffraction (XRD) analysis confirmed the preservation of the crystalline phase and revealed minor variations in lattice parameters, indicating successful dopant incorporation without disturbing the host structure. Fourier transform infrared (FTIR) spectroscopy was employed to identify functional groups and assess molecular interactions between the dopant and the TGS lattice. Optical transparency and absorption behaviour were evaluated using ultraviolet–visible (UV–Vis) spectroscopy, which demonstrated enhanced optical transmission in the visible region for the doped samples. The optical band gap values were estimated from absorption data and showed concentration-dependent variation. The results indicate that controlled malachite green doping can effectively tailor the structural stability and optical properties of TGS crystals, making them suitable for optoelectronic and photonic device applications.

Keywords: Single Crystals, FTIR, Optical devices, Functional groups

EL-031

Nonlinear Optical and Photoluminescence Studies of Malachite Green Doped Triglycine Sulphate Single Crystals

Sathish S, Praveen Joshwa Ramesh, Rajesh Paulraj*

Centre for Crystal Growth, Department of Physics, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai – 603110

***Corresponding author e-mail:** rajeshp@ssn.edu.in

ABSTRACT

Malachite green doped triglycine sulphate (TGS) single crystals were synthesized by the slow evaporation method using two different dopant concentrations to investigate their nonlinear optical and photoluminescence properties. The incorporation of malachite green into the TGS lattice was found to significantly influence the optical response of the crystals. Second harmonic generation (SHG) efficiency was evaluated using the Kurtz–Perry powder technique, and the doped crystals exhibited enhanced nonlinear optical activity compared to the undoped sample. The variation in SHG output with dopant concentration indicates the role of molecular polarization and defect modulation in improving nonlinear behaviour. Photoluminescence (PL) spectra revealed characteristic emission bands arising from dopant-related electronic transitions, demonstrating improved luminescence efficiency. The observed PL intensity and emission wavelength shifts were found to be concentration dependent. These findings suggest that malachite green doped TGS crystals possess promising nonlinear and luminescent properties, supporting their potential application in frequency conversion and photonic devices.

Keywords: Slow evaporation, Photoluminescence, Photonic devices

EL-032

Growth, Optical and Electrical Studies Of β-Alanine Crystals

K.K. HemaDurga[1], Dr. N. Srinivasan[1], Dr. Sayee Kannan Ramaraj[2]

[1]*Department of Physics, Thiagarajar College, Madurai-9.*

[2]*Department of Chemistry Thiagarajar College, Madurai-9.*

ABSTRACT

β-alanine (3-aminopropanoic acid) is a non-essential naturally occurring amino acid, which is manufactured directly by the human body and does not need to be obtained through the diet. β-alanine is found in animal foods such as fish, chicken, beef etc. The amino group is attached to the β-carbon atom instead of the α-carbon of alanine. β -alanine crystals are obtained by slow evaporation technique. The saturated solution of beta alanine was stirred well using a hot plate magnetic stirrer for 2h and filtered. The crystals were obtained by allowing the solution to evaporate slowly without any disturbance for 30 days. Otherwise, the supersaturated solution (s=1.05) may be kept in constant temperature bath to yield crystals quickly. The photograph of the grown crystal is shown in fig.1. Single crystal XRD studies reveal that β-alanine crystallizes in a centrosymmetric orthorhombic space group Pbca. The various functional groups of β-alanine were identified by FTIR spectrum. The sharp peak at 2108 cm^{-1} is due to the combination of asymmetric stretching and torsional oscillation of NH_3 group. The zwitterionic nature of β-alanine was evident from NH_3^+ absorption band. The UV-Vis transmission spectrum and the associated Tauc plot reveal the optical band gap to be 4.77eV. The SHG test for the grown β-alanine crystal was carried out by using powder Kurtz and Perry technique. From the experiment, it is noticed that there is no green light (no SHG emission) emitted from the sample since it crystallizes in a Centrosymmetric space group. With the help of impedance studies, the grain effect appears as the first semicircle in the Nyquist plot. The semiconductor plot divulges bulk capacitance and hence used to calculate dielectric relaxation time and electronic conduction behaviour of the crystal. The results of crystal growth, optical and electrical characterization will be discussed in detail.

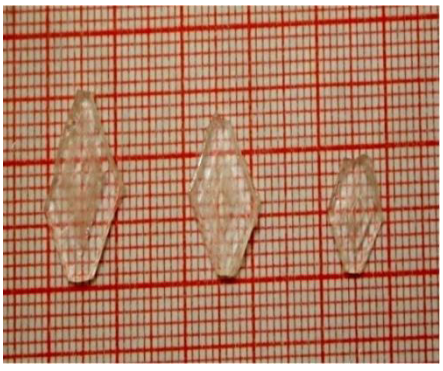


Fig.1. Grown β-alanine crystal

Functional Integration of Sensors, Arduino and Python Programming: Blueprint of a Low-Cost Early Warning for Underground Hard Rock Mines

Rahul Rout, Aman Markande, Falguni Sarkar*, Chandan Biswal

Department of Mining Engineering, National Institute of Technology, Rourkela, Odisha, India

***Corresponding author e-mail:** fresearchnitr@gmail.com

ABSTRACT

Principal hazards in underground metalliferous mines are typically characterized by fire, inundation, strata collapse, inadequate illumination and high noise level etc. These hazards sometimes exhibit disastrous consequences or accident-prone situations, which require modern composite early warning systems for prompt risk mitigation to safeguard the lives of the miners. In this study, development of a hybrid type (combination of wired and wireless structures) early warning system comprising audio-visual alarm and WhatsApp alert service had been attempted. To design this early warning and data transmission-based communication system, Arduino UNO and various Python Libraries like PySerial and PyWhatkit have been integrated. In this context, the developed prototype model was successfully tested and the response times were measured against the incidence of fire breakout, water inrush, inadequate lighting, and intolerable noise at an underground metalliferous mine. The designed system is expected to become trailblazer for mine management and mine's key personnel who can activate the disaster management protocol as soon as warning is received and save precious lifes.

Keywords: Principal hazards, Early warning system, Risk mitigation

References:

1. F. Sarkar et al., J. Inst. Eng. (India): Ser. D, 102 (2021) 39–46.
2. Y. S. Dohare et al., IETE Tech. Rev., 32 (2015) 140–150.
3. A. Jha et al., Saf. Health Work, 13 (2022) 40–50.
4. S.-M. Kim et al., Appl. Sci., 10 (2020) 5018.

EL-034

Solvent-Thermal Annealing-Induced Grain Growth in Triple-Cation Halide Perovskite Thin Films for Enhanced Solar Cell Performance

Mukundan R. Pillai*, Nithin Xavier, Jean Maria Fernandes, Soumya Dutta

Department of Electrical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India, 600036

***Corresponding author e-mail:** ee22d305@smail.iitm.ac.in

ABSTRACT

Metal halide perovskites have gained significant attention for photovoltaic applications due to their high absorption coefficients, tunable bandgaps, and long carrier diffusion lengths [1]. However, non-radiative recombination at grain boundaries and defects limits device performance [2], making improved crystallinity and larger grain size essential. Solvent engineering strategies have previously been employed under controlled low-humidity and oxygen-restricted conditions to optimize film formation and device reproducibility in regular n–i–p architectures [3]. In this work, triple-cation halide perovskite thin films were prepared using two post-deposition approaches: direct thermal annealing and solvent-thermal annealing in dimethyl sulfoxide (DMSO) vapor. Unlike earlier reports, this study explores solvent-thermal annealing-assisted recrystallization under comparatively higher moisture conditions, emphasizing the robustness of the method. Scanning electron microscopy (SEM) analysis shows significantly enlarged grains for solvent-thermal-annealed films relative to thermally annealed films (Figure 1), suggesting reduced grain-boundary recombination and improved charge transport in perovskite solar cells (PSCs) fabricated using these films.

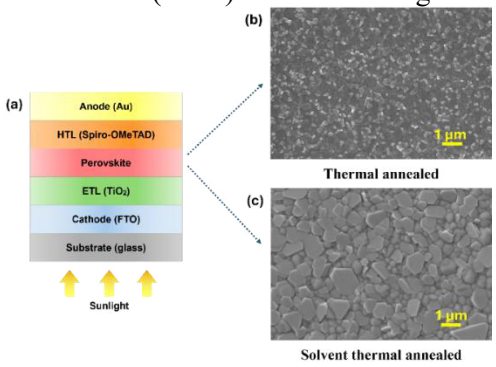


Fig. 1 (a) Schematic representation of the perovskite solar cell architecture; SEM images of the (b) thermally annealed and (c) solvent-thermal-annealed perovskite films.

References:

1. Ajay Kumar Jena, Ashish Kulkarni, Tsutomu Miyasaka, Chem. Rev., 119 (2019), 3036–3103.
2. Tejas S. Sherkar, Cristina Momblona, Lidón Gil-Escrig, Jorge Ávila, Michele Sessolo, Henk J. Bolink, L. Jan Anton Koster, ACS Energy Lett., 2 (2017), 1214–1222.

Enhanced Second order Nonlinear Optical Properties of Hematene Nanosheets

Thameemunnisha Beevi M[1], Arjun Greeshlal[1], Junaid Masud Laskar*[1]

[1]*Nanophotonics and Quantum Meta-Optics Group, Centre for Nanophononics, Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** junaidmb@srmist.edu.in

ABSTRACT

Atomically thin non–van der Waals materials have attracted considerable interest for nonlinear photonic applications owing to their thickness-dependent electronic structure and symmetry-breaking effects. In particular, the second-order nonlinear susceptibility (χ^2) is a key material parameter governing the efficiency of second harmonic generation (SHG) and related frequency-conversion processes, such as spontaneous parametric down-conversion (SPDC). Materials exhibiting large χ^2, optical transparency at the fundamental and harmonic wavelengths, and structural non-centrosymmetric are therefore highly desirable for integrated nonlinear and quantum photonic platforms. Hematene, a two-dimensional derivative of hematite (α-Fe_2O_3), emerges as a promising candidate due to its reduced dimensionality, surface reconstruction, and modified optical and magnetic properties. In this work, we present a systematic investigation of the SHG response of hematene nanosheets with particular emphasis on near-infrared excitation. Hematene nanosheets were synthesized via controlled liquid-phase exfoliation, yielding well-defined hexagonal nanosheets with tunable thickness achieved by varying the exfoliation duration. Thickness reduction enhances quantum confinement and increases the surface-to-volume ratio, leading to effective inversion symmetry breaking and strong surface-induced nonlinear polarization—essential prerequisites for second-order nonlinear optical processes. Structural and vibrational properties were examined using Raman spectroscopy and FTIR analysis, while photoluminescence measurements reveal optically active defect and surface states. Optical absorption studies demonstrate enhanced transparency of hematene nanosheets in the near-infrared region (1100–1600 nm), favoring efficient nonlinear frequency conversion. SHG experiments performed using a nanosecond pulsed Nd:YAG laser reveal a measurable SHG signal arising from intrinsic non-centrosymmetric and thickness-induced surface nonlinearities. From these measurements, the effective second-order nonlinear susceptibility (χ^2) was experimentally determined, providing a quantitative evaluation of the nonlinear optical efficiency. These results establish hematene nanosheets as promising materials for near-infrared nonlinear photonic applications, including SPDC and quantum light source development.

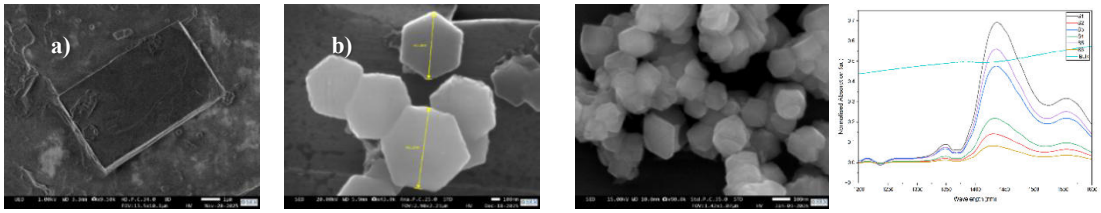


Fig. 1 The FESEM images illustrate the morphological evolution from (a) bulk Fe_2O_3 to the synthesized nanostructures: (b) Fe_2O_3 hexagonal nanoplates, and (c) Fe_2O_3 hexagonal nanosheets. (d) Absorption Spectra.

References:

1. Nature Nanotechnology, 13 (2018) 602–609.
2. ACS Appl. Opt. Mater. 2023, 1, 3, 660–668.
3. Peng, Z. H., Cotrufo, M., Xu, D. *et al*. *Nature Photonics* 19, 1376–1384 (2025).
4. Appl. Phys. Lett. 118, 183102 (2021).

EL-036

A Double Interlocking Strategy for Narrowband Ultra-Violet Emitters (CIEy ≈ 0.029) with Dual Functionality for Efficient OLEDs

Keerthika P, Seung Won Han[3], Ankit Kumar[1], Venkatramaiah Nutalapati[6], Kenkera Rayappa Naveen[5], Jun Yeob Lee*[2,3,4] and Rajendra Kumar Konidena*[1]

[1]*Organic Materials Laboratory (OML), Department of Chemistry, Indian Institute of Technology-Patna, Bihta Kappa Rd, Patna, Dayalpur Daulatpur, Bihar 801106, India*

[2]*Department of Display Convergence Engineering, Sungkyunkwan University2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi, 16419, Republic of Korea*

[3]*School of Chemical Engineering, Sungkyunkwan University 2066, Seobu-ro, Jangan gu, Suwon, Gyeonggi, 16419, Korea*

[4]*Institute of Energy Science and Technology, Sungkyunkwan University,2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi, 16419, Korea*

[5]*Department of Polymer and Process Engineering, Indian Institute of Technology Roorkee, Saharanpur Campus, Saharanpur 247001, Uttar Pradesh, India*

[6]*SRM Institute of Science and technology (Deemed to be university)-Andhra Pradesh*

***Corresponding author e-mail:** leej17@skku.edu; rajsan@iitp.ac.in; rkonidena531@gmail.com.

ABSTRACT

Ultraviolet (UV) organic emitters are crucial for next-generation organic light-emitting diodes (OLEDs), but achieving short-wavelength emission (<400 nm) with narrow full-width-at-half maximum (FWHM <30 nm) remains challenging. In this work, we introduce a strategic double interlocking to develop a narrowband UV emitter using 4-(2,11-di-*tert*-butylindolo[3,2,1-jk]carbazol-5-yl)-N,N-diphenylaniline (tBuICzTPA) as a reference material, where the phenyl units in triphenylamine were interlocked to yield a UV emitter 2',11'-di-*tert*-butyl-2,5'-biindolo[3,2,1-jk]carbazole (tBuICzICz). This design restricts the free rotation of the phenyl units and reduces the donor strength of triphenylamine in reference material tBuICzTPA, effectively suppressing vibronic coupling and increasing singlet energy simultaneously. As a result, tBuICzIC**z** exhibited a 17 nm blue-shift along with a narrowed FWHM of 16 nm. The tBuICzICz emitter demonstrated pure UV emission with a peak at 398 nm and an FWHM of 24 nm. OLED of tBuICzICz achieved an external quantum efficiency (EQE) of 4.2% and CIEy~0.029. Additionally, its wide band-gap and triplet-energy enabled as a host for green phosphorescent OLEDs, achieving an EQE_{max} of 18.5% and a current efficiency of 51.3 cd/A. Notably, the green phosphorescent OLED demonstrated extremely low efficiency roll-off of 1.0% at 3,000 cd/m^2. This simple yet effective strategy paves the way for further development of efficient narrowband UV emitters, which can exhibit dual functionality as emitter and host.

Keywords: UV emitter; Narrowband; OLEDs; Dual-Functionality; Supressed roll-off

References:

1. K. P. Keerthika et al., Chem. Commun., 61 (2025) 12554–12557.

Stimuli-Responsive Molecular Systems for Nanoscale Energy Harvesting Prospects

Pritam Sadhukhan[1], Osamu Sato*[2], Shinji Kanegawa[2], Suhrit Ghosh*[1], Anuja Datta*[3]

[1]*Indian Association for the Cultivation of Science (IACS), Jadavpur, Kolkata, India 700032*

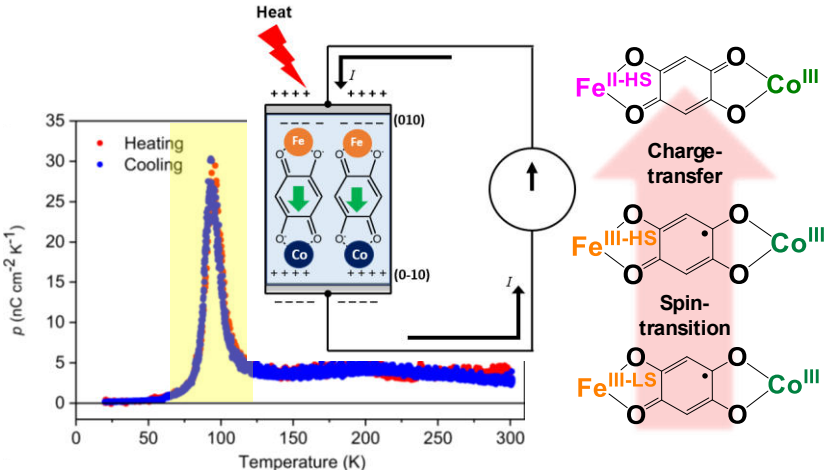
[2]*Kyushu University, ITO Campus, Mootoka, Nishi-ku, Fukuoka, Japan 819-0395*

[3]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:**sato@cm.kyushu-u.ac.jp, psusg2@iacs.res.in, psuad4@iacs.res.in

ABSTRACT

Polar molecular systems exhibiting switchable polarization hold promise for advanced applications in ferroelectric memory, pyroelectric sensing, and nanoscale energy harvesting. Yet, the intrinsic electronic correlations within conventional ferroelectrics pose significant challenges to material design and property modulation. Dynamic molecular crystals provide a compelling alternative, as phenomena like spin crossover and intramolecular charge transfer trigger pronounced electronic density redistributions that facilitate polarization switching. Building on this principle, we introduce a new class of materials, molecular electronic pyroelectrics, that exhibit polarization changes induced by electronic reorganization rather than lattice distortions. These materials demonstrate versatile light- and heat-responsive pyroelectric behaviour, paving the way for next-generation, molecule-based energy-harvesting systems.[1,2] More intriguingly, soft polymer systems also enable precise control of temperature-dependent spontaneous polarization in donor-acceptor π-architectures via reversible, thermally driven supramolecular assembly-disassembly transitions.[3] This approach provides a novel pathway for achieving and modulating electronic pyroelectricity in flexible, biocompatible organic materials.



References:

1. P. Sadhukhan et. al., *Nature Communications*, vol 12 (2021) 4836.
2. P. Sadhukhan et. al., *Nature Communications*, vol 14 (2023) 3394.
3. P. Sadhukhan et. al., *Chemical Communications*, vol 61 (2025) 5289.

Phenothiazine-Linked Benzodithiophene Hole Transport and Interface Passivation Materials for Perovskite Solar Cells

Akashkumar saravanan, Ravikumar Guruswamy, Sivasankar Parameswaran,

G.T. Senthil Andavan, Ananthanarayanan Krishnamoorthy*

Organic & Perovskite Photovoltaics Laboratory (OPPV), Department of Chemistry

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203

***Corresponding author e-mail:** as6237@srmist.edu.in, ananthak@srmist.edu.in

ABSTRACT

Perovskite solar cells (PSCs) have achieved high efficiency (around 26%, device level) but their poor stability under ambient conditions remains a key challenge for their commercialization. The two main reasons for the poor stability are a) surface defects and b) interfacial instability. To address these challenges, we have designed and synthesised two new organic small molecules having N-methoxy triphenyl-aminated phenothiazine units, coupled with sulfur-rich methoxy benzodithiophene units in donor-π-donor (D1-π-D2) and donor-π-donor-π-donor(D1-π-D2-π-D1) configurations. These molecules act as both hole transport material and interfacial passivation agents. Studies such as steady-state photoluminescence and time-resolved photoluminescence reveal that these molecules enable efficient hole extraction, and as confirmed by X-ray photoelectron spectroscopy studies, they effectively passivate defects such as under coordinated Pb^{2+} ions. Devices employing these molecules achieved a maximum power conversion efficiency of 18.52%. These devices also exhibited better stability. Unencapsulated devices retained almost 80 % of their initial PCE after 1000 hours.

Keywords: dual functionality, multisite nitrogen and sulfur chemistry, D1−π−D2−π−D1 configuration, energy level engineering, defect passivation, perovskite solar cells

Reference:

1. Li, N et al., Chem. Soc. Rev. 2020, 49 (22), 8235−8286.
2. Wang, R. et al., Adv. Funct. Mater. 2019, 29 (47), 1808843.
3. Saraswathi G et al., Energy Fuels 2023, 37, 18, 14303–14314

EL-039

Enhance the Efficiency of n-ZnO /p-Si Thin Silicon Solar Cell Through Silver Caped Silica Nanoparticle Mirror

Veda Samhitha Lakshmipurapu*, Kavya Nair, A. Sandeep Kumar Reddy, Arijit Bardhan Roy

SRM Institute of Science and Technology, Kattankulathur, Chennai

***Corresponding author e-mail:** vl8192@srmist.edu.in

ABSTRACT

Thin crystalline silicon (c-Si) based n-ZnO/p-Si heterojunction solar cells offer promising prospects for lightweight and flexible photovoltaic applications. However, the reduced absorber thickness limits photon confinement, leading to increased optical losses and reduced device efficiency. In this work, a silver-capped silica (Ag–SiO_2) nanoparticle back reflector structure is numerically investigated with particular emphasis on the influence of silver (Ag) shell thickness varying from 0.05 nm to 1 nm. Finite Element Method (FEM)-based optical simulations were carried out over the wavelength range of 300–1100 nm under AM 1.5 illumination. The study evaluates reflectance, absorbance, and electric field distribution for different Ag thickness values. The results indicate that ultra-thin Ag layers (≈0.05 nm) provide limited plasmonic interaction, resulting in weaker light scattering and modest reflectance reduction. As the Ag thickness increases, enhanced localized surface plasmon resonance (LSPR) improves backscattering and optical path length inside the silicon layer, thereby increasing absorption and reducing reflectance. An optimal thickness region is observed before parasitic absorption in thicker Ag layers (approaching 1 nm) begins to counteract the optical gains. The analysis demonstrates that controlled tuning of Ag thickness significantly modifies the electric field intensity distribution and hotspot formation within the junction region. Improved light confinement directly enhances photon absorption and carrier generation, contributing to better optical performance of the thin silicon heterostructure. The proposed thickness-optimized Ag–SiO_2 nanoparticle mirror provides an effective nanophotonic strategy for reducing reflection losses and improving light management in thin-film silicon solar cells without introducing surface recombination defects. The integrated reference for 200nm difference between Ag and SiO_2 for each model is seen to be giving lesser reflectance and increased absorption than 100nm difference between Ag and SiO_2, especially Ag having thickness varying from 0.4nm to 0.7nm in 200nm difference between Ag and SiO_2.

Keywords: Ag thickness optimization, Silver-capped silica nanoparticle, Thin c-Si solar cell, Plasmonic back reflector, FEM simulation, Light trapping enhancement.

References:

1. Green, M. A., *Solar Cells: Operating Principles, Technology, and System Applications*, Prentice-Hall, 1982.
2. Battaglia, C., Cuevas, A., & De Wolf, S., "High-efficiency crystalline silicon solar cells: status and perspectives," *Energy & Environmental Science*, vol. 9, pp. 1552–1576, 2016.
3. Özgür, Ü. et al., "A comprehensive review of ZnO materials and devices," *Journal of Applied Physics*, vol. 98, 041301, 2005.

EL-040

Surfactant-Mediated Structural Evolution and Band Gap Engineering of Hierarchical BiOCl Nanostructures

Sibin C S[1], Mani Rahulan K[2], Santhi K*[1]

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*Nanophotonics Research Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India*

***Corresponding author e-mail:** santhichak@gmail.com

ABSTRACT

This study investigates the influence of Cetyltrimethylammonium bromide (CTAB) as a capping agent in the Co-precipitation method of Bismoclite (BiOCl) nanostructures synthesis. X-ray diffraction (XRD) analysis shows that all synthesized samples maintains a crystalline tetragonal phase within the P4/nmm space group. For the pristine sample (BOC - T1), calculated lattice parameters (a = b = 3.8926 Å, c = 7.3873 Å) showed minimal deviation from standard reported values. The introduction of CTAB significantly reduced the crystallite size from 33.51 nm (BOC-T1) to 22.24 nm (BOC-T3). This reduction is attributed to CTA^+ cations capping the surface charge of nuclei, which effectively limits the ion diffusion and prevented self-aggregation of the nano structures.

Field Emission Scanning Electron Microscopy (FESEM) shows a structural evolution from discrete 2D nanoplates in pristine BiOCl to complex hierarchical assemblies. While pristine samples exhibit irregular polygonal shapes, high CTAB concentrations promote the assembly of ultra-thin square shaped nanoplates into highly transparent structures. Optical properties investigated via UV–Vis diffuse reflectance spectroscopy demonstrate successful band gap engineering. The indirect band gap was tuned from 2.81 eV (BOC-T1) down to 2.64 eV (BOC-T3). This decrease in band gap is likely arises from surfactant-mediated changes happened in crystallite size and surface states. This study highlights the efficacy of CTAB-assisted synthesis in tailoring the morphology and electronic properties of BiOCl for advanced optoelectronic applications.

References:

1. Ji-Ming Song, Chang-Jie Mao, He-Lin Niu, Yu-Hua Shen, Sheng-Yi Zhang, CrystEngComm, 12 (2010) 3875–3881.
2. Hui Li, Shichen Xu, Zhipeng Huang, Jiawei Huang, Jun Wang, Long Zhang, Chi Zhang, Mater. Chem. C, 6 (2018) 8709-8716.
3. Chunchun Li, Yikai Xu, Xinyuan Li, Ziwei Ye, Chaoyi Yao, Qinglu Chen, Yuanfeng Zhang, Steven E. J. Bell, Adv. Mater. Interfaces, 7 (2020) 2000391.
4. Yugesh Singh Thakur, Aman Deep Acharya, Sakshi Sharma, Amisha, Sagar Bisoyi, Bhawna, Sandeep Singh Manhas, Mater. Sci. Semicond. Process., 177 (2024) 108376.

Achieving White Light Emission from A Hydrazone Through Three Different Channels: AIE,Solvatochromism and Excitation Wavelength

Jayashree Venkatesh, Rakshantha Srithar and Susnata Pramanik*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** susmatap@srmist.edu.in

ABSTRACT

Reported herein is a hetero-bis-hydrazone that comprising two different diones which emit independently in the blue and orange regions, resulting in white light emission in solution. Two ESIPT moieties simultaneously emitting in the blue and orange regions led to white light. The presence of four tautomers, two from each, was crucial to achieve this. Interestingly, the white light emission was achieved using three channels: AIE, solvatochromism, and tuning of the excitation wavelengths in a partially aggregated solution (f_w = 30%). These results will pave the way for designing new molecular frameworks that can emit white light under multiple experimental conditions.

Keywords: white-light emission, ESIPT, hydrazones, multi-channel emission

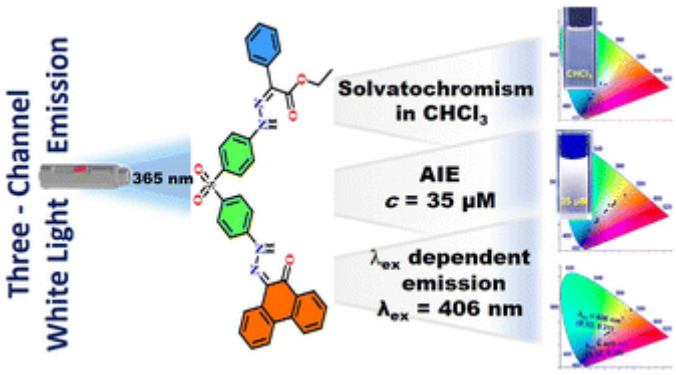


Fig. 1 White-light emission through three independent photophysical channels.

References:

1. B. Shao, H. Qian, Q. Li and I. Aprahamian, *J. Am. Chem. Soc*., 2019, **141**,8364–8371;
2. M. N. Kumar, D. L. Lyngkhoi, S. Gaikwad,J. Samanta, R. Ahamed, S. Khatua and S. Pramanik, *Chem. Commun.,*2023, **59**, 14122–14125.

EL-042

Multi-colour and Red Emissions from a Small Donor-Acceptor Molecule by Breaching Kasha's Rule

Prathaban G[1], Akanksha Sharma[2], Soumen De[2], and Susnata Pramanik[1]*

[1]*SRMIST, Kattankulathur,*

[2]*IISER, Thiruvananthapuram*

ABSTRACT

We present a compact organic fluorophore (MW 260 Da) that defies Kasha's rule by exhibiting dual excited-state emissions. Built on an acenaphthylene scaffold with donor–acceptor substitution, the molecule shows simultaneous S1 and S3 emissions, enabling excitation-dependent colour variation from blue to red. This behaviour is accompanied by huge Stokes shifts (>5000 cm^{-1}) and minimal spectral overlap, ensuring distinct multicolour outputs. In solution, the emission is strongly charge-transfer in nature and highly sensitive to solvent polarity, while in the solid state, the molecule retains efficient red emission. Time-dependent density functional theory (TDDFT) calculations support the experimental findings, revealing two bright states separated by a dark intermediate that suppresses internal conversion and stabilizes dual emission pathways. This study highlights how a small molecular design can achieve versatile photophysical behaviour typically reserved for larger systems. The results open avenues for practical applications in multicolour OLEDs, ratiometric bioimaging, anti-counterfeiting technologies, and photodynamic therapy. By combining simplicity of structure with complex excited-state dynamics, this work establishes a new benchmark in molecular photophysics.

Keywords: Anti-kasha, multicolour emission, charge transfer

References:

1. M. Kasha, Characterization of Electronic Transitions in Complex Molecules. Discuss Faraday Soc. 1950, 9, 14.
2. P. Demchenko, V. I. Tomin, P.-T. Chou, Breaking the Kasha Rule for More Efficient Photochemistry. Chem. Rev. 2017, 117, 13353–13381.
3. Y. Shen, Z. An, H. Liu, B. Yang, Y. Zhang, Excitation-Dependent Multicolour Luminescence of Organic Materials: Internal Mechanism and Potential Applications. Angew. Chem. Int. Ed. 2023, 62, e202214483

A Mechanistic Insight into the Emission Behavior of Boron Difluorohydrazones (BODIHYs): Suppression of Kasha's Rule

Rakshantha Srithar[1], Naveen Kumar M[1], Renitta Benny[2], Sudhakar Gaikwad[2], Soumen De[3], and Susnata Pramanik*

[1]*SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

[2]*R.Benny,S.De School of Chemistry, Indian Institute of Science Education and Research (IISER), Thiruvananthapuram, Kerala695551, India*

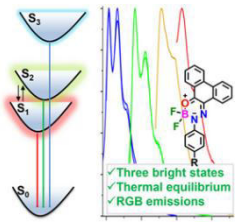
E-mail:soumende@iisertvm.ac.in

[3]*S.Gaikwad, Department of Chemistry, University of Cambridge, Cambridge CB21EW, UK*

***Corresponding author e-mail:** susmatap@srmist.edu.in

ABSTRACT

Single-component luminophores showing excitation-wavelength–dependent emissions are highly attractive for both fundamental studies and advanced optoelectronic applications. Such systems often deviate from Kasha's rule, enabling emission from higher excited states. Herein, we report boron difluorohydrazone (BODIHY) derivatives that exhibit clear excitation-dependent multicolor fluorescence, covering the full red-green-blue (RGB) range. Combined experimental and theoretical investigations reveal that this unusual color tunability originates from three emissive ("bright") excited states, namely S_1, S_2, and S_3. Time-dependent density functional theory (TDDFT) calculations show that the energy gap between S_2 and S_3 exceeds 3000 cm^{-1} (0.37 eV), which favors radiative decay from $S_3 \rightarrow S_0$ over competing internal conversion. For BODIHY 1, the smaller gap between S_1 and S_2 (< 2000 cm^{-1}, 0.25 eV) suggests partial thermal equilibrium between these two states. In contrast, BODIHY 2 exhibits three well-separated emissive excited states, allowing independent fluorescence from each state. Distinct excitation spectra, fluorescence lifetimes, and photoluminescence quantum yields (PLQYs) for the emission bands further support the presence of three independently emissive excited states, leading to unprecedented excitation-controlled RGB luminescence in small organic molecules.



Keywords: BODIHY, Excitation-wavelength dependent emission, anti-Kasha

References:

1. H. Qian, M. E. Cousins, E. H. Horak, A. Wakefield, M. D. Liptak, I. Aprahamian, Nat. Chem. 2017, 9, 83.
2. M, N. K., D. L. Lyngkhoi, S. Gaikwad, J. Samanta, R. Ahamed, S. Khatua, S. Pramanik, Chem. Commun. 2023, 59, 14122.

EL-044

Atomistic Tuning of Optoelectronic and Chiroptical Properties in π-Conjugated Systems

Gayathri Jothish Kumar[1], Anjan Bedi[1,2*], and Goutam Kumar Kole[1]*

[1]*Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu - 603203, India.*

[2]*Department of Radiology, University of Texas Southwestern Medical Center, Dallas, TX 75390, USA*

***Corresponding author email**: goutamks@srmist.edu.in, gj4273@srmist.edu.in

ABSTRACT

Tuning of optoelectronic and chiroptical properties in heteroaromatic π-conjugated systems by an atomistic approach is an important area of research from the viewpoint of designing materials for the advancements in organic electronics. Enhancement of triplet yields in organic materials is intriguingly challenging, though it could have manifold utility in several applications like singlet fission (SF), thermally activated delayed fluorescence (TADF), room-temperature phosphorescence (RTP), etc. Recently, it was known that improvement in those applications could be attained by using materials that are aromatic in their first excited triplet state. But synthetic developments of such stable systems are non-trivial, which can be comprehended from their scarce examples in literature. Diheterolodiheteroles are such 4nπ antiaromatic systems which are stable in ambient conditions. However, any development towards modulating the triplet yield or the rate of intersystem crossing require further research. Therefore, we have designed, synthesised, and structurally characterized a series of fluorene-based diheterolodiheteroles to understand the problem. Additionally, we could alter the heteroatoms of the π conjugated systems to understand the result through the photophysical characterizations (Abs, Em, τ, ϕPL) in combination with computational analysis through density functional theory (DFT), etc. In addition, chiroptical activity have also been amplified by changing the hetero atoms in chalcogenophenyl substituents in multi-substituted acenes, leading to the development of circularly polarised luminescence (CPL) emitters. In short, we have synthesized and explored photophysical properties and the chiroptical activity of these tetraaryl tetracenes in an atomistic manner by varying the heteroatoms in the chalcogenophenyl substituents, which could be a potential candidate for CPL emitters.

Keywords: Singlet fission; diheterolodiheteroles; chiroptical activity; tetraaryl tetracenes; fluorene

References:

1. D.J. Schipper, L.C.H. Moh, P. Müller, and T. M. Swager, Angew. Chem. Int. Ed., (2014), 53, 5847-5851 (b) A. Bedi, S. Debnath, S.S. Zade. Chem. Commun., (2014), 50, 13454
2. A. Bedi, L. J. W. Shimon, O. Girdon, J. Am. Chem. Soc. (2018), 140, 8086–8090 ,Y. Xiao, J. T. Mague, R. H. Schmehl, F. M. Haque, R. A. Pascal, Jr., Angew. Chem. Int. Ed. (2019), 58, 2831–2833
3. G.J. Kumar, B. Bogoslavsky, S. Debnath, A. Bedi. Molecules, (2023), 28, 5074.

EL-045

Investigation of Energy gap, Optical Conductivity, real and imaginary dielectric values of Nano composite from UV- Visible Spectroscopy

Kalyani Chilamakuri[1*], Raju Panthagani[1]

[1]*Department of Physics, Geethanjali College of Engineering and Technology, Keesara, Hyderabad -501301 India,*

***Corresponding e-mail**: kalyani15chilamakuri@gmail.com*

ABSTRACT

Pure Copper oxide (CuO) and Nano composite (1-x)$Zn_{0.7}Al_{0.2}Mn_{0.1}O$+ xCuO (x= 0.1, 0.3 ,0.5,1) samples were successfully synthesized and characterized to find the influence of CuO in $Zn_{0.7}Al_{0.2}Mn_{0.1}O$ on their structural and surface properties. X-ray diffraction (XRD) analysis confirmed that all samples retained the monoclinic tenorite phase of CuO, with characteristic diffraction peaks corresponding to standard JCPDS data, indicating high phase purity and structural stability after activation. While pristine CuO exhibited sharp and intense diffraction peaks, the Nano composite samples showed slight peak broadening and reduced intensity, suggesting a decrease in crystallite size and the introduction of lattice strain and defect states with increasing activation. These structural modifications are indicative of defect engineering without phase transformation. Complementary FT-IR analysis revealed the presence of oxygen-containing functional groups such as hydroxyl, carbonyl, and C–O groups on the nano composite samples, with their intensity increasing as CuO content, confirming enhanced surface functionalization. The combined structural, dielectric and spectroscopic results demonstrate that Nano composites effectively modify the dielectric constant, energy band gap and optical conductivity as CuO concentration increases. which is expected to improve performance in catalysis, adsorption, and energy-related applications engineer Phonon Glass Electron Crystal systems.

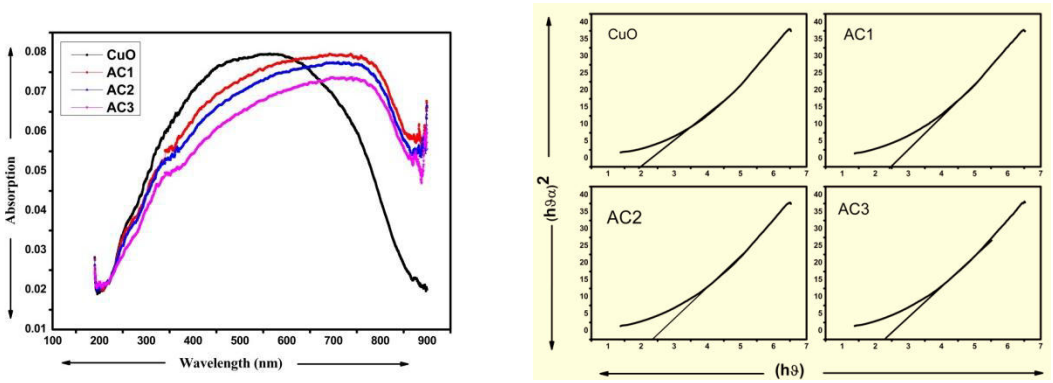


Figure1: Absorption spectrum and Optical Band Gap Analysis of Pure CuO and Nano composite (1-x)$Zn_{0.7}Al_{0.2}Mn_{0.1}O$+ xCuO

Keywords: XRD; SEM; FTIR; Energy Gap; Optical Conductivity; Dielectric constant;

References:

1. Ahmad, M. et al., Ceram. Int., 49 (2023), 115019–115028.

EL-046

3D Plasmonic Ag Nanodendrites as Highly Efficient SERS Substrates for Ultra-Trace Detection of Ascorbic Acid

Dhatchayani Murugan[1], Akash Sharma[1], Sumit Saxena[2], Lakshya Daukiya[3], Debabrata Sarkar[4], Shailendra K. Saxena[1],Vivek Kumar [5*] and Anand M. Shrivastav[1 *]

[1]*Optics and NanoElectronics (ONE) Laboratory, Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203, India.*

[2]*Department of Applied Science and Humanities, Invertis University, Bareilly, Uttar Pradesh-243123, India*

[3]*Department of Physics, Central University of Rajasthan, Ajmer - 305817, India*

[4]*Applied Nanophysics Laboratory, Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203, India.*

[5]*Applied Nanomaterials and Devices Laboratory, Department of Physics, Indian Institute of Information Technology, Design & Manufacturing, Kancheepuram, Chennai-600127, India*

***Corresponding author e-mail:** vivek@iiitdm.ac.in , anandmos@gmail.com

ABSTRACT

A rapid, cost-efficient, single-step metal-assisted growth (MAG)1 method is employed to synthesize well-defined Ag dendrites on a silicon substrate. The sharply branched dendritic nanostructures support extremely dense 3D plasmonic hotspot networks, offering excellent performance in surface-enhanced Raman scattering (SERS)2. These substrates are subsequently applied for the label-free, ultrasensitive detection of l-ascorbic acid (vitamin C)3. In addition to electromagnetic enhancement, the sensing mechanism also relies on charge transfer interactions that modulate characteristic vibrational modes, enabling quantitative analysis. The platform supports a broad detection range (10–9 M to 10–3 M) and a lower detection limit of 7.182 nM of ascorbic acid concentration. Owing to its simplicity, analytical robustness, and high sensitivity, the proposed Ag dendritic SERS system is well-suited for portable diagnostic technologies and real-time biochemical monitoring.

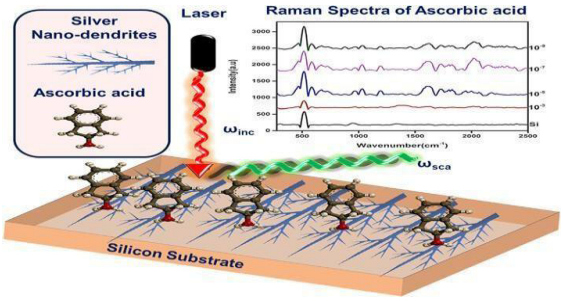


Fig. 1 Graphical representation of silver Nanodendrites SERS substrates for Detection of Ascorbic Acid

Keywords: surface-enhanced Raman spectroscopy, metal-assisted growth, plasmonics, nanodendrite, ascorbic acid

References:

1. D. Murugan et al., *Nano Ex.*, 2024, 5, 045004.
2. H. Wei et al., *Anal. Chem.*, 2018, 90, 3227–3237.

Interface Engineering on Vertically Stacked MoS_2/In_2S_3 Photodiode for High Performance Photodetector

Naskath Sithara H,[1] Vinoth E,[2] Navaneethan M,[2] Archana J[1]*

[1]*Center of Excellence in Materials for Advanced Technologies, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India- 603203.*

[1]*Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India- 603203.*

***Corresponding author email:** jayaram.archana@gmail.com

ABSTRACT:

Vertically stacked heterojunction paves notable built-in electric field at the interface of photodiode resulting in low charge separation and reduction in carrier recombination. Hence, the MoS_2/In_2S_3 heterojunction photodiode was successfully fabricated by optimizing growth parameters in an indigenous CVD technique. The formation of MoS_2 and β-In_2S_3 phases was confirmed through Raman spectroscopy. All the characteristic vibrational modes of both materials are distinctly present in the heterojunction sample, confirming successful stacking without structural degradation. The A_{1g} mode of MoS_2 is observed to be blue shifted of about 0.2 cm^{-1}, which signifies the weak van der Waals interfacial coupling between MoS_2 and In_2S_3. Furthermore, the phonon lifetime is found to decrease specifically for this mode, attributed to the increased electronic concentration at the interface leading to enhanced electron-phonon scattering. Photoluminescence (PL) spectroscopy reveals prominent band-to-band as well as defect-mediated transitions in In_2S_3. In the case of MoS_2, the characteristic A and B excitonic emissions are observed along with trionic features and defect-related transitions. The electrical transport characteristics demonstrate significant enhancement in photodetection performance for the heterojunction device compared to pristine MoS_2. The I-V measurements under illumination confirm improved photoresponse due to efficient interfacial charge separation. Notably, the responsivity shows a substantial increase from 3.85 mA/W (pure MoS_2) to 642 mA/W in the MoS_2/In_2S_3 heterojunction, highlighting the advantage of vertical heterostructure engineering for high-performance photodetector applications.

Keywords: vertical heterojunction, blue-shift, interfacial coupling, phonon lifetime.

References:

1. Sandoval, S. Jiménez, D. Yang, R. F. Frindt, and J. C. Irwin. "Raman study and lattice dynamics of single molecular layers of MoS 2." *Physical Review B* 44, no. 8 (1991): 3955.
2. Zhou, Kai-Ge, Freddie Withers, Yang Cao, Sheng Hu, Geliang Yu, and Cinzia Casiraghi. "Raman modes of MoS2 used as fingerprint of van der Waals interactions in 2-D crystal-based heterostructures." *ACS nano* 8, no. 10 (2014): 9914-9924.

Realization of Surface Plasmon Polariton Modes in Graphene coated Conducting Media

Gishamol Mathew[1*], Louie Frobel P. G.[2]

[1] *Maharaja's College, Ernakulam, Kerala, India, 682 011*

[2] *St.Alberts College, Ernakulam, Kerala, India, 682 018*

***Corresponding author e-mail:**mathew.gishamol@maharajas.ac.in

ABSTRACT

Surface Plasmon Polaritons (SPPs) at an interface of a metal and a dielectric can support light propagation and confinement beyond the diffraction limit. The practical implementation of these metallic plasmonic devices suffers significant losses and poor controllability. To overcome the lack of functionality of metallic based devices in integrated photonic circuits especially at THz frequencies, the strong alternative is Graphene, i.e. a monolayer of carbon atom bound in hexagonal structure. It was reported that Graphene plasmons have low-loss in the THz and mid- IR frequencies and can be better confined in smaller regions when compared to metal plasmons. The functionality of Graphene can be modified by chemical doping, electrical and magnetic fields, and bias voltage. In this work, the authors considered Graphene coated metallic structures. Both theoretical and numerical analysis has performed on the dispersion of SPP modes. The results showed that SPP modes are excited at Graphene interfaces and could be tuned by material selection and the frequency of operation. Also, long range SPP modes are identified at these structures which makes it suitable for active plasmonic waveguides.

Keywords: Graphene plasmons, Propagation distance, Dispersion, THz Propagation

References:

1. Maier,S. ,Adv. Materials. 2001, 13, 19, 1501-1505
2. Kim, J. et.al. , Nano Lett. 2012, 12, 11, 5598-5602
3. Lin, C. et.al., Reviews in Physics 2021, 6, 100054
4. Kim, J and Choi, S., Optic Express 2011, 19, 24, 24557-24562

Green Synthesis of Semiconductor-Embedded PCL Nanofibers Fabricated by Electrospinning for Optoelectronic Applications

Madathy Babu S[1], Padmaja S*[1], Sowmiya S[1]

[1]*SRM Valliammai Engineering College, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** padhdhu.sri2025@gmail.com

ABSTRACT

The development of sustainable nanostructured materials has gained significant attention due to their potential applications in environmental and optoelectronic technologies. In this study, polycaprolactone (PCL)/Zinc Sulphide (ZnS) composite nanofibers were successfully fabricated via the electrospinning technique using a naturally derived sulfur precursor during synthesis. The approach offers an environmentally friendly pathway for producing semiconductor-embedded polymer nanofibers. The prepared nanofibers were systematically characterized to evaluate their structural, morphological, optical and electrical properties. X-ray diffraction analysis confirmed the formation of crystalline ZnS within the PCL matrix, while scanning electron microscopy revealed uniform and bead-free nanofibrous structures with well-distributed ZnS nanoparticles. The incorporation of ZnS significantly influenced the crystallinity and surface morphology of the nanofibers. Optical studies indicated enhanced absorption behaviour, suggesting potential applications in photocatalysis, sensing, and optoelectronic devices. The use of a bio-derived sulfur source provides a sustainable alternative to conventional chemical precursors, reducing environmental impact while maintaining effective nanostructure formation. This work demonstrates a simple and eco-friendly strategy for producing polymer–semiconductor hybrid nanofibers, opening new possibilities for green nanomaterial synthesis and functional applications.

Keywords: Electrospinning; PCL/ZnS Nanofibers; Bio-derived Sulfur Source; Polymer Nanocomposites; Sustainable Nanomaterials; Optoelectronic Applications

References:

1. Shyju S., Akash M. Chandran, *ACS Appl. Electron. Mater.*, **6** (2024) 8987–8997.
2. Gopal Panthi, Arun Gyawali, *Hydrogen*, **5** (2024) 403–413.
3. Y. E. Bulbul, N. Dilsiz*Fibers Polym.*, **25** (2024) 1701–1712.
4. Jingjing Tian, Thomas E. Paterson, Jingjia Zhang, Yingxing Li, *Int. J. Mol. Sci.*,**24** (2023) 14420
5. S. Saudi, S. R. Bhattarai, U. Adhikari, S. Khanal, J. Sankar, S. Aravamudhan, N. Bhattarai, *Nanoscale*, **12** (2020) 23556–23570.

Low Dimensional Nanostructures Based Bi_2S_3/P-Si(100) Heterojunction Photodiodes For Photodetector Applications

Gokul P[1], Archana J[2], Vinoth E[1*] , Navaneethan M[1]

[1]*Nanotechnology Research Centre,*

[2]*Center of Excellence in Materials for Advanced Technologies,*
SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** vinothe1@srmist.edu.in

ABSTRACT

Bi_2S_3 nanostructures, with a high absorption coefficient of 10^5 cm^{-1} and an optical bandgap of ~1.3 eV, present promising opportunities for broad-band photodetector applications. These low-dimensional nanostructures are grown on p-Si (001) substrates using optimized chemical vapor deposition (CVD) parameters. X-ray diffraction confirms the orthorhombic phase with high crystallinity. The nanorods exhibit enhanced charge transfer due to their interconnected network, improving device performance. The I-V characteristics demonstrate rectifying behavior, with illumination producing a photocurrent of 379.65 µA. The photodetector shows a responsivity of 506 mA/W and a detectivity of 9.546×10^{12} Jones, indicating high sensitivity and efficiency in photodetection applications. The photocyclability characteristics were confirmed by over 10 seconds of light on and off cycles, producing constant current in both dark and illuminated conditions, demonstrating consistent behavior under varying light exposure. These notable figure of merits of the fabricated device paves the way for better optoelectronics devices.

References:

1. Li, Y., Zeng, A., Ali, R., Dou, H., Ou, Q., Ma, H., & Wang, H. E. (2025). Low-temperature CVD synthesis of single-crystalline bismuth sulfide (Bi 2 S 3) microrods for efficient photodetection. *Chemical Communications*, *61*(100), 19840-19844
2. Zeng, A., Ali, R., Fu, S., Liu, L., Rasool, A., Liu, C., ... & Wang, H. E. (2025). Single-crystalline bismuth sulfide microrods for efficient visible light photodetection. *Journal of Materials Chemistry A*, *13*(3), 1772-1778.

EL-051

Chirality in New Hybrid Cu-Halides: Synthesis and Functional Properties

Sukalpo Dey[1], Priya Ranjan[1], Rajashi Halder[1], Anuja Datta[2,3]*

[1]*School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, 2A and 2B Raja S. C. Mullick Road, Kolkata, India-700032*

[2]*Technical Research Center, Indian Association for the Cultivation of Science, 2A and 2B Raja S. C. Mullick Road, Kolkata, India-700032*

[3]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai, 603203, India*

ABSTRACT

Over the past decade, chirality in two-dimensional hybrid perovskites has largely been studied in systems where chiral organic spacers impose their handedness onto the inorganic framework.1,2 In contrast, this work explores chirality that arises without any intrinsically chiral building blocks focusing on how lattice distortions and ordering at larger length scales can break inversion symmetry and produce chiral structures. Since the absence of an inversion centre is a defining feature of chirality, such symmetry breaking is closely connected to functional properties such as ferroelectricity in polar systems, as well as piezoelectric and pyroelectric responses. The material system investigated is the zero-dimensional hybrid perovskite analogue $[MePPh_3]_2\ CuX_4$, where the halide *X*is varied between Cl and Br. Single-crystal X-ray diffraction is used to determine crystal structures and relate lattice distortions to functional behaviour, while powder X-ray diffraction showed phase purity, batch reproducibility, and polymorph selection. Modified synthetic routes allow the isolation of previously unreported polymorphs that crystallize in space groups different from those described in the literature. The bromide analogue which crystallizes in a polar, non-centrosymmetric space group show functional responses consistent with its symmetry, including prominent electroactive properties. In contrast, the chloride analogue adopts a centrosymmetric, nonpolar space group showing no electroactivity. Optical Rotatory Dispersion, Circular Dichroism, Circularly Polarized Luminescence, and ground-state Circular Dichroism are also examined in detail in solution and thin films Overall, this work aims to clarify how lattice distortions in achiral hybrid frameworks can generate emergent chirality and associated optical and polar responses, while establishing careful experimental strategies to distinguish intrinsic chiral behaviour from extrinsic anisotropic effects.

Keywords: Chirality, Piezoelectricity, Ferroelectricity, Cu-Halide

References:

1. Long et al., Nature Reviews Materials, volume 5, pages 423–439 (2020)
2. Barman et al., Chem. Commun., 2023, 59, 10283

EL-052

Design and Simulation of Patch Antenna for 5G Millimetre Wave Applications

Dhananjeyan R*, Vaijinth V A*, Victor R*, Vikash Babu S*, Yogesh N*

Department of Electronics and Communication Engineering, SRM Valliammai Engineering College, Kattankulathur, 603203, India.

ABSTRACT

This paper presents a design of a compact patch antenna operating at 28 GHz for 5G millimetre-wave applications. The proposed design is based on a microstrip patch incorporating a slot and a defected ground structure to enhance bandwidth and gain. The proposed millimetre wave antenna is designed on a Rogers RT Duroid 5880 substrate having a relative dielectric permittivity of 2.2 and thickness of 0.8 mm. The simulation results demonstrate that the return loss of -18.70dB in the frequency range of 26.867-28.975 GHz, and it provides a bandwidth of 2.1 GHz. The proposed antenna yields 73% of the radiation efficiency within the desired operating frequency band. The antenna has a high gain of 4.337dBi with unidirectional radiation pattern. All the proposed designs are simulated in computer simulation technology (CST) software. The proposed design demonstrates high performance, making it a strong candidate for integration into 5G millimetre wave applications.

Keywords: Microstrip Patch Antenna, 5G, millimetre-wave

EL-053

A Hierarchical Self-Assembly-Induced Solid-State White-Light Emission from a Solution- Processed Single Polymer

Poonguzhali B, [1] Mohammed Vajith Ali, [1] Ravindran E [1] *

[1] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology,*

Kattankulathur-603203, Chengalpattu District, Tamil Nadu

***Corresponding author e-mail**: ravindre@srmist.edu.in

ABSTRACT

Researchers worldwide have invested significant effort in developing organic light-emitting diodes (OLEDs) for future display and lighting applications. However, achieving efficient and optimized white OLEDs by integrating diverse organic emitters across the visible spectrum is challenging. This study demonstrates the efficient operation of nondoped white OLEDs triggered by molecular tuning of copolymers (PTNAA 0.1 to PTNAA 50), thereby enriching the aggregation-induced emission (AIE) characteristics in a solution-processed single polymer. Remarkably, the synthesized copolymer, PTNAA 0.1, generates a bright and stable dual-band white light with a solid-state photoluminescence quantum yield (PLQY) of 87.7%, displaying a unique "nanoring-like" hierarchical self-assembly potentially driven by J-aggregate formation. Furthermore, PTNAA-based copolymers effectively diminish charge carrier trapping owing to their ambipolar charge transport characteristics, enabling efficient electroluminescence (EL). A solution-processed single-polymer-based OLED device fabricated with PTNAA 0.1 exhibited bright white light luminescence with an external quantum efficiency (EQE) of 6.75% with CIE coordinates of (0.33, 0.32), and maximum luminescence, current, and power efficiencies of 10553 cd m^{-2}, 9.68 cd A^{-1}, and 4.34 lm W^{-1}, respectively. Moreover, theoretical (DFT and TD-DFT) studies confirm the competent energy transfer from fluorene to the PTNAA-gens. Our results corroborate materials design for solution-processed WOLEDs and concrete advances in solid-state lighting and display technologies.

Keywords: Solution process white light emission, Single polymer, aggregation-induced emission (AIE), hierarchical self-assembly, Fourier resonance energy transfer (FRET).

References:

1. L. Chen, Y. Jiang, H. Nie, R. Hu, H. S. Kwok, F. Huang, A. Qin, Z. Zhao, B. Z. Tang, ACS Appl. Mater. Interfaces 2014, 6, 17215
2. N. Thejokalyani, S. J. Dhoble, Renew. Sustain. Energy Rev 2014, 32, 448.
3. E. Ravindran, E. Varathan, V. Subramanian, N. Somanathan, J. Mater. Chem. C 2016, 4, 8027; b) E. Ravindran, N. Somanathan, J. Mater. Chem. C 2017, 5, 4763;

EL-054

Corncruzer: An Autonomous Iot-Enabled Precision Seeding Rover for Corn Cultivation

Chandni Kumari[1], Jayalakshmi M[2], Kavya S[3], Amshavalli M[4]

Erode Sengunthar Engineering College, Perundurai, Erode – 638 057.

***Corresponding author e-mail:** [1]chandnimgr2005@gmail.com,[2] jayalakshmim2905@gmail.com, [3]kaviyasundar32@gmail.com , [4]amshavalli1498@gmail.com

ABSTRACT

The CornCruzer is an advanced, fully autonomous smart rover that is intended to monitor, explore, and navigate cornfields with less human interaction. With the rising problem of labor shortages in modern agriculture and the need for greater efficiency, automation has become the key to improving productivity, precision, and decision-making. The CornCruzer aims to solve these problems by incorporating advanced sensing, navigation, and communication technologies into a small rover system that can function effectively in the challenging environment of cornfields. The main purpose of CornCruzer is to help farmers gain accurate and real-time information about their fields, making routine monitoring easier. The system continuously collects and analyzes environmental and spatial information, which improves the practice of precision agriculture.CornCruzer's sensing infrastructure is centered on a LiDAR module that offers high-resolution spatial information for environmental mapping and obstacle detection. In a conventional corn field, there are many navigational hazards such as closely packed crop rows, irregular terrain, and unexpected obstacles like weeds, rocks, and irrigation system components. The LiDAR sensor continuously provides distance information and point cloud data, allowing the rover to detect obstacles, estimate their distance, and perform autonomous obstacle avoidance maneuvers to ensure safe passage without damaging crops or the rover. For maintaining accurate alignment along the crop rows, CornCruzer also uses a set of infrared sensors placed at strategic locations. These sensors are able to detect variations in contrast between soil, crop, and boundaries of the field, thus enabling the rover to stay aligned along the center of the crop rows during its navigation.CornCruzer is a scalable and efficient solution for precision agriculture applications.

CM-001

Numerical Review on Dynamic Factor Evaluation of Pick and Carry Crane Cabin Structure

Masilamani R*[1], Logeshwaran T [2], Avinash T[3], Dasaradhan S[4]

[1]*Karpagam College of Engineering, Coimbatore, Tamil Nadu, India, 641032*

***Corresponding author e-mail:** masilamani.r@kce.ac.in

ABSTRACT

Pick and carry cranes are commonly used in construction and material handling, but the vibration and dynamic loads acting on their cabin structure are often ignored during design. These dynamic effects directly influence the operator comfort, safety and long term fatigue of the structure. This review mainly focus on the numerical identification of the Dynamic Amplification Factor (DAF) for the crane cabin by using simulation and analytical methods. Many previous studies used simplified static or linear models which cannot capture the real vibration pattern when the crane moves on rough terrain or during braking. Recent developments in finite element (FE) and modal analysis tools like ANSYS and Abaqus made it possible to study these effects more precisely. The novelty of this work is in collecting and comparing different numerical approaches to evaluate DAF without full scale testing. The review also point out the research gap where no clear link exists between field vibration data and computed dynamic factor values. The results from literature shows that the DAF value usually increase with boom angle, speed and terrain irregularity. Overall, the study highlight the importance of including dynamic factor in cabin design to improve structural safety, reliability and reduce maintenance failures in mobile cranes.

Keywords: Pick and carry crane, Dynamic factor, Cabin structure, Finite element modeling, Modal analysis, Vibration response, Structural fatigue, Simulation

References:

1. Zou M, Chen M, Zhu L, Li L, Zhao W, Ocean Eng. 268 (2023) 113376.
2. Žnidarič A, Kalin J, Struct J Civ. Health Monit. 10 (2020) 00407-2.
3. Zhuo Y, Qi Z, Xu J, Vib. Eng J. Technol. 10 (2022) 00774-8.
4. Zhuang C, Wen H, Ni X, Zhang D, Bao Y, Huang H, Machines 10 (2022) 1148.
5. Zhu L, Meiyan Z, Chen M, Li L, Ocean Eng. 242 (2021) 109443.
6. Zhu H, Du Z, Wu J, Sun Z, World Patent Inf. 68 (2022) 102092.

CM-002

Climate-Aware Materials Informatics for Designing Corrosion-Resistant Coatings under Future Environmental Scenarios

Vignesh Jagajeevan[1], Vidhyalakshmi Sivakumar[1]*

[1]*Department of Civil Engineering, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Chennai, Tamil Nadu, India*

***Corresponding author e-mail:** vidhyalakshmis.sse@saveetha.com

ABSTRACT

Climate change is altering environmental exposure conditions that govern corrosion processes, yet current corrosion-resistant coating designs remain largely optimized for historical or present-day environments. This study presents a climate-aware materials informatics framework for the design of corrosion-resistant coatings tailored to future environmental scenarios. The approach integrates climate projections, environmental degradation indicators, and experimentally derived corrosion performance data into a data-driven materials design workflow. Machine learning models are employed to identify non-linear relationships between evolving environmental variables—such as temperature rise, humidity fluctuations, salinity intensification, and atmospheric pollutant levels—and coating degradation mechanisms. These relationships are then used to guide the optimization of coating composition, microstructure, and functional additives for enhanced long-term durability. Case studies demonstrate that coatings optimized using climate-aware informatics exhibit superior resistance under projected future exposure conditions compared to conventionally designed systems. The proposed framework provides a forward-looking strategy for developing corrosion-resistant materials that remain robust under climate-induced environmental change, offering critical insights for sustainable infrastructure design and environmental engineering applications.

References:

1. S. Tiwari, K. Dash, N. Park, and N. G. S. Reddy, Coatings 15 (2025) 888.
2. N.-L. Tran, T.-H. Nguyen, V.-T. Phan, and D.-D. Nguyen, Adv. Mater. Sci. Eng. (2021) 6967550.
3. Y. Seechurn, Artificial Intelligence, Engineering Systems and Sustainable Development (2024) 207–218.

CM-003

DFA-based fault severity tracking in bearing with standard material grade used in Induction Motor

Anindya Basu[1]*, Sourav Sarkar[2], Santanu Das[3]

[1]*Siliguri Institute of Technology Diploma College, Siliguri, West Bengal, India, 734009*

[2] *School of Material Science and Nanotechnology, Jadavpur University, Kolkata, India*

[3]*Electrical Engineering, Jalpaiguri Govt. Engineering College*

Jalpaiguri, West Bengal, India

***Corresponding author e-mail:** anijpg4@gmail.com

ABSTRACT

Bearing-related failures constitute a major cause of unexpected induction motor breakdowns, resulting in unplanned downtime, increased maintenance costs, and reduced operational reliability in industrial drive systems. This study experimentally investigates the propagation of bearing faults in an induction motor using a bearing of standard grade of material to evaluate its influence on degradation behaviour. A dedicated laboratory test rig comprising a three-phase squirrel-cage induction motor, controlled loading arrangement, and data acquisition system is developed to generate progressive bearing degradation under sustained operating conditions. Stator current signals are continuously acquired during motor operation, enabling a non-invasive monitoring framework without the use of additional mechanical sensors. The recorded current signals are analysed using Detrended Fluctuation Analysis (DFA) to characterise the evolving nonlinear dynamics associated with fault initiation and propagation. The DFA scaling exponent is employed as a condition indicator to quantify changes in long-range correlations of the current signal as the bearing transitions from a healthy state to advanced fault stages. Experimental results reveal that variations in bearing material properties significantly affect the fault evolution pattern, as reflected in systematic changes in the DFA exponent. The proposed experimental methodology demonstrates the effectiveness of DFA-based motor current signature analysis for tracking bearing fault progression. It provides a practical foundation for real-time condition monitoring and predictive maintenance of electric drive systems.



Fig. 1 (a) Bearing of Induction Motor (b) Experimental Setup

Keywords: Induction Motor; Bearing Fault; Material; DFA analysis; Motor current signature analysis

References:

1. K. N. Jayasena, B. Batkhishig, B. Nahid-Mobarakeh, and A. Emadi, Proc. IEEE Int. Symp. Ind. Electron. (ISIE), (2025) 1–7.
2. S. Das, A. K. Pradhan, A. Kedia, S. Dalai, B. Chatterjee, and S. Chakravorti, IEEE Trans. Ind. Electron., 65 (2018) 7322–7331.

CM-004

Exploring Transport Properties and Rare-Earth-Substitution-Enhanced Magnetism in XFeSb (V, Nb, Ta) Intermetallics for Renewable Energy and Spintronics Applications

Klinton Brito K[1], Srinivasan M[1]*

[1]*Department of Physics, SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai*

***Corresponding author e-mail:** srinisastri@gmail.com

ABSTRACT

The semiconducting half-Heusler alloys XFeSb (X = V, Nb, Ta) are non-magnetic and achieved figures of merit of 0.8, 0.68, and 0.68 for VFeSb, NbFeSb, and TaFeSb, respectively, at 1200 K. To induce magnetism in the XFeSb (X = V, Nb, Ta) half-Heusler alloys, aliovalent substitution with Gd was employed. A 2×2×2 supercell consisting of 24 atoms was constructed, and the impact of Gd on the magnetic properties of XFeSb alloys was studied. The magnetic properties of the compounds $X_{1-y}GdyFeSb$ and XFe1-yGdySb were examined for y = 0.125, where all compounds exhibited magnetic moments greater than 8 μB. At y = 0.25, all compounds transformed from a conventional to a primitive unit cell, and at y = 0.375, the compounds transitioned from cubic to tetragonal structures. The obtained figures of merit, along with the tailored magnetic properties after Gd substitution, confirm that the investigated half-Heusler alloys VFeSb, NbFeSb, and TaFeSb are potential candidates for thermoelectric and spintronic applications.

Keywords: thermoelectric, spintronic, DFT

References:

1. K. K. Brito, J. J. Muthukumaran, S. Manickam, and J. B. Sudharsan, J. Phys. Chem. Solids, (2025) 113286.

CM-005

Machine Learning-Driven Design and Applications of Carbon Quantum Dots in Environmental and Energy Nanotechnology

Kalpukuri Manohar, Gunasekaran Venugopa*

Advanced Nanomaterials and System Lab, Department of Materials Science, School of Technology, Central University of Tamil Nadu, Thiruvarur – 610 005, Tamil Nadu, India.

*** Corresponding author e-mail**: gunasekaran@cutn.ac.in

ABSTRACT

Carbon quantum dots (CQDs) have emerged as an exciting class of Zero-dimensional nanomaterials exhibiting outstanding optical, electrical, and surface properties. Their nanoscale size (<10 nm), high aqueous dispersibility, tunable photoluminescence, and environmental benignity have made them highly suitable for diverse applications ranging from sensing and water purification to energy conversion and biomedical imaging. Recently, the integration of computational modeling and machine learning (ML) has revolutionized the understanding and optimization of CQDs. ML algorithms enable predictive control over CQD synthesis, surface modification, and property tuning, while First-principles simulations reveal quantum-level mechanisms that govern photoluminescence, charge transport, and catalytic activity. This review systematically examines recent progress in machine-learning-assisted CQD design and computational modeling, drawing insights from theoretical and experimental studies. It emphasizes the role of ML in correlating synthesis parameters with quantum yield, optimizing doping strategies, and accelerating materials discovery. Furthermore, the review highlights emerging environmental and energy applications, such as pollutant sensing, photocatalysis, and hydrogen evolution, as well as bioimaging and drug delivery prospects. Finally, key challenges related to synthesis scalability, data standardization, and model interpretability are discussed. By merging data-driven and physical approaches, the review outlines a roadmap for sustainable and intelligent design of CQD-based nanomaterials in future green technologies.

Keywords: Carbon quantum dots; machine learning; computational modeling; fluorescence; water remediation; electrochemistry; bioimaging; nanomaterials; quantum yield; artificial intelligence

References:

1. M. El-Azazy et al., Coord. Chem. Rev., (2024).
2. L. Wu, Y. Xiao, M. Ghosh, Q. Zhou, and Q. Hao, ES Mater. Manuf., 9 (2020) 34–39.

CM-006

Semiconductor to metallic transition with possible magnetism in coved armchair BP nanoribbons

Ankita Nemu*, Neeraj K. Jaiswal, Pankaj Srivastava

Department of Engineering Sciences, ABV-Indian Institute of Information Technology and Management (IIITM), Gwalior, India

***Corresponding author e-mail:** ankita.nemu@gmail.com

ABSTRACT

Defects are intrinsic to nanomaterials under realistic synthesis and operational conditions, often playing a pivotal role in tuning their physicochemical properties. This study examines the impact of coved-edge defects on the structural and electrical characteristics of armchair BP nanoribbons (ABPNR) using density functional theory-based first-principles computations. These edge-modified structures are energetically favourable, according to the binding energies, indicating that they could be viable for experiments. The presence of coved-edge defects leads to significant changes in the electronic structure, exhibiting semiconducting and metallic properties with magnetic ground state depending on the defect location. In particular, as the ABPNR-P-cv-pristine structure indicates, coved-edge changes can result in a change from a direct to an indirect band gap and induce n-type doping characteristics. Defective nanoribbons have electronic band gaps between 0.36 eV and 1.50 eV, which is a wide tunability that is ideal for device integration. These results show that ABPNR electronic and magnetic characteristics can be modulated using edge-defect engineering, which has significant implications for the design of upcoming nanoscale semiconductors and spintronic components.

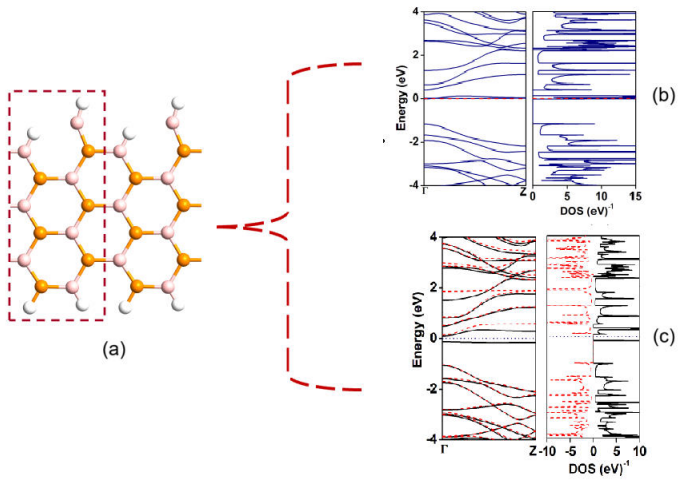


Fig.1 (a) Optimized geometry of coved ABPNR-P-cv (pristine) (b) Electronic band structure and DOS (c) Spin-polarized band structure and DOS

Keywords: Boron phosphide; nanoribbon; electronic structure; coved edge; spintronic

References:

1. J. Yu, W. Guo, Appl. Phys. Lett., 106 (2015).
2. Nemu, N. K. Jaiswal, J. Mol. Grap. Model., 121 (2023).

CM-007

Hafnium based ferromagnetic half metals for spintronic and thermoelectric device applications.

Harshit[1], Klinton Brito K[2], Srinivasan M[2]*,

[1]*Department of EEE, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai*

[2]*Department of Physics, SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai*

***Corresponding author e-mail:** srinisastri@gmail.com

ABSTRACT

In this study, we investigate the spintronic and thermoelectric properties of half-Heusler alloys HfMnZ (Z = Sn, Sb, Bi) using density functional theory. Initially, we have optimized the cubic structure of the considered crystal alloys for various magnetic phases. Through calculations, we obtained that minimum ground state energy in ferro-magnetic phase. Using generalized gradient approximation, we studied the electronic properties of the alloys HfMnZ (Z = Sn, Sb, Bi) and we obtained the band gap in spin up channel. For HfMnSn, the calculated band gap value is 0.77 eV, 1.09 eV for HfMnSb and the band gap value of HfMnBi is 0.29 eV in spin up channel. The presence of band gap only in the spin up channel confirms the half-metallic nature of the considered alloys. Also, the band gap are indirect in nature for HfMnSn and HfMnSb alloys whereas for HfMnBi the direct band gap is observed. The positive integer total magnetic moment values of HfMnZ (Z = Sn, Sb, Bi) confirms the ferro magnetic nature of the materials. We have also studied the transport properties of the alloys HfMnZ (Z = Sn, Sb, Bi) with the ZT values 0.52, 0.6 and 0.29 respectively. Our results shows that the half-Heusler alloys HfMnZ (Z = Sn, Sb, Bi) are suitable for spintronic and thermoelectric applications.

Keywords: Magnetism, spintronics, Wien2k

References:

1. K. K. Brito, J. J. Muthukumaran, S. Manickam, and J. B. Sudharsan, J. Phys. Chem. Solids, (2025) 113286.

CM-008

Tantalum Based Ferrimagnetic Half Metals for Spintronic and Thermoelectric Device Applications.

Saakitheyen K K[1], Klinton Brito K[2], Srinivasan M[2]*,

[1]*Department of ECE, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai*

[2]*Department of Physics, SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Chennai*

***Corresponding author e-mail:** srinisastri@gmail.com

ABSTRACT

The half Heusler alloys TaMnZ (Z = As, Sb, Bi) are stable in the ferrimagnetic cubic phase. The band dispersion plots suggest that the compounds TaMnAs, TaMnSb and TaMnBi are half metals with indirect band gap having the band gap energies of 1.13 eV, 1.24 eV and 1.12 eV respectively in the spin down channel. As the materials have 100 % spin polarization with an integer magnetic moment of −1 μB, they are suitable for making spintronic devices such as spin transistors and spin-flip flops. The materials have low lattice thermal conductivity which was confirmed by Slack's equation. The obtained thermoelectric figure of merit for p-type TaMnAs, TaMnSb and TaMnBi is 0.7, 0.6 and 0.8 respectively at 1200 K. Similarly, the figure of merit obtained for n-type TaMnAs, TaMnSb and TaMnBi is 0.6, 0.64 and 0.8 respectively at the same temperature. The favourable heat and spin transport properties of these alloys show that they are the potential characters to figure out better thermoelectric and spintronic performance.

Keywords: DFT, Half metals, Materials Science

References:

1. K. K. Brito, J. J. Muthukumaran, S. Manickam, and J. B. Sudharsan, J. Phys. Chem. Solids, 192 (2025) 113286.

CM-009

Machine Learning-Assisted Image-Based Crack Detection and Self-Healing Evaluation in Functional Self-Healing Materials

Srishti Singh[1], Neelam Singh[2]*

[1]*Aayojan Schools of Architecture, Jaipur, Rajasthan, India, 302022*

[2]*SRM Institute of Science and Technology, Delhi-NCR Campus, Ghaziabad, Uttar Pradesh, India, 201204*

***Corresponding author e-mail:** neelams@srmist.edu.in

ABSTRACT

Crack formation in materials significantly impacts structural performance and service lifetime. Self-healing materials (SHMs) aim to autonomously repair damage, offering extended durability. Recent advances in machine learning (ML) and deep learning (DL) enable automated crack detection and evaluation from image data, improving monitoring and accelerating materials development. This research integrates a DL crack detection pipeline with self-healing assessment in SHMs, proposing a deep convolutional network model trained on high-resolution crack images to quantify crack width and monitor healing progression over time. The framework leverages cloud computing for scalable data processing and transfer learning for model generalization. Experimental results demonstrate high accuracy of 91% in crack segmentation and meaningful correlation between model outputs and physical healing metrics.

Keywords: Self-Healing materials (SHMs), Machine Learning, Deep Learning, Cloud Computing, Transfer Learning.

CM-010

Quantum Kernel-Driven Learning of Nanoscale Transport Dynamics in Engineered Nanomaterials

Aarthi S[1]*, Sujarani Rajendran[2]

[1]*CSED, School of Computing, SRM Institute of Science and Technology, Tiruchirappalli*

[2]*Department of Computer Science and Engineering, SASTRA Deemed University, Kumbakonam*

***Corresponding authors e-mail:** aarthis6@srmist.edu.in, rsujarani4@gmail.com

ABSTRACT

Predicting transport regimes in nanostructured materials remains challenging due to nonlinear quantum effects, scattering mechanisms, and high-dimensional parameter coupling. Classical machine learning struggles with strongly quantum-confined nanoscale systems where transport behavior exhibits complex nonlinear dependencies. Existing approaches fail to capture coupled nanoscale interactions inherent in quantum transport phenomena. The proposed research presents Hybrid quantum-classical framework combining ZZ feature maps with full entanglement connectivity to model coupled atomic-scale interactions. In this study, we generated 200 synthetic nanomaterial samples with 4 critical features including Grain size (5-100 nm), Quantum confinement energy (0.01-2.0 eV), Defect density (0-1 defects/nm³), and External electric field strength (0-2 V/nm). The architecture includes a 4-qubit ZZ feature map with 3 repetitions and full entanglement with the objective to classify the Binary transport regime (147 diffusive, 53 ballistic samples) and implemented in a Qiskit-based quantum kernel with fidelity metric, coupled to classical SVM. The Quantum Kernel Performance indicates the accuracy of 72.0%, Precision (diffusive): 73.5%, Recall (diffusive): 97.3% and Support vectors: 119/150 training samples. However the classical kernel outperforms with 2.7% in terms of accuracy than quantum kernels. The results indicate that while quantum kernels do not universally outperform classical methods in idealized settings, they offer a clear advantage in nanoscale learning tasks characterized by strong nonlinear coupling, phase sensitivity, and noise that is indicated with an increase in accuracy of 4%.

Keywords: Quantum machine learning; Quantum kernel; Nanotechnology; Nanoscale transport; Noise robustness; Phase interference; Hybrid quantum–classical learning

References:

1. G. Percebois, Ph.D. Diss., Univ. Strasbourg, (2023).
2. S. Lorber et al., Phys. Rev. Appl., 22 (2024) 014041.
3. S. M. Mastoor and A. A. K. Kordbacheh, arXiv, (2025) arXiv:2506.

CM-011

Atomistic Insights into the Role of Gd/W Co-doping on the Electronic Structure and Phase Stability of $La_2Mo_2O_9$: A First-Principles Supercell Investigation

Amogh U Lanjewar[1]*, Smita Acharya[1]

[1]*Advanced Material Research Laboratory (AMRL), Department of Physics, RTM Nagpur University, Nagpur, Maharashtra, India*

***Corresponding author e-mail:** amoghlanjewar@gmail.com

ABSTRACT

This study employs first-principles Density Functional Theory (DFT) to fundamentally understand how multisite co-doping influences the phase stability and electronic properties of the $La_2Mo_2O_9$ (LMO) oxide-ion conductor. While LMO is a promising material, its structural phase transition limits its performance. Our approach investigates the $La_{2-x}Gd_xMo_{1.7}W_{0.3}O_9$ (LMGW) system to decode the synergistic effects of substituting Gd on La sites and W on Mo sites at an atomic level. The primary challenge in modeling such a chemically complex system lies in accurately capturing the local atomic distortions and electronic interactions introduced by the dopants. To address this, our computational framework, implemented within the Quantum Espresso package [1], is centered around a robust supercell approach. A critical and foundational step of our work is the determination of an optimal supercell geometry that balances physical accuracy with computational feasibility. For this, we are leveraging the Supercell Optimization for Heisenberg Exchange Calculations (SUPERHEX) methodology [2]. This allows us to construct a supercell that minimizes spurious periodic interactions and provides the most reliable representation of the doped material's structure. Subsequently, we will conduct in-depth analyses of the electronic structure, including the band gap and density of states (DOS), to reveal how co-doping modulates the orbital hybridization and bonding characteristics. These calculations are designed to provide direct insight into the mechanisms governing oxygen vacancy formation and mobility, which are the cornerstones of ionic conductivity. To ensure our theoretical models are grounded in physical reality, the LMGW compositions (x = 0 to 0.4) have been synthesized and experimentally validated. This computationally-driven investigation aims to establish a clear structure-property relationship, offering a predictive pathway for the rational design of next-generation solid-state ionic conductors.

Keywords: $La_2Mo_2O_9$; Density Functional Theory (DFT); Co-doping; Supercell Optimization.

References:

1. P. Giannozzi et al., J. Phys.: Condens. Matter, 21 (2009)
2. M. Alaei, A. R. Oganov, Phys. Rev. B, 111 (2024)

CM-012

Tuning the Transport Characteristics of Boron Phosphide Monolayers via Ad-Atom Functionalization and Substitutional Doping: A DFT - NEGF Study

K S Bharath Shirpi Thasan, D. John Thiruvadigal*

Computational Materials Science and Nano Devices Simulation Laboratory, Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail:** johnd@srmist.edu.in

ABSTRACT

Monitoring toxic gas levels in the environment is essential for ensuring environmental safety, managing industrial processes, and detecting hazardous gases early. This current investigation explores the transport characteristics of the boron phosphide (BP) monolayer and surface functionalized BP monolayer via ad-atom and substitutional doping. In this work, we employ Density Functional Theory (DFT) combined with Non-Equilibrium Green's Function (NEGF) formalism to systematically investigate the sensing behavior of BP-based nanoscale devices toward hydrogen-containing toxic gases. DFT calculations reveal strong adsorption energies and significant charge transfer between BP surfaces and target gas molecules, leading to pronounced modifications in the electronic density of states. NEGF transport simulations further demonstrate that these adsorption-induced perturbations result in measurable changes in transmission spectra and current–voltage characteristics, enabling highly sensitive detection. Our simulations reveal that BP devices exhibit high sensitivity towards the targeted gas molecules through pronounced modulation of transmission spectra and conductance. Importantly, our modified BP systems demonstrate exceptional sensitivity, with ad-atom decorated BP C-BP achieving 98.6% sensitivity and substitutionally doped BP Si-BP reaching 97% sensitivity toward ammonia detection. These enhancements underscore the critical role of surface modification in tailoring BP's electronic response to the target system. These findings highlight boron phosphide as a promising candidate for hydrogen-based toxic gas sensors, and underscore the effectiveness of DFT–NEGF methodologies in guiding the design of advanced nanoscale sensing architectures.

Keywords: DFT, NEGF, Boron Phosphide, Transport Properties

References:

1. J. Pang, Q. Yang, X. Ma, L. Wang, C. Tan, D. Xiong, H. Ye, and X. Chen, Phys. Chem. Chem. Phys., 19 (2017) 30852.
2. H. Dou, J. Sun, G. Zhang, and J. Leng, Physica B, 618 (2021) 413176.

CM-013

AI-Driven Design and Optimization of Advanced Functional Thin-Film Materials for Energy and Electronic Applications

Vidhushavarshini Sureshkumar[1], M.Kiruthiga Devi[2], Adethya Muralidharan[2]

Department of Computer Science and Business Systems, Rajalakshmi Institute of Technology (RIT), Chennai -124. vidhushasuresh@gmail.com

Department of CSE, SRM Institute of Science and Technology, Vadapalani, kiruthim6@srmist.edu.in

ABSTRACT

Developing functional, advanced thin-film materials is the foundation of the next generation of technologies for energy conversion, storage and electronic devices. Unfortunately, the development of these materials requires lengthy, costly experimentation and limited scalability, which presents significant challenges for researchers developing these advanced thin-films. Conventional trial-and-error methods do not adequately reflect the complexity of the relationship between processing, structure and performance of thin-films. As a result, there is a substantial gap between the identification of new materials and their application as commercial products. In this paper, we describe an integrated Artificial Intelligence (AI) based approach to the development and optimisation of functional thin-film devices, which incorporates Materials Informatics and Machine Learning-Assisted Design. The proposed framework consists of a four-layer pipeline: 1) Collecting data from laboratory experiments, computer simulations or publications; 2) Feature engineering to develop encodings of process and structure; 3) AI Model development using regression, deep learning and Bayesian optimisation; 4) Closed-loop optimisation which uses feedback for continuous refinement. This framework provides predictive mapping between fabrication parameters (i.e., thickness, crystal quality, defect density, etc.) and key performance metrics (i.e., electrical conductivity, charge carrier mobility and energy efficiency). The key element of this work is the integration of Process Parameters, Material Properties & Device Properties into an AI-based Scaled workflow that allows for Data-Driven Decisions throughout the lifecycle of Thin Films. Examples are provided using Energy Devices (solar cells, solid-state batteries, and functional coatings) and Electronic Technologies (transistors, sensors, flexible electronics). Collaboration between Academia and Industry through Standardization can help create a pathway to Autonomous Materials Design and to hastening the real-world implementation of AI-based Thin Film Technology for Energy and Electronic Systems.

Keywords: AI-Driven Materials Design; Functional Thin Films; Materials Informatics; Machine Learning-Assisted Optimization

CM-014

Copper and Zinc Doped Black Phosphorene Nanosheets as Promising Nanocarriers for Dacarbazine Delivery: A DFT Investigation

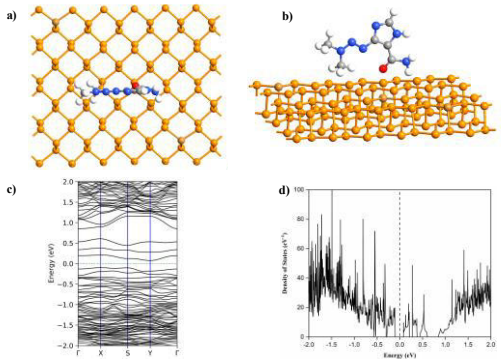
B. Anitha, R. Mugunthini, D. John Thiruvadigal, K. Janani Sivasankar*, R.M. Hariharan*

Computational Materials Science and Nano Devices Simulation Laboratory, Department of Physics and Nanotechnology, SRM University, Kattankulathur, Chennai-603 203, India.

Corresponding author e-mail: jananik@srmist.edu.in, hariharr@srmist.edu.in

ABSTRACT

Black phosphorene (BP) is a promising two-dimensional nanomaterial for biomedical applications owing to its tunable band gap, high surface area, and biocompatibility; however, its instability under ambient conditions limits practical use. In this study, density functional theory (DFT) calculations were employed to investigate the structural, electronic, and adsorption properties of copper (Cu)- and zinc (Zn)-doped black phosphorene nanosheets (BPNS) for drug delivery applications targeting metastatic melanoma. Doping at three different concentrations was performed to enhance the stability and electronic tunability of BPNS. The optimized doped systems were further examined for their interaction with the anticancer drug dacarbazine. Adsorption energy, charge transfer, frontier molecular orbitals, and density of states were analyzed to elucidate drug–nanocarrier interactions. The results reveal that Cu-doped BPNS exhibits stronger adsorption and moderate charge transfer, indicating a predominantly physisorption-driven and reversible drug loading mechanism suitable for controlled drug release. This study demonstrates the potential of metal-doped BPNS as efficient nanocarriers for targeted cancer therapy.



Keywords: Black phosphorene, DFT, Metal doping, Drug delivery, Metastatic melanoma

References:

1. Tahereh Mahboobi & Mohammad Reza Zardoost & Mohammad Reza Toosi, Journal of Molecular Modeling, (2020) 26: 269

CM-015

First-Principles Exploration of Nb_2C MXene for Two-Dimensional Drug Delivery Nanocarriers

Madhumitha G[1], Rooban P[1], Anitha B[1], Janani Sivasankar K[1]*

[1]*Computational Material Science and Nano Devices Simulation Laboratory, Department of Physics and Nano technology, SRM University, Kattankulathur, Chennai – 603 203, India.*

***Corresponding author e-mail:** jananik@srmist.edu.in

ABSTRACT

Two-dimensional (2D) MXenes have emerged as promising nanocarriers for drug delivery systems due to their large surface area, tunable electronic properties, and excellent structural stability. In this work, density functional theory (DFT) calculations are employed to investigate Nb_2C MXene as a potential nanocarrier material. Initially, the structural, electronic, and dynamical properties of pristine Nb_2C are systematically examined. The electronic characteristics of pristine Nb_2C are analyzed using total density of states (DOS), partial density of states (PDOS), and band structure calculations, confirming its metallic nature and high electronic conductivity. Phonon dispersion analysis is further performed to verify the dynamical stability of the pristine system, ensuring its feasibility for nanomedical applications. To enhance and tailor the intrinsic properties of Nb_2C, substitutional sulfur (S) doping is introduced at carbon sites. Two even dopant concentrations, namely 2S- and 4S-doped Nb_2C, are considered, resulting in multiple distinct configurations. The effect of sulfur doping on the electronic structure is systematically analyzed through DOS and PDOS calculations. The results reveal that S incorporation significantly modifies the electronic states near the Fermi level, indicating improved charge redistribution and electronic tunability. These features suggest enhanced drug–nanocarrier interactions, highlighting pristine and S-doped Nb_2C MXene as stable and promising platforms for drug delivery applications.

Keywords: MXene; Nb_2C; Density Functional Theory; Sulfur Doping; Nanocarrier; Drug Delivery System; Electronic Properties.

References:

1. Q. Xu, J. Ma, W. Khan, et al., Chem. Commun., 56 (2020) 6648.
2. M. A. S. Sakr, H. Abdelsalam, N. H. Teleb, M. A. Saad, O. H. Abd-Elkader, Y. Liu, and Q. Zhang, J. Mol. Graphics Modell., 136 (2025) 108937.

CM-016

Exploring Zr_2C MXene as a Two-Dimensional Nanocarrier for Drug Delivery: A First-Principles Study

P. Rooban, G. Madhumitha, K. Janani Sivasankar, C. Preferencial kala*,

Computational Material Science and Nano Devices Simulation Laboratory, Department of Physics and Nano technology, SRM University, Kattankulathur, Chennai – 603 203, India.

***Corresponding author e-mail:** preferec@srmist.edu.in

ABSTRACT

MXene materials have attracted significant attention in drug delivery research due to their two-dimensional structure, large surface area, and tunable surface chemistry. Among them, Ti_2C and Nb_2C MXenes have been extensively investigated using Density Functional Theory (DFT) to understand their adsorption behavior, surface modification, and drug–material interaction mechanisms, demonstrating excellent drug loading capacity and controlled release characteristics. In contrast, Zr_2C MXene remains relatively unexplored despite its promising potential in biomedical applications.

In this work, pure Zr_2C MXene is systematically studied as a nanocarrier for the anticancer drug cisplatin using first-principles calculations performed with the Vienna Ab initio Simulation Package (VASP). The structural stability of Zr_2C is assessed through phonon dispersion analysis, confirming its dynamical stability. Electronic properties are analyzed using density of states and band structure calculations to understand the interaction mechanism upon drug adsorption. Molecular dynamics simulations are employed to evaluate the thermal stability and interaction behavior of the Zr_2C–cisplatin complex. Furthermore, adsorption energy calculations are performed to identify the most energetically favorable binding site of cisplatin on the Zr_2C surface. The results demonstrate strong drug adsorption, stability, and favorable electronic characteristics, highlighting Zr_2C MXene as a stable, biocompatible, and efficient two-dimensional nanocarrier for advanced drug delivery applications.

Keywords: MXene, drug delivery, Density Functional Theory (DFT), Ti_2C, Zr_2C, Nb_2C.

Reference:

1. Zhu et al. (2021). Thoracic Cancer, 12(24), 3340–3355.
2. Sakr et al. (2025). Journal of Molecular Graphics and Modelling, 136, 108937.
3. Esquivel-Castro et al. (2022). Journal of Drug Delivery Science and Technology, 77, 103837.

CM-017

First-Principal Study of Toxic Gas Sensing on ZrS_2 Monolayer

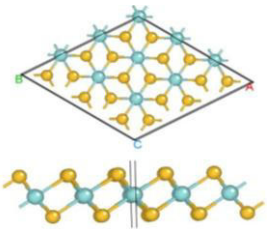
S. Sharon sneha, Dr. C. Preferencial kala*

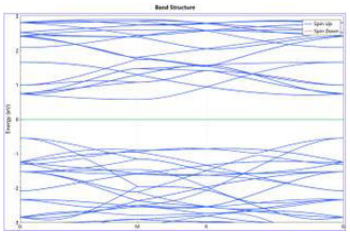
Computational Material Science and Nano Devices Simulation Laboratory, Department of Physics and Nanotechnology, SRM University, Kattankulathur, Chennai – 602 203, India.

*** Corresponding author e-mail:** preferec@srmist.edu.in

ABSTRACT

In recent years, air pollution has been considered one of the major concerns, caused by the release of toxic gases from various semiconductor industries, Industrial activities, vehicle emissions, fossil-fuel combustion, and chemical processing. The release of these harmful gases into the atmosphere can trigger human health issues and, in some conditions, lead to death. There is a need for efficient detection technologies to identify these gases. Among these emerging sensing materials,2D materials like TMDCs attracted attention for potential detection due to their high surface-to-volume ratio, structural flexibility, and tunable bandgap, allowing the design of fast, selective and stable gas sensing platforms. Zirconium disulfide (ZrS_2) is a layered transition metal dichalcogenide (TMDC) with the chemical formula ZrS_2. This 2D ZrS_2 exhibits an indirect bandgap and structural stability, making it a promising candidate for gas sensing applications. In particular, defects such as doping, vacancies enhance the charge-transfer performance, improving sensitivity towards toxic gas detection. Here, we systematically optimized the ZrS_2 structure using the DFT approach and investigated its electronic and gas-sensing properties.





Keywords: Density functional theory (DFT), Gas adsorption, ZrS_2 monolayer, vacancies.

References:

1. X.-Q. Lin, Z.-H. Han, X. Zhang, J.-X. Yang, and Y.-G. Yao, Phys. Chem. Chem. Phys., 2025.
2. X. Tian, S. Wang, H. Li, M. Li, T. Chen, X. Xiao, and Y. Wang, Sens. Diagn., 2 (2023) 361.
3. H. Li et al., Sci. Rep., 2 (2012) 595.
4. S. Zhao, J. Xue, and W. Kang, arXiv, 2013.

CM-018

Enhanced H_2S Detection Using Selenium Vacancy-Induced $MoSe_2$ Monolayer: A Density Functional Theory Analysis

Viveka N[1], Preferencial Kala C [1]*

[1]*Department of Physics and Nanotechnology, Computational Materials Science and Nano Devices Simulation Laboratory, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu 603203, India*

***Corresponding author e-mail:** preferec@srmist.edu.in

ABSTRACT

The detection of hazardous gases, such as hydrogen sulfide (H_2S), is critically important for ensuring safe industrial operations, environmental protection, and human health. In this study, the electronic properties and gas-sensing behavior of a selenium (Se) vacancy-created $MoSe_2$ monolayer are studied using density functional theory (DFT) calculations. The introduction of a Se vacancy significantly alters the intrinsic electronic structure of the pristine MoSe2 monolayer, resulting in a noticeable reduction in the band gap and a corresponding decrease in electrical resistance. This modification enhances the material's conductivity and sensing performance. The presence of the Se vacancy leads to substantial charge redistribution around the defect site, generating highly active adsorption centers that promote stronger interactions with the target H_2S gas molecule. Comprehensive analyses, including band structure, total and projected density of states (TDOS and PDOS), electron density difference (EDD), electron localization function (ELF), and Mulliken population analysis, reveal pronounced charge transfer between the H2S molecule and the defective MoSe2 surface. These results confirm that the interaction is significantly stronger than that observed for the pristine monolayer. The Se-vacancy $MoSe_2$ monolayer exhibits a strong adsorption energy of approximately -1.0 eV toward H2S, indicating a chemisorption-dominated sensing mechanism. Despite the strong binding strength, the system maintains favorable desorption characteristics, with a calculated recovery time of 32.5 seconds at an elevated temperature of 373 K. This balance between strong adsorption and efficient desorption highlights the material's potential for reusability with thermal assistance. Overall, the findings demonstrate that the defect-created MoSe2 monolayer is a promising candidate for selective, sensitive, and reusable H_2S gas sensing applications.

Keywords: DFT, $MoSe_2$ monolayer, selenium vacancy, charge transfer, adsorption energy, and recovery time.

References:

1. Cui, Z., K. Yang, Y. Shen, Z. Yuan, Y. Dong, P. Yuan, and E. Li, App. Sur. Sci, 613 (2023).
2. L. Sun, J. Dong, F. Tian, J. Zhang, and L. Chen, Langmuir, 40(24) (2024).

CM-019

First-Principles Investigation of Spinterface Magnetism and Spin Transport in 2D Molecular–Fe_3GeTe_2 Junctions

Ardhendu Dey[1], Arijit Sen[1]*

[1] *SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** arijits@srmist.edu.in

ABSTRACT

Two-dimensional ferromagnetic Fe_3GeTe_2 (FGT) combines metallic conductivity, strong perpendicular anisotropy, and stable spin polarization, positioning it as a promising van der Waals electrode for molecular spintronics. Here, we investigate a 2D molecular layer adsorbed on monolayer FGT and explore its interfacial magnetic and electronic response using first-principles density-functional theory (VASP). Differential charge and spin-density analyses reveal localized π–d hybridization and interfacial spin redistribution, indicating that molecular adsorption perturbs surface Fe-derived moments without suppressing the intrinsic ferromagnetic metallicity. Spin-resolved band structures confirm a clear majority/minority channel separation near the Fermi level. To probe spin-transport functionality, a two-probe molecular junction is constructed and simulated using QuantumATK within the nonequilibrium Green's function formalism. The current–voltage response exhibits strong spin selectivity between parallel and antiparallel magnetic configurations, demonstrating efficient spin filtering driven by the FGT electrodes, consistent with earlier predictions of giant magnetoresistance in FGT-based molecular junctions. These results highlight monolayer FGT as a robust mixed-dimensional platform for molecular spin devices

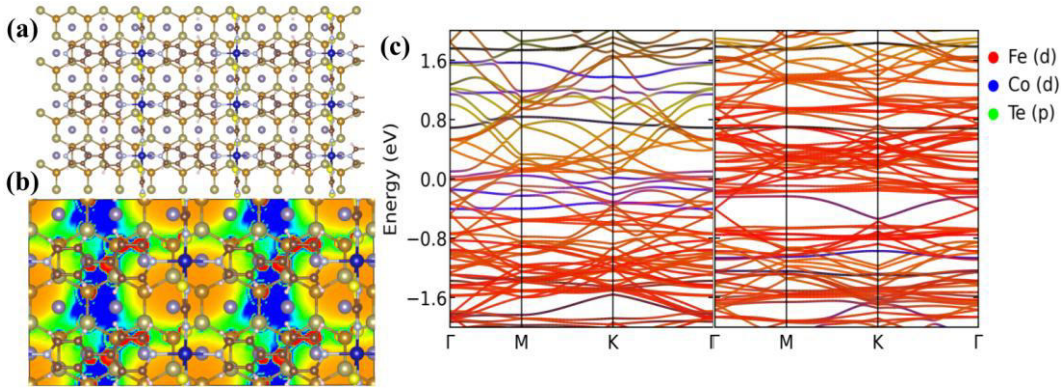


Fig. (a) Atomic structure of a 2D molecular overlayer adsorbed on ferromagnetic Fe_3GeTe_2. (b) Spatial spin-polarization map illustrating interfacial spin redistribution. (c) Spin-resolved electronic band structure, showing spin-up and spin-down dispersions, orbital projected.

References:

1. Andre K. Geim, Konstantin S. Novoselov, The rise of graphene, Nat. Mater. 6 (3) (2007) 183–191.

CM-020

Magnetism and Spin-Filtering in Benzene-Modified MTe_2 Monolayers

Divya Anand[1], Ardhendu Dey[1], Arijit Sen[1]*

[1] *SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** arijits@srmist.edu.in

ABSTRACT

Two-dimensional magnetic MTe_2 compounds (M = Cr, V, Fe, Mn) provide a versatile platform for molecular spintronics. We examine benzene adsorption on monolayer MTe_2 using VASP, focusing on in- terfacial charge redistribution, spin polarization, and transport modulation. Differential spin-density maps reveal localized π–d hybridization between benzene and surface metal sites, altering interfacial magnetic moments in a metal-dependent manner. Non-equilibrium Green's function calculations on molecular two- probe devices show a strong contrast between parallel and anti-parallel current–voltage responses, con- firming robust spin filtering across different MTe_2 hosts. Quantitative magnetic analysis is demonstrated for $CrTe_2$. Exchange parameters are extracted through the four-state energy mapping approach, and the resulting Heisenberg Hamiltonian is treated with Monte Carlo simulations. A Curie temperature of ~160 K is obtained, consistent with temperature-dependent magnetization trends and confirming moderate two- dimensional ferromagnetism. These results highlight benzene-functionalized MTe_2 as a promising molec- ular-magnetic platform where adsorption chemistry and spin-polarized transport are closely coupled.

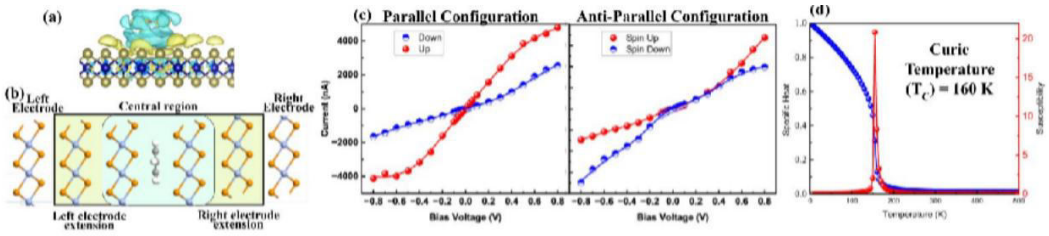


Fig. (a) Calculated differential spin density of benzene adsorbed on a $CrTe_2$ monolayer. (b) Two-probe transport configuration with benzene in the scattering region. (c) Spin-polarized I–V responses for parallel and antiparallel magnetic alignments. (d) Temperature-dependent magnetization behavior of $CrTe_2$, yield- ing a Curie temperature of about 160 K.

References:

1. A. K. Geim and K. S. Novoselov, Nat. Mater., 6 (2007) 183–191.
2. Y. Liu, S. Kwon, G. J. de Coster, R. K. Lake, and M. R. Neupane, Phys. Rev. Mater., 6 (2022) 084004.
3. H. Zhou, Y. Zhang, and W. Zhao, ACS Appl. Mater. Interfaces, 13 (2021) 1214–1221.
4. L. Webster and J.-A. Yan, Phys. Rev. B, 98 (2018) 144411.

CM-021

Enhanced Waste Heat Recovery in Industrial Systems using Optimized Thermoelectric Generators

Kunal Kishore[1]*, Tanmoy Maiti[1]

[1]*Indian Institute of Technology Kanpur, Kalyanpur, Kanpur, Uttar Pradesh, India, 208016*

***Corresponding author e-mail:** kunalk21@iitk.ac.in

ABSTRACT

Thermoelectric generator (TEG) has emerged as a promising solution for sustainable energy generation by efficiently converting waste heat into electricity. However, their widespread application is hindered by limited performance due to multitude of losses and other design factors. Hence, assessing their performance under realistic operating scenarios is crucial for harnessing their full potential. This study presents a comprehensive numerical simulation of TEG performance under isoflux heat source boundary conditions, utilizing finite element modelling (FEM). Critical design parameters are optimized to maximize power output and efficiency, including leg geometry, contact resistance, external load resistance, and fill fraction (FF). Additionally, fin design adjustments are implemented to optimize FF and convective heat transfer, enhancing the performance of the thermoelectric (TE) module. Here we have explored the use of high-performance silicon-germanium (SiGe) based p-type and n-type alloys selected for their exceptional thermal stability at elevated temperatures. A vast surge of approximately 80% is achieved with a maximum power output of 11.9W alongside a total potential drop between two ends was observed to be around 36.5V for a single n-p TE module with 256 legs. The maximum power conversion efficiency was observed to be around 10% for the same. In conjunction, heat transfer processes within a thermal power plant boiler are simulated to visualize realistic functioning conditions. The simulation focuses on heat loss in thermal power plant boilers operational at high temperatures, which reduces their efficiency. The strategic placement of TEGs helps to convert waste heat into electricity efficiently, enabling their potential integration into commercial systems for waste heat recovery.

Dynamic Conductance of Chiral Molecular Junctions: A First-Principles Study

Thingujam Yaiphalemba Meitei*, Ardhendu Dey, J. John Donald Raj, Saikumar k, Arijit Sen

Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur PO, Chennai 603203, Tamil Nadu, India

***Corresponding author e-mail:** thyaip@gmail.com

Owing to significant advances in the nanofabrication techniques over the last few decades, the realization of nanodevices has often turned out to be more feasible with less complexity. This attaches importance to the exploration of several quantum transport phenomena [1-5], one of which lies apparently in the study of dynamic conductance of nanodevices to help better understand the ultrafast transient dynamics. In the present work, we examine the chirality aspect in dynamic conductance of single molecular devices (Fig. 1) from first-principles. Besides, the overall effect of temperature on the transient transport of electrons in chiral molecular junctions is investigated for improved thermal stability and device performance.

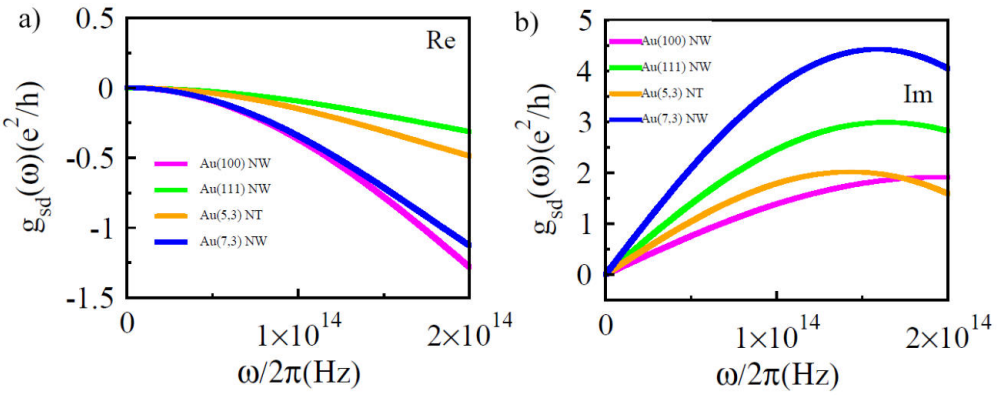


Fig. a) Real and b) Imaginary part of the dynamic conductance associated with chiral molecular junctions

References:

1. A. K. Slimane, P. Reck, and G. Fleury, Phys. Rev. B, 101 (2020) 235413.
2. D. Kienle, M. Vaidyanathan, and F. Léonard, Phys. Rev. B, 81 (2010) 115455.
3. B. Wang, J. Wang, and H. Guo, Phys. Rev. Lett., 82 (1999) 398.

CM-023

Transport characteristics of pure HfS2 monolayers influenced by cobalt doping: A DFT study

Selvamani E[1], Preferencial Kala C[1]*, John Thiruvadigal D[1]

[1]*Computational Materials Science and Nanodevices Simulation Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India*

***Corresponding author e-mail:** preferec@srmist.edu.in

ABSTRACT

Transition metal dichalcogenides (TMDs) show remarkable potential for thermoelectric energy conversion, attributed to their adjustable electronic structures and low lattice thermal conductivity, which result from significant d-electron correlations and phonon scattering. Using first-principle calculations of density functional theory (DFT) with the NEGF method, we have studied the electronic and thermal properties of both pristineHfS2 and cobalt (Co) doped monolayers. The stability of the pure HfS2 and cobalt-doped HfS2 is verified by formation energy analysis, and the thermal stability is revealed by ab initio molecular dynamics simulations. The electronic structure calculation indicates that the monolayer HfS2 and Co-HfS2 are indirect band gap semiconductors with a band gap of 1.20 eV and 0.90 eV. Non-Equilibrium Green's Function is used to analyse the electron and phonon transmission to compute the dimensionless figure of merit (ZT), thermal conductivity of electrons and phonons, electrical conductance (Ge), and Seebeck coefficient (S). The thermoelectric figure of merit was greatly boosted with the incorporation of a cobalt dopant and was determined with chemical potential as a function of temperature. These results indicate that modifying the Co-HfS2 system demonstrates the greatest potential for thermoelectric applications.

Keywords: NEGF, electrical conductance, phonon thermal conductance, figure of merit.

References:

1. Xiong, K. wei, RSC. adv., 13.12 (2023): 7972-7979.2.
2. Li, B. ke, Phys. Chem. C, 126.1 (2021): 525-533.

CM-024

Engineering Silicon-Doped Graphdiyne with Amino Acid Derivatives: A DFT Study Toward Targeted Drug Delivery

R. Mugunthini, K. Iyakutti, D. John Thiruvadigal, K. Janani Sivasankar*, R.M. Hariharan*

Computational Materials Science and Nano Devices Simulation Laboratory, Department of Physics and Nanotechnology, SRM University, Kattankulathur, Chennai-603 203, India.

***Corresponding author e-mail**: jananik@srmist.edu.in, hariharr@srmist.edu.in

ABSTRACT

The development of efficient nanocarriers remains a crucial step in advancing targeted drug delivery strategies for neurological disorders. Graphdiyne (GDY), a novel two-dimensional carbon allotrope with intrinsic sp–sp² hybridization, offers outstanding stability, tunable electronic properties, and versatile functionalization potential, making it an excellent candidate for biomedical applications. In this work, we show a potential carrier for neuroactive drug delivery using a DFT-designed nanoplatform based on silicon-doped graphdiyne (Si-GDY) functionalized with amino acid derivatives. By inducing localized electronic states and symmetry breaking within the graphdiyne lattice, silicon substitution improves the material's surface reactivity and adsorption capacity. Stable drug loading is made possible by surface functionalization with biologically relevant amino acid derivatives, which enhances hydrophilicity and interfacial compatibility. Electronic structure analysis, charge transfer characteristics, and solvation-related properties further support the suitability of the functionalized Si-GDY system for biological environments. Overall, this study establishes amino-acid-functionalized silicon-doped graphdiyne as a promising nanocarrier, providing a fundamental computational framework for future development of targeted drug delivery systems for neurodegenerative disorders.

Keywords: Graphdiyne, Silicon, DFT, Drug delivery, neurodegenerative disorders.

References:

1. Tabandeh, Z.; Reisi-Vanani, A. Diam. Relat. Mater. 2021, 119, 108564.
2. Mugunthini, R.; Anitha, B.; Sneha, J.; Hariharan, R. M.; Iyakutti, K.; Thiruvadigal, D. J.; Sivasankar, K. J. J. Mol. Graph. Model. 2025, 109201.

CM-025

Aluminum-Doped Penta-Graphene as a Promising Two-Dimensional Material for Hydrogen Storage

Vinotha S, Abinaya V, John Thiruvadigal D*

Department of physics and Nanotechnology, SRM institute of Science and Technology, Tamilnadu, India, 603203

***Corresponding author e-mail:** johnd@srmist.edu.in

ABSTRACT

Hydrogen storage remains a major technological challenge in realizing a hydrogen-based energy economy. Two-dimensional materials have attracted significant attention due to their high surface area and tunable physicochemical properties. Among these materials, penta-graphene a carbon allotrope composed exclusively of pentagonal carbon rings exhibits intrinsic buckling, structural stability, and unique electronic characteristics that make it a promising hydrogen storage platform. This work summarizes recent advances in hydrogen adsorption on pristine, doped, and particularly Al-doped penta-graphene, with emphasis on gravimetric hydrogen storage capacity, adsorption mechanisms, and reversibility. Aluminum doping enhances hydrogen adsorption through charge transfer–induced polarization while maintaining a low atomic mass, thereby preserving high gravimetric efficiency. Reported studies indicate that Al-doped penta-graphene can achieve gravimetric hydrogen storage capacities of approximately 6–7 wt%, approaching targets for reversible on-board hydrogen storage. Remaining challenges include dopant clustering, thermal stability, and experimental realization, which must be addressed to enable practical hydrogen storage applications based on Al-functionalized penta-graphene.

References:

1. Zhang, S.; Zhou, J.; Wang, Q.; Chen, X.; Kawazoe, Y.; Jena, P. Proc. Natl. Acad. Sci. U.S.A. 2015, 112, 2372–2377.
2. Hao, J.; Zhang, Y.; Wang, Y.; Sun, Q. Int. J. Hydrogen Energy 2021, 46, 25533–25542.
3. Ali, A.; Hussain, T.; Ahuja, R. Int. J. Hydrogen Energy 2022, 47, 36190–36203.
4. Ao, Z. M.; Peeters, F. M. J. Appl. Phys. 2009, 105, 074307.
5. Shevlin, S. A.; Guo, Z. X. Chem. Commun. 2013, 49, 1094–1096.

CM-026

Halogen Doped Boron Nitride Nanosheets as Metal-Free Electrocatalysts for Hydrogen Evolution Reaction

Sneha. J, Abinaya. V, K. Janani Sivasankar, D. John Thiruvadigal*

Computational Material Science and Nanodevices Simulation Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India

***Corresponding author e-mail:** johnd@srmist.edu.in

ABSTRACT

Hydrogen production through water splitting is a crucial approach for generating clean and sustainable energy. Boron nitride nanosheets (BNNS) are chemically stable two-dimensional materials; however, their application in water splitting is limited due to their wide band gap and lack of active sites. In this work, we investigate the effect of halogen doping (F, Cl, Br, and I) on the catalytic performance of BNNS for the hydrogen evolution reaction (HER) using density functional theory calculations. Pristine and doped BNNS structures were fully optimized, and their stability was examined through formation energy analysis. The catalytic activity was evaluated by studying hydrogen adsorption behavior and the free energy of hydrogen adsorption (ΔG_H*). Compared to pristine BNNS, halogen-doped BNNS exhibits significantly improved hydrogen adsorption characteristics, indicating enhanced HER activity. Charge density difference analysis reveals effective charge redistribution around the dopant sites, identifying them as active centers for hydrogen adsorption. The results demonstrate that halogen doping is an effective strategy for activating inert BNNS and highlight its potential as a stable, metal-free catalyst for hydrogen production.

References:

1. Gadore, V.; Mishra, S. R.; Singh, A. K.; Ahmaruzzaman, M. RSC Adv. 2024, 14, 3447–3472.
2. Wan, Q.; Wei, F.; Ma, Z.; Anpo, M.; Lin, S. Adv. Theory Simul. 2019, 2, 1800174.
3. Liu, Y.; Zhang, X.; Yuan, Z.; An, L.; Liu, B. Z. Sustainable Energy Fuels 2026.
4. Alam, K. M.; Kumar, P.; Kar, P.; Goswami, A.; Thakur, U. K.; Zeng, S.; Vahidzadeh, E.; Cui, K.; Shankar, K. Nanotechnology 2020, 31, 084001.

CM-027

Intrinsic Polarization Effects in Janus 2D Aluminum Nitride for Energy Applications

V. Abinaya[1], J. Sneha[1], K. Janani Sivasankar[1], D. John Thiruvadigal [1]*

[1]*Computational Material Science and Nanodevices Simulation Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India.*

***Corresponding author e-mail:** johnd@srmist.edu.in

ABSTRACT

Two-dimensional Aluminum Nitride (AlN) is a wide-bandgap, polar material with intrinsic piezoelectric and electronic properties that are attractive for energy-related nanoscale applications. In this work, we explore surface polarization engineering in monolayer AlN through asymmetric Janus functionalization using fluorine and hydroxyl terminations. Using first-principles density functional theory calculations, we examine how breaking out-of-plane mirror symmetry influences the electronic structure and electrostatic potential of 2D AlN. The Janus configuration exhibits a distinct potential gradient across the atomic thickness, indicating the formation of an intrinsic built-in electric field. Furthermore, asymmetric surface functionalization leads to noticeable work-function differences between the two sides of the sheet, suggesting directional charge separation. Charge redistribution analysis reveals polarization-induced electron transfer between the functionalized surfaces, while the semiconducting nature of AlN is preserved. These findings highlight the potential of Janus 2D AlN as an intrinsically polarized material platform for self-powered energy harvesting and sensing applications, and provide a foundation for further device-oriented investigations.

References:

1. Lu A.-Y., Zhu H., Xiao J., Chuu C.-P., Han Y., Chiu M.-H., Cheng C.-C., Yang C.-W., Wei K.-H., Yang Y., Wang Y., Sokaras D., Nordlund D., Yang P., Muller D. A., Chou M.-Y., Zhang X., Li L.-J., Nat. Nanotechnol., 12 (2017) 744–749.
2. Dong L., Lou J., Shenoy V. B., ACS Nano, 11 (2017) 8242–8248.
3. Zhang C., Gong C., Nie Y., Min K.-A., Liang C., Oh Y. J., Zhang H., Wang W., Hong S., Colombo L., Wallace R. M., Cho K., J. Appl. Physics, 123 (2018) 244302.
4. Sevik C., Çağın T., Phys. Rev. B, 82 (2010) 045202

CM-028

Halogen-Substituted-Driven Band Engineering in Mixed-Metal Chalcohalides $CuBiSeI_2$

Manivannan Saminathan[1], Kathirvel Venugopal[1]*

[1] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India*

***Corresponding author e-mail:** kathirvv@srmist.edu.in

ABSTRACT

The rapid growth in global energy necessitates the development of efficient renewable energy technologies. Mixed-anion halide-chalcogenide materials are promising for energy applications due to their structural complexity and low thermal conductivity. Recently, CuBiSeCl2 was reported to exhibit glass-like thermal transport, but its large band gap (~1.3 eV) limits the carrier transport and thermoelectric performance. With this motivation, halogen substitution as a band-engineering strategy is attempted by replacing Cl atoms with I atoms to design CuBiSeI2. First-principles calculations show that CuBiSeI2 crystallizes in the orthorhombic pnma (NO. 62) structure, consisting of CuSe2I2 tetrahedra and BiSe6I6 polyhedra with formal oxidation states Cu1+, Bi3+, Se2-, and I1-. The PBE+U with vdW corrections predicts a direct band gap of 0.47 eV, nearly threefold smaller than that of CuBiSeCl2. Phonon stability, negative formation energy, and satisfied Born criteria confirm synthesizability. The compound exhibits an enhanced power factor of up to 1.17 mW m-1 K-2 at 600 K, highlighting its potential as a promising thermoelectric material among mixed-anion chalcohalides.

Keywords: Thermoelectric, electron, Phonon, transport properties, first principle calculation

Reference:

1. Cara J. Hawkins, Jon A. Newnham, Batoul Almoussawi, Nataliya L. Gulay, Samuel L. Goodwin, Marco Zanella, Troy D. Manning, Luke M. Daniels, Matthew S. Dyer, Tim D. Veal, John B. Claridge, Matthew J. Rosseinsky, Chem. Mater., 36 (2024) 4530–4541.

CM-029

Density Functional Theory Investigation of WS_2 for Drug Delivery Applications

Ruba Devi M, Sneha J, Janani Sankar and John Thiruvadigal D*

Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Tamil Nadu, 603 203 India

***Corresponding author e-mail:** johnd@srmist.edu.in

ABSTRACT

Two-dimensional transition metal dichalcogenides (TMDs) have attracted significant attention for biomedical and nanoelectronics applications due to their tunable electronic properties, large surface area, and chemical stability. In this work, a comprehensive first-principles density functional theory (DFT) investigation is carried out to explore the structural, electronic, and adsorption characteristics of a WS_2 monolayer for potential nanocarrier applications. Geometry optimization confirms the thermodynamic stability of pristine WS_2 with a hexagonal lattice structure. Electronic band structure and density of states analyses reveal a direct band gap of approximately 1.8 –2.1 eV at the K-point, consistent with previously reported experimental and theoretical results. The interaction between WS_2 and selected drug molecules is examined through adsorption energy, charge transfer, and charge density difference analyses. The results indicate favourable adsorption with moderate binding strength, ensuring stable drug loading while allowing controlled release. Furthermore, changes in the electronic properties upon adsorption suggest enhanced sensitivity and improved carrier–drug interactions. These findings highlight the potential of WS_2 monolayers as efficient nanocarriers for drug delivery and pave the way for further experimental and theoretical investigations in biomedical nanotechnology.

References:

1. Mahmud A. Y., Yashir S., Zubair M., Nanoscale Adv. 6 (2024) 1347–1362.
2. Manzeli S., Ovchinnikov D., Pasquier D., Yazyev O. V., Kis A., Nat. Rev. Mater. 2 (2017) 17033.
3. Cheng L., Yuan C., Shen S., Yi X., Gong H., Yang K., Liu Z., ACS Nano 9 (2015) 11090–11101.
4. Bu Y., Sun M., Phys. Chem. Chem. Phys. 27 (2025) 14397–14409.
5. Moradpur-Tari E., Sarraf-Mamoory R., Yourdkhani A., Physica B: Condens. Matter 650 (2023) 414568.
6. Bishal G., Moradian R., Comput. Condens. Matter 18 (2019) e00352.

CM-030

First-Principles Study of Structural, Electronic, and Magnetic Properties of Tetragonal Ce-Based Pnictides

Narayanan Namboodiri Puthusseri[1], Pankaj Bhalla[1]*

[1]*Department of Physics, School of Engineering and Sciences, SRM University AP, Amaravati 522240, India*

***Corresponding author e-mail:** pankaj.b@srmap.edu.in

ABSTRACT

We present a first-principles density functional theory (DFT) investigation of the structural, electronic and magnetic properties of the tetragonal CeX_2Y_2 (X = Co, Ni, and Fe; Y = P, As, and Sb) compounds, crystallizing in the $ThCr_2Si_2$-type structure (space group I4/mmm) [1]. The crystal structure was fully optimized using the plane-wave pseudopotential method within the generalized gradient approximation (GGA) [2], yielding lattice parameters consistent with the expected tetragonal symmetry. Based on the relaxed structure, self-consistent electronic structure calculations were performed. The electronic band structure and density of states were analyzed with particular emphasis on the role of Ce-4f states and Co-3d states on the total magnetic behaviour of the compound. The calculated density of states reveals a significant contribution from Ce-4f and Co-3d orbitals near the Fermi level, indicating a complex interplay between localized and itinerant electronic states. Inclusion of SOC leads to noticeable band splitting and modification of the near-Fermi-level band dispersion, which is relevant for understanding relativistic effects in Ce-based intermetallic compounds. These results provide a reliable computational baseline for further investigations of magnetism and possible topological features in CeX_2Y_2 and related materials. The present study serves as a starting point toward exploring correlation-driven and spin–orbit–induced phenomena in Ce-based pnictides.

References:

1. H. Hu, Y. Jiang, D. Liu, Y. Chen, A. M. Tsvelik, Y. Xu, K. Haule and B. A. Bernevig, arXiv, 2025, 2411.13647.
2. D. Joubert, Phys. Rev. B, 1999, 59, 1758–1775.

CM-031

Halogen-Driven Modulation of Electronic and Thermoelectric Properties in $TiOX_2$ Monolayers: A DFT Study

Bhavya Janghel*, S.M. Saini

National Institute of Technology, Raipur, Chhattisgarh, India, 492010

***Corresponding author e-mail:** bjanghel.phd2024.phy@nitrr.ac.in

ABSTRACT

Two-dimensional $TiOX_2$ (X = Cl, Br, I) monolayers are investigated using first-principle calculations to examine their stability in term of structural, mechanical and dynamical. The electronic structure is also investigated for energy gap analysis and thermoelectric performance. $TiOX_2$ monolayers is confirmed through elastic constant and phonon dispersion analysis. We found that the band gap decreases with the substitution of I and Br in place of Cl i.e. $TiOCl_2$ (2.04eV) to $TiOBr_2$ (1.53 eV) and $TiOI_2$ (0.295 eV). Corresponding changes in the electronic density of states near the Fermi level influence carrier transport behavior. Thermoelectric transport properties are calculated using Boltzmann transport theory within the constant relaxation time approximation. Among these monolayers the highest ZT value is obtained in $TiOCl_2$ (≈2.7), which suggests its potential suitability for thermoelectric applications. Overall, this work provides a systematic comparison of halogen-dependent property modulation in 2D $TiOX_2$ monolayers.

References:

1. Pernilla Helmer, Martin Dahlqvist J. Mater. Chem. C, 13 (2025), 4769
2. M. Menderes Aly¨orük, Computational Condensed Matter, 42 (2025) e01005

CM-032

Study of 2D Janus Cdxi (X=Cl, Br) Monolayers for Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance

Jeevanlal Sahu*, S. M. Saini

National Institute of Technology, Raipur, Chhattisgarh, India, 492010

***Corresponding author e-mail:** jsahu.phd2024.phy@nitrr.ac.in

ABSTRACT

Two-dimensional (2D) materials have emerged as promising candidates for thermoelectric applications. Their reduced dimensionality can enhance the Seebeck coefficient and suppress lattice thermal conductivity, which leads to an improved thermoelectric figure of merit (ZT), making them potential candidates for waste heat recovery. Using Density functional theory (DFT) combined with Boltzmann transport theory, the thermoelectric properties of Janus CdXI (X=Cl, Br) monolayers are systematically investigated. Phonon dispersion analysis and elastic constant calculations confirm the dynamical and mechanical stability of these monolayers. The calculated electronic structures reveal the direct band gaps of 2.41 (3.24) eV and 2.53 (3.37) eV for CdClI and CdBrI using PBE (HSE06) functionals, respectively. These investigated monolayers exhibit the ultra-low lattice thermal conductivity of 0.356 W/mK and 0.386 W/mK, at room temperature for CdClI and CdBrI, respectively. The high Seebeck coefficient (~1550 μV/K) combined with ultralow lattice thermal conductivity leads to an excellent thermoelectric performance. At 1000 K, the predicted ZT values are 3.61 (p-type) and 2.69 (n-type) for CdClI, and 3.83 (p-type) and 4.03 (n-type) for CdBrI. These results indicate that CdClI and CdBrI have high potential for thermoelectric applications, and this work provides theoretical support for the future experimental studies.

References:

1. Delong Li, Youning Gong et al. Nano-Micro Letters, 12 (2020) 36.
2. Ali Obies Muhsen Almayyali, Sarab J. Musa et al. Materials Science in Semiconductor Processing, 199 (2025) 109834

CM-033

Oxide TE-Predictor: An Interpretable Machine Learning Framework to Accelerate the Design of Oxide-Perovskite Thermoelectric Materials

Shivam Aggarwal* and Tanmoy Maiti

Plasmonics and Perovskite Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Kanpur Uttar Pradesh, India 208016

***Corresponding author e-mail:** shivzagg20@iitk.ac.in

ABSTRACT

Thermoelectric (TE) generators convert waste heat from industries, furnaces, and engines into electricity, providing a sustainable energy solution. Oxide perovskites are promising TE materials due to their thermal stability and environmentally benign nature, but their low figure of merit (zT) limits device efficiency. Designing high-zT oxide perovskite material is crucial for enhancing TE performance. This study employed machine learning (ML) to predict the TE properties of ABO_3 oxide perovskites. A dataset of over 110 perovskite compositions, curated from literature, including experimental data on the Seebeck coefficient, electrical conductivity, thermal conductivity, and zT at various temperatures. Various elemental and structural properties were used to featurize the chemical composition. The positional average elemental property (PAEP) approach was employed to capture site-specific effects and improve model accuracy. Several ML models were trained to predict TE properties, including, random forest, XGBoost, extra trees, and AdaBoost regressor. The best-performing models achieved an R^2 score above 0.90, ensuring high prediction accuracy. A graphical user interface (GUI), Oxide TE-Predictor was developed to integrate these models, enabling real-time temperature-dependent TE property predictions for any given ABO_3 composition. To the best of our knowledge, this is the first ML-based study to predict the zT of oxide perovskites. This work highlights the potential of ML in accelerating the discovery of high-performance TE materials, providing a data-driven alternative to traditional trial-and-error experimental methods.

CM-034

Zr-Induced Enhancement of Thermoelectric Performance in Li-Based Quaternary Heusler Alloys

Lokanksha Suktel[1]*, S. M. Saini[1]

[1]*National Institute of Technology, Raipur, Chhattisgarh, India, 492010*

***Corresponding author e-mail:** lsuktel.phd2022.phy@nitrr.ac.in

ABSTRACT

We have conducted a comprehensive study of the Li-based quaternary Heusler alloy $LiZr_xHf_{1-x}PdAl$ (x=0, x=0.25, x=0.5, x=0.75, x=1), for examining the effect of Zr substitution on its electronic, structural, thermoelectric, and elastic properties. Density Functional Theory (DFT) and the Boltzmann transport equation are employed to evaluate the parameters of these alloys. The energy band structure revealed an indirect band gap, and the proximity of the valence band to the Fermi energy level indicated a p-type semiconducting nature. These alloys are a good thermoelectric material because of their semiconducting nature, high figure of merit (ZT), high electrical conductivity (σ), and low thermal conductivity (κ). Notably, the maximum ZT of ~0.77 is obtained for x = 0.5 composition of the alloy. These results demonstrate that Zr substitution effectively tunes the electronic and transport properties of LiHfPdAl, making $LiZr_xHf_{1-x}PdAl$ a promising candidate for thermoelectric applications.

References:

1. S. Perumal, T. Ghosh, A. Singh, V. Umesh, K. Biswas, S. Perumal, M. Samanta, T. Ghosh, U.S. Shenoy, A.K. Bohra, Joule 3 2565.
2. N. Estaji, M. Afshar, Mater. Res. Express 8 (2021) 46527.

CM-035

Cellular Automata Modelling of Layered Ternary Carbides and Nitrides

A. Bhavadharani[1], D. K. Sheena Christy[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** sheenac@srmist.edu.in

ABSTRACT

Layered ternary carbides and nitrides (MAX phases) are crystalline materials distinguished by their unique layered architectures, offering remarkable potential in advanced materials science. In this study, we introduce a cellular automata (CA) framework to simulate the structural growth of MAX phases on a two-dimensional grid. By encoding the lattice dynamics into CA rules, we replicate the spatial evolution of MAX architectures, capturing the interplay between transition-metal, A-group, and carbon/nitrogen layers. We analyse the periodicity inherent in these CA-generated structures, reflecting the ordered stacking observed in MAX phases. Furthermore, we investigate the reversibility of the CA rules to examine whether the growth process can be computationally reversed, which is an essential property for theoretical modelling and nanofabrication.

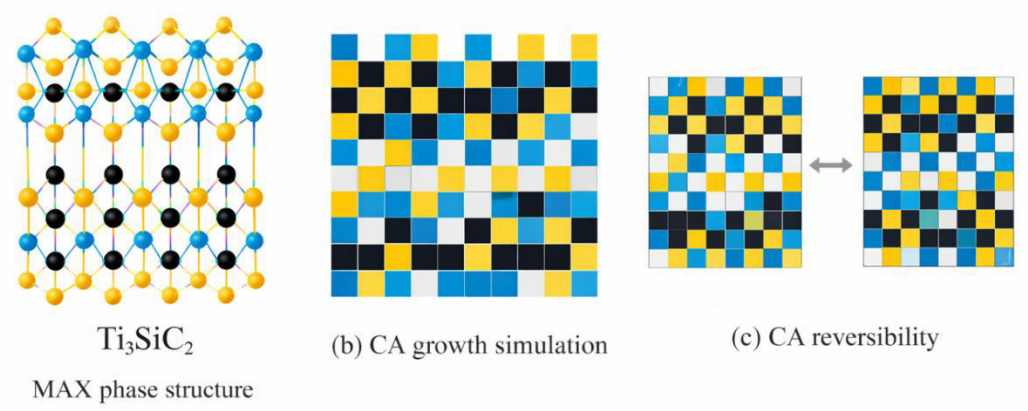


Fig. 1. Schematic representation of a MAX phase (Titanium silicon carbide)

References:

1. K. Bhattacharjee, N. Naskar, S. Roy and S. Das, Nat. Comput., 2020, 19, 433–461.
2. S. V. Krivovichev, Crystallogr. Rep., 2012, 57, 10–17.
3. M. S. Alam et al., RSC Adv., 2024, 14, 26995–27041.
4. M. C. Gallant, M. J. McDermott, B. Li and K. A. Persson, Chem. Mater., 2024, 37, 210–223.
5. Y. Zhi, Y. Jiang, D. Ke, X. Hu and X. Liu, Materials, 2024, 17, 1370.

CM-036

A Traceable Digital Thread for UAV Propulsion: MBSE Architecture Linked with Performance Simulation

Wen-Chuan, Yen[1], Yen-Cheng, Lin[1], Jen-Yo, Li[1], Po-Hung, Lin[2], Yueh-Heng, Li[1,2]*

[1]*Institute of Space Systems Engineering, National Cheng Kung University, Tainan, Taiwan, 701*

[2] *Department of Aeronautics and Astronautics, National Cheng Kung University, Tainan, Taiwan, 701*

***Corresponding author e-mail:** yueheng@mail.ncku.edu.tw

ABSTRACT

Modern engineering systems increasingly depend on advanced materials, smart devices, and rapid development cycles, making traceable digital workflows essential for turning innovations into reliable hardware. In this study, we develop a model-based digital-twin framework that serves as a computational "digital backbone" for integrating requirements, architecture, and quantitative data. We use a single-rotor Wankel rotary engine designed for fixed-wing UAV propulsion as our case study. CATIA® MAGIC with the Magic Grid methodology is employed to construct a consistent and traceable system model across requirements, functions, structures, and key parameters, all based on published engine data and previous research[1-3].

In parallel, a MATLAB-based performance model is implemented following literature frameworks to simulate pressure–volume behavior and primary performance metrics, providing numerical evidence for requirements verification. Requirements are written with standardized sentence patterns to improve completeness and testability. The resulting model-based systems engineering (MBSE) artifacts—including requirement, behavior, and structural diagrams—clearly represent subsystem interactions and parameter flows, while simulation outputs are linked back into the MAGIC model to enable direct compliance checking. This study demonstrates an initial closed-loop integration between system-level MBSE and computational simulation, offering a scalable pathway for accelerating engineering design cycles and supporting future integration of advanced materials and functional devices through a unified digital thread.

References:

1. O. A. Kutlar, F. Malkaz, Energies, vol. 12, 2019, no. 21.
2. F. Lu, N. B. Yu, "Triangular rotor engine", 1990.
3. L. Boggero, P. D. Ciampa, and B. Nagel, AIAA Aviation 2021 Forum, 2021, p. 3076.

CM-037

Graph-Splicing as a Digital Twin for Nanoscale Fabrication

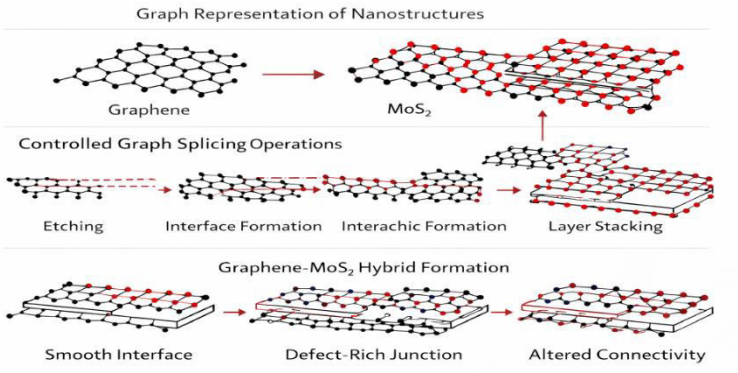
Abdul Alima.A[1], D. K. Sheena Christy[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** sheenac@srmist.edu.in

ABSTRACT

Nanofabrication of advanced functional materials and devices involves cutting, etching, joining, and recombination processes at nanometer scales, where atomic-level structure and interface topology strongly influence material performance. Although atomistic simulation approaches such as density functional theory and molecular dynamics provide high-fidelity physical insights, they are computationally intensive and limit systematic exploration of fabrication pathways. Furthermore, continuum-scale models lack the discrete structural representation required to capture topological reconfiguration during fabrication. In this work, we introduce a graph-splicing-based digital twin framework for computational modeling of nanoscale fabrication processes. Nanoscale materials are represented as graphs, with vertices corresponding to atoms and edges representing interatomic bonds, while fabrication operations such as etching, interface formation, and layer stacking are formalized as rule-based cut-and-recombine graph splicing operations. A graphene–MoS_2 hybrid nanostructure is used as a case study to demonstrate how different splicing rules encode fabrication choices and produce distinct structural outcomes, including smooth interfaces, defect-rich junctions, and altered connectivity pathways. The proposed framework supports systematic, rule-driven exploration of fabrication sequences and provides a lightweight computational layer that complements physics-based simulations, enabling pre-fabrication screening, defect analysis, and interface optimization in functional nanomaterials and nanoscale device architectures.



References:

1. Y. Xia, J. A. Rogers, K. E. Paul and G. M. Whitesides, Chem. Rev., 1999, 99, 1823–1848.
2. K. S. Novoselov et al., Proc. Natl. Acad. Sci. U.S.A., 2005, 102, 10451–10453.
3. G. Păun, Discrete Appl. Math., 1996, 70, 57–79.
4. R. Freund, G. Păun, G. Rozenberg and A. Salomaa, Theory Comput. Syst., 1999, 32, 69–112.
5. R. Rama and K. G. Subramanian, Int. J. Comput. Math., 2012, 89, 513–531.

CM-038

Rh-Doped $TiCo_{1-x}Ir_xSb$ (x = 0,0.25,0.75,1) Half-Heusler Alloys: High-Efficiency Thermoelectric Materials for Sustainable Energy Applications

Shreya Mehta[1]*, S. M. Saini[1]

[1]*National Institute of Technology, Raipur, Chhattisgarh, India, 492010*

***Corresponding author e-mail:** shreyamehta0418@gmail.com

ABSTRACT

This study aims to enhance the TE performance of half-Heusler (HH) alloys using doping strategy to enable the use of these materials for sustainable energy harvesting applications. First principles calculations are employed to systematically analyse the influence of Rh doping on the transport behaviour of $TiCo_{1-x}Rh_xSb$ (x=0,0.25,0.75,1) HH alloys. The introduction of Rh at the Co site leads to substantial changes in the electronic band structure in the vicinity of the Fermi level without compromising the semiconducting nature of the system. The mechanical stability of all investigated compositions is confirmed through the calculated elastic constants, satisfying the Born stability criteria and ensuring structural robustness under operating conditions. In addition, the optical properties, including the complex dielectric function and associated optical constants, reveal strong optical absorption and favourable dispersion behaviour over a broad energy range, indicating that Rh-substituted TiCoSb alloys are also promising for optoelectronic applications. Thermoelectric transport properties are evaluated using the Boltzmann transport equation by considering a temperature-dependent relaxation time. The Rh-doped TiCoSb alloys exhibit a substantial enhancement in thermoelectric performance, achieving a maximum conversion efficiency of approximately 15% at elevated temperatures. This improvement is primarily attributed to the combined effect of enhanced electrical transport and a pronounced reduction in lattice thermal conductivity. The calculated thermoelectric parameters show good agreement with available experimental and previously reported theoretical data on undoped TiCoSb, which validate the present approach. Overall, the results establish Rh substitution in $TiCo_{1-x}Rh_xSb$ (x=0,0.25,0.75,1) as an effective strategy for simultaneous band and phonon engineering, enabling the Rh-doped TiCo1-xRhxSb (x=0,0.25,0.75,1) HH as a multifunctional material for advanced energy conversion applications.

References:

1. B. Abdelkebir, Z. Charifi, H. Baaziz et al. Phys. B Condens. Matter, vol. 688, (2024) 416166.
2. T. Sekimoto, K. Kurosaki et al. J. Alloys Compd., vol. 394, (2005) 122–125.

CM-039

Mechanistic Insights into Gas Selectivity of Noble Metal Functionalized WO_3 from First-Principles Calculations

Ananya Garg[1], Rahul Agarwal[1], Nilesh Jaiswal[1], Gaurav Malik[2], Satyendra Kumar Mourya[1]*

[1]*Smart Material & Sensing Devices (SMSD) Lab, Department of Electrical & Electronics Engineering, Birla Institute of Technology & Science Pilani, Rajasthan 333031, India*

[2]*School of Semiconductor Science & Technology and Semiconductor Physics Research Center, Jeonbuk National University, Jeonju, 561-756, Republic of Korea*

***Corresponding author e-mail:** satyendra.mourya@pilani.bits-pilani.ac.in

ABSTRACT

Tungsten trioxide (WO_3) is widely employed in chemiresistive gas sensors; however, the mechanistic role of noble metal functionalization in governing gas selectivity and electronic response at specific crystal surfaces remains insufficiently understood. In this study, density functional theory (DFT) calculations are performed to systematically investigate the interaction of H_2, CO, CO_2, and NO_2 with pristine as well as Pt- and Pd-functionalized monoclinic WO_3 (001) surfaces. The (001) surface is selected due to its thermodynamic stability and frequent experimental relevance in WO_3-based sensing materials. All calculations are carried out using periodic slab models within the generalized gradient approximation (GGA-PBE), with full structural relaxation to ensure consistent and reliable comparison among different gas–surface configurations. Gas adsorption behavior is evaluated using adsorption energy, Bader charge transfer, and projected density of states as key sensing descriptors. Noble metal functionalization is found to significantly enhance gas–surface interactions relative to pristine WO_3, accompanied by pronounced charge redistribution and the emergence of metal-induced electronic states near the Fermi level. Clear quantitative trends are established linking adsorption strength with charge transfer magnitude and electronic structure modification, enabling prediction of sensor response polarity and relative sensitivity. Pt decoration exhibits stronger interaction with reducing gases, whereas Pd functionalization yields comparatively balanced interaction with oxidizing species, indicating distinct selectivity pathways governed by metal–adsorbate bonding characteristics. The surface-resolved, multi-gas comparative framework adopted in this work establishes direct structure property relationships that move beyond empirical noble metal selection. The predicted electronic and adsorption descriptors are directly relevant to resistance-based sensing mechanisms, providing practical guidance for experimental optimization of selective and stable WO_3-based gas sensors.

References:

1. S. Ma et al., ACS Appl. Nano Mater. 7 (2024) 15298–15307.
2. Y. Yang et al., New J. Chem. 49 (2025) 5266–5278.
3. V. C. Nguyen, H.-Y. Cha et al., Sensors 23 (2023) 3465.
4. X. Zhang, Y. Zhao et al., Nano-Micro Lett. 15 (2023) 47.

CM-040

Material-Aware Computational Modeling of VAT-Based Detumbling Control for a 3U CubeSat

Chanakarn Phoopat, Bing-Han Huang, Yueh-Heng Li*

Department of Aeronautics and Astronautics, National Cheng Kung University, Tainan, Taiwan, 701

***Corresponding author e-mail:** yueheng@mail.ncku.edu.tw

ABSTRACT

Vacuum Arc Thrusters (VATs) is a micro-propulsion device for CubeSat attitude control due to their compact architecture, solid-based furl, and ability to perform without relying on the outside environment. The conventional Attitude Determination and Control System (ADCS) usually depends on the magnetic torquer of a reaction wheel for the detumbling phase after launching the satellite. However, these devices have limitations in a deep space environment or when subjected to momentum saturation. Thruster-based detumbling using pulse plasma actuation, therefore, provides a viable alternative for post-deployment stabilization [1].

This research illustrates a simulation-based study on VAT-assisted detumbling control for a 3U CubeSat, with an emphasis on material-dependent thruster behavior and simple discrete control strategies. Copper (Cu) is adopted as the baseline cathode material, as it has been widely demonstrated in experimental VAT systems [2], while tungsten (W) is considered as a comparative material due to its higher melting point and erosion resistance reported in prior studies [3]. Material effects are incorporated through impulse-bit modeling that captures variability and degradation characteristics associated with different electrode materials.

The three-degree-of-freedom (3-DOF) rigid-body attitude dynamics model with realistic pulsed VAT actuation is developed. Two low-complexity detumbling control laws, which are Bang-Bang control and Logic-Based control, are used and evaluated under identical initial tumbling conditions. Logic-based control is widely used and follows established on-off thruster control principles, which require minimal tuning and computational effort [4]. The efficiency of two control laws is assessed in terms of angular-rate convergence, detumbling time, and firing activity.

Simulation results show that decreasing the angular rate of the satellite by using VAT is feasible under the limitation of the impulse bit constraints, and that material-dependent thrust characteristics significantly influence control performance. Bang-Bang control rapidly reduces the angular rate but results in higher firing frequency, while logic-based control exhibits improved robustness to impulse variability and material degradation.

References:

1. N. A. Gatsonis, Y. Lu, J. Blandino, M. A. Demetriou, J. Spacecraft Rockets, 53 (2016) 57–75.
2. Y.-H. Li, J.-Y. Pan, G. Herdrich,Acta Astronautica, 172 (2020) 33–46
3. J. Schein, N. Qi, R. Binder, M. Krishnan, J. K. Ziemer, J. E. Polk, A. Anders, Proc. Int. Electric Propulsion Conf. (IEPC) (2001) IEPC-01-228.

CM-041

Unlocking High Thermoelectric Performance in 2D GaN/WSeTe van der Waals Heterostructures: DFT + NEGF study

K.A. Jeeva Vergin Raj[1], D. Ramkumar[1], K Janani Sivasankar[1], D. John Thiruvadigal[1], R.M.Hariharan[1]*

[1]*Computational Materials Science and Nano Devices Simulation Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai-603 203, India.*

***Corresponding author e-mail:** hariharr@srmist.edu.in

ABSTRACT

The thermoelectric performance of Gallium Nitride (GaN) is fundamentally limited by its elevated thermal conductivity and reduced electrical conductance, thereby reducing its efficiency for power production from thermal gradients. To overcome these constraints, we propose the GaN/WSeTe vdW heterostructure (vdWHs) to reduce thermal lattice conductivity and improve efficiency. This study employs density functional theory (DFT) to investigate structural, electronic, and thermal transport properties of vdWHs. The stability of both pristine and hybrid systems has been assessed by analyzing their energy and thermodynamic stability. The adhesion energy has been computed for the hybrid system, to confirm the most stable stacking configuration of GaN/WSSe vdWHs. Among the different stacking configurations, the Se-4 and Te-3 stacking models exhibit the highest binding energies of -1192 meV and -1032 meV, respectively, and demonstrate staggered (type-II) band alignment, facilitating the separation of charge carriers at the interface. The electronic transport channels at the interface mitigate electron scattering, resulting in elevated Ge of vdWHs and intermediate thermopower between |S|GaN and |S|WSSe. The interface scattering of κph has been diminished in Se-4 and Te-3 vdWHs, resulting in ZT values of 3.61 and 2.42 at elevated temperatures (900K). The results suggest that the GaN/WSSe van der Waals heterostructure possesses considerable promise for thermoelectric applications.

Keywords: DFT, Thermoelectric figure of merit, Seebeck coefficient, vdW Heterostructure

CM-042

Machine Learning-Assisted Optimization of CdS/Zn(O,S) Window Layers for CdTe Solar Cells using SCAPS-1D.

Nihal J Dsouza[1], Mahesha M.G.[1*]

[1]*Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, 576104, India*

***Corresponding author e-mail:** mahesha.mg@manipal.edu

ABSTRACT

Parasitic absorption in the CdS window layer and carrier recombination at the heterointerface limit the efficiency of conventional Cadmium Telluride (CdTe) solar cells. This work investigates alternative window layer architectures to reduce these losses. The performance of a standard CdS/CdTe baseline device is compared with two optimized designs: a CdS/ZnO/ZnS bilayer stack and a composite window structure incorporating a linearly graded Zn(O,S) layer. Device simulations were carried out using SCAPS-1D, supported by a machine learning-assisted optimization approach. A Gaussian Process Regression model with an active learning strategy was used to explore the design space and optimize window layer thickness distributions within a fixed total thickness of 60 nm. The optimization focused on a combined efficiency-fill factor metric to balance photocurrent enhancement against resistive losses. Simulation results establish performance benchmarks for the baseline device and enable direct comparison with the proposed architectures. The CdS/ZnO/ZnS bilayer shows an increase in conversion efficiency due to improved spectral transmission, but this improvement is accompanied by a reduction in fill factor. In contrast, the CdS/graded-Zn(O,S) window architecture demonstrates superior overall performance relative to both the baseline and bilayer designs, primarily due to reduced lattice mismatch and improved spectral utilization. These results indicate that graded bandgap Zn(O,S) window layers provide a more effective route for enhancing CdTe thin-film solar cell performance than discrete bilayer structures.

References:

1. M. Burgelman, P. Nollet, and S. Degrave, Thin Solid Films, 361–362 (2000) 527–532.
2. M. Gloeckler, A. L. Fahrenbruch, and J. R. Sites, Proc. 3rd World Conf. Photovolt. Energy Convers., 1 (2003) 491–494.
3. C. E. Rasmussen and C. K. I. Williams, Gaussian Processes for Machine Learning, MIT Press (2005).
4. F. Pedregosa et al., Scikit-Learn: Machine Learning in Python (2018).
5. S. K. Sengar, Int. J. Sci. Res., 13 (2024) 662–665.

CM-043

Computational Screening of $Ti_3C_2T_x$ and $Ti_3C_2T_x$–Ag MXenes for Heavy-Metal Adsorption: Langmuir-Freundlich Isotherm Analysis in Python

Vishwas Kumar[1], Nitin K. Puri[2], Rishu Chaujar[1*]

[1] *Nanomaterials Research Laboratory (NRL), Department of Applied Physics, Delhi Technological University, Delhi, 110042, India*

[2] *National Institute of Electronics and Information Technology (NIELIT), Patna, India*

***Corresponding author e-mail:** chaujar.rishu@dtu.ac.in

ABSTRACT

The rapid growth of industrialization, urbanization, and intensive agriculture has accelerated the release of persistent and emerging environmental pollutants, including heavy metals, pharmaceuticals and microplastics, creating complex contamination pathways, long-term ecological and public-health risks. Sustainable remediation strategies are therefore required that are both high-performance and scalable. In this study, we evaluate two 2D MXenes ($Ti_3C_2T_x$ and $Ti_3C_2T_x$–Ag) as computationally favourable nanomaterials for water treatment, using Python-based isothermal adsorption modelling with synthetic equilibrium datasets generated over a wide concentration range and fitted via nonlinear regression (SciPy curve fitting) to Langmuir and Freundlich isotherms. Beyond capacity-only screening (q_{max}), we introduce mechanistically informed performance criteria to evaluate practical remediation value: (i) intrinsic surface activity via surface density (normalized adsorption capacity per BET area), (ii) thermodynamic interaction regime using adsorption enthalpy thresholds to distinguish weak physisorption, mixed/ion-exchange behaviour, and strong chemisorption and (iii) process feasibility using the Langmuir separation factor (R_l) to identify favourable adsorption conditions over concentration ranges. For pristine $Ti_3C_2T_x$, the modelled results show a broad removal spectrum and strong adsorption for Ni, Mn, Cr and Hg which is again characterized by well-defined saturation plateaus under Langmuir fitting. Overall, this fully computational framework highlights $Ti_3C_2T_x$–Ag as a high-performance candidate for As/Ni/Zn remediation and $Ti_3C_2T_x$ as a versatile sorbent across multiple metals, providing actionable isotherm parameters for adsorption-system design without requiring experimental synthesis or wet-lab testing.

References:

1. O. J. Ajala, J. O. Tijani, R. B. Salau, A. S. Abdulkareem, and O. S. Aremu, Results Eng., 16 (2022) 100671.
2. A. Kagalkar, S. Dharaskar, N. Chaudhari, V. Vakharia, and R. R. Karri, Sci. Rep., 15 (2025) 15563.

CM-044

Machine Learning Integrated MoS_2-Functionalized AlGaN/GaN HEMT for Ultra-Sensitive Mercury Ion Detection under UV illumination

Shruti Jha[1], Amit Kumar Goyal[1], Nipun Sharma[2], Adarsh Nigam*[1]

[1]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Udupi Karnataka India, 576104*

[2]*Leibniz Institute of Solid State and Materials Research, Dresden, Germany.*

***Corresponding author e-mail:** adarsh.nigam@manipal.edu

ABSTRACT

This work presents a machine-learning-enabled framework for automated qualitative and quantitative detection of Hg^{2+} ions using chronoamperometric drain-current responses from a MoS_2-functionalized AlGaN/GaN HEMT sensor operated under UV illumination, which offers ppt-level limits of detection excellent sensitivity of 548 µA/ppb. Here, time-series I_{DS} signals from blank and contaminated solutions are segmented into fixed windows and transformed into low-dimensional statistical features. Further, supervised classification models are trained to discriminate safe versus contaminated conditions. Additionally, regression models are developed to estimate Hg^{2+} concentration within the sensor's linear detection range. Window-level predictions are aggregated using majority voting to obtain robust curve-level decisions. Among the evaluated models, a Support Vector Machine with an Radial Basis Function (RBF) kernel demonstrates superior performance, achieving an accuracy of 87.04% and a curve-level accuracy of 88.89% compared to k-Nearest Neighbours and Random Forest models. Model generalization is assessed using a leave-one-group-out cross-validation strategy, ensuring robustness across distinct sensing curves. Furthermore, coarse multiclass classification is performed to enable concentration-level discrimination within the linear operating range. The proposed hybrid framework achieves high event-level classification accuracy and low regression error relative to the device limit of detection, demonstrating robust decision making under realistic noise and variability. By combining ultra-sensitive sensing response from fabricated MoS_2 functionalized AlGaN/GaN HEMT with both ML-based classification and regression, this approach advances toward intelligent, low-cost, and field-deployable mercury monitoring nodes for real-time water quality surveillance.

References:

1. Kichul Lee et al., Advanced Functional Materials, Adv. Funct. Mater. (2025) e19859.
2. Adarsh Nigam, Nipun Sharma, Dmitry Lobanov, Alexey Novikov, and Mahesh Kumar, IEEE Trans. of Elect. Dev. vol 67 (2020) page no.5693 – 5700
3. Jiao Chen, Xiaolong Xiong, Jingru Ye, Xinjia Shuai, Jun Zhou, Qingqing Liu, Cheng zhi Huang, Hui Liu, Sensor and Actuator B: Chemical, 431 (2025), 137385

CM-045

Analysing the State of Lead Halide Perovskites through 38,000 Photovoltaic Device Records

Muthuganesh M[1], Hasantheeka S[1]., Sujit Kumar*[1]

[1]*Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai-603203*

***Corresponding author e-mail:** sujitk@srmist.edu.in

ABSTRACT

Lead halide perovskite solar cells (PSCs) have achieved remarkable laboratory efficiencies, yet their industrial translation remains restricted by limited understanding of the composition–processing–performance relationship. Here, we present a large-scale meta-analysis of ~38,000 $APbX_3$ devices, classified into $MAPbI_3$, $FAPbI_3$, alternative-cation $APbI_3$, and multicomponent $APbX_3$, to identify common processing trends and critical determinants of performance. We first trace the temporal evolution of Pb-halide PSCs, consolidating key milestones into a unified and accessible framework. Energy-loss analysis highlights Pb–iodide perovskites as distinct within the halide family, exhibiting the lowest Voc losses and underscoring the need to replicate their favourable electronic structure with environmentally benign alternatives. Device-level analysis shows that high-efficiency outcomes are more frequently realized in n–i–p configurations, particularly for compositions requiring moderately high annealing temperatures, whereas achieving similar gains in p–i–n devices demands thermally robust hole-transporting layers. A comprehensive evaluation of deposition methods, solvent systems, additives, quenching strategies, annealing protocols, and processing environments identifies solvent coordination chemistry and thermal treatment as the most influential parameters governing device performance. Collectively, these findings establish a statistically robust framework for rational perovskite design, emphasizing scalable high-crystallinity film growth, composition-specific engineering, and stable interfacial designs as enablers of industrial deployment.

Keywords: Perovskite Solar cell, Photovoltaics, Efficiency, Data analysis, Processing Parameters, Feature Importance Analysis.

CM-046

Design Analysis of a 4H-SiC Trench U-MOSFET with Breakdown Point Transfer Technology

Kaustubh Pandey, Adarsh Nigam, Sunil Rathore, Amit Kumar Goyal, Pramod Martha*

Manipal institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India

***Corresponding author e-mail:** pramod.martha@manipal.edu

ABSTRACT

Power semiconductor devices form the backbone of modern power electronic systems, enabling efficient energy conversion across applications ranging from electric vehicles to renewable energy systems. Among power devices, the Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) is widely used due to its voltage-controlled operation and fast switching characteristics. Though silicon-based power MOSFETs face fundamental limitations from the properties of Si, especially the trade-off between breakdown voltage and specific on-resistance. Silicon carbide (4H-SiC) has emerged as a transformative wide-bandgap semiconductor material enabling high-voltage and high-power applications, with a critical electric field approximately ten times higher than silicon $E_{critical}$ =3.0 × 10^6 V/cm for SiC vs 2.5-3.0 ×10^6 V/cm for Si. This characteristic allows higher breakdown voltages with thinner, more highly doped drift regions and lower specific on-resistance, while its superior thermal conductivity and high-temperature capability make it suitable for demanding applications. Trench-gate U-MOSFETs offer improvements over planar devices by eliminating the JFET region resistance and increasing channel density through reduced cell pitch. Conventional Si trench MOSFETs, however, suffer from electric field crowding at trench oxide corners, limiting breakdown voltage and stressing the gate dielectric. Incorporating SiC with terminal design techniques such as breakdown point transfer (BPT) and p-shield/corner-oxide field moderation addresses these issues and improves the VB–$R_{on,sp}$ trade-off. This work presents a TCAD simulation study of an all-4HSiC trench U-MOSFET to design and validate previously reported performance improvements using calibrated wide bandgap physics models in Sentaurus TCAD. This includes detailed device design with accurate mobility and impact ionization physics. Further characterization of DC electrical behavior through transfer (I_{DS}-V_{GS}), output (I_{DS}-V_{DS}), and breakdown study is carried out. Finally, a comparison with the recently proposed devices is presented, and future device optimization possibilities are discussed.

References:

1. B. Duan, X. Yang, J. Lv, and Y. Yang, IEEE Trans. Electron Devices, vol. 65 (2018), 3388–3393.
2. B. J. Baliga, Fundamentals of Power Semiconductor Devices. New York, USA: Springer, 2008.
3. B. J. Baliga, IEEE Trans. Electron Devices, 1998.
4. H. Chen, Y. Zhang, J. Electron. Sci. Technol., 21 (2023), 100224.
5. H. Fu, Z. Wei, S. Liu et al., Microelectronics Reliability, 123 (2021), 114249.

CM-047

Machine Learning Assisted MoS_2-Functionalized HEMT for UV-Enhanced Ultra-Sensitive Hg^{2+} Detection

Shruti Jha[1], Amit Kumar Goyal[1], Nipun Sharma[2], Adarsh Nigam*[1]

[1]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Udupi Karnataka India, 576104*

[2]*Leibniz Institute of Solid State and Materials Research, Dresden, Germany.*

***Corresponding author e-mail:** adarsh.nigam@manipal.edu

ABSTRACT

This work presents a machine-learning-enabled framework for automated qualitative and quantitative detection of Hg^{2+} ions using chronoamperometric drain-current responses from a MoS_2-functionalized AlGaN/GaN HEMT sensor operated under UV illumination, which offers ppt-level limits of detection excellent sensitivity of 548 μA/ppb. Here, time-series I_{DS} signals from blank and contaminated solutions are segmented into fixed windows and transformed into low-dimensional statistical features. Further, supervised classification models are trained to discriminate safe versus contaminated conditions. Additionally, regression models are developed to estimate Hg^{2+} concentration within the sensor's linear detection range. Window-level predictions are aggregated using majority voting to obtain robust curve-level decisions. Among the evaluated models, a Support Vector Machine with an Radial Basis Function (RBF) kernel demonstrates superior performance, achieving an accuracy of 87.04% and a curve-level accuracy of 88.89% compared to k-Nearest Neighbours and Random Forest models. Model generalization is assessed using a leave-one-group-out cross-validation strategy, ensuring robustness across distinct sensing curves. Furthermore, coarse multiclass classification is performed to enable concentration-level discrimination within the linear operating range. The proposed hybrid framework achieves high event-level classification accuracy and low regression error relative to the device limit of detection, demonstrating robust decision making under realistic noise and variability. By combining ultra-sensitive sensing response from fabricated MoS_2 functionalized AlGaN/GaN HEMT with both ML-based classification and regression, this approach advances toward intelligent, low-cost, and field-deployable mercury monitoring nodes for real-time water quality surveillance.

References:

1. Kichul Lee et al., Advanced Functional Materials, Adv. Funct. Mater. (2025) e19859.
2. Adarsh Nigam, Nipun Sharma, Dmitry Lobanov, Alexey Novikov, and Mahesh Kumar, IEEE Trans. of Elect. Dev. vol 67 (2020) page no.5693 – 5700
3. Jiao Chen, Xiaolong Xiong, Jingru Ye, Xinjia Shuai, Jun Zhou, Qingqing Liu, Cheng zhi Huang, Hui Liu, Sensor and Actuator B: Chemical, 431 (2025), 137385.

CM-048

CM Finite-Difference Steepest Descent (FDSD) Method for Modeling Light Propagation in Structures with Metal Nanoparticles

Jevgenijs Kaupužs*[1], Svitlana Bugaychuk[2], Majid Taki[2], Pavels Onufrijevs[1], Oleksandra Gridyakina[3], Tomasz Wolinski[3], Janusz Parka[4]

[1]*Institute of Physics and Materials Science, Riga Technical University, Riga, Latvia, LV-1048*

[2]*PhLAN, University of Lille, Lille, France, 59655*

[3]*Faculty of Physics, Warsaw University of Technology, Warsaw, Poland, 00-665*

[4]*Faculty of Advanced Technologies & Chemistry, Military University of Technology, Warsaw, Poland, 00908*

***Corresponding author e-mail:** jevgenijs.kaupuzs@rtu.lv

ABSTRACT

We investigate light propagation in structures with regularly arranged metal nanoparticles based on Maxwell's equations for electromagnetic waves. Recently, we proposed a numerical method for solving such problems [1], which has now been substantially improved. Unlike the finite-difference time-domain (FDTD) method, which solves time-dependent wave equations, our approach directly computes stationary electromagnetic field amplitudes from a system of linear algebraic equations, offering enhanced numerical stability.In this work, we present a new and significantly more efficient solution strategy compared with the Gaussian elimination method used previously. The proposed algorithm is based on an iterative steepest descent method combined with several optimization procedures, leading to a major improvement in computational efficiency. This advancement enables the effective treatment of data-intensive problems involving reflection, scattering, and absorption of electromagnetic waves in complex structures, including solar cells and hybrid liquid-crystal devices [2]. The method is validated by demonstrating convergence to the analytical Mie solution for a spherical particle. In this benchmark test, our approach shows substantially better performance than standard FDTD simulation software.

References:

1. J. Kaupužs, et.al., Coatings, 14 (2024) 1612.
2. S. Bugaychuk, et.al., Appl. Nanoscience, 10 (2022) 4965.

CM-049

White Light Emission Generation by Engineering Dopant Stoichiometry in Metal-Organic Frameworks using FRET-Mapped Optimization and Shanno Radii Method

Christo Raymonde E[1], Selva Boopalan A[2], Shailendra K Saxena [3*], Annie Sujatha R [4*]

[1] *Department of Networking and Communications, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu Dt – 603203, Tamil Nadu, India.*

[2] *Nanophotonics Research Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu Dt – 603203, Tamil Nadu, India.*

[3] *Optical and Nano-Electronics Lab, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu Dt – 603203, Tamil Nadu, India.*

ABSTRACT

Achieving precise chromaticity control in white-light-emitting materials is traditionally an exhaustive experimental challenge due to complex, non-linear energy transfer dynamics. This work addresses this bottleneck by integrating physics-based kinetics with global optimization. Unlike traditional black-box models, our pipeline maps code components directly to established physical laws, including Förster (FRET) and Dexter transfers, Arrhenius-driven thermal quenching, and Shannon ionic radii for lattice compatibility. By co-doping Eu^{3+} and Tb^{3+} into a blue-emitting Y-MOF host, we utilize a Differential Evolution algorithm to navigate the multi-dimensional parameter space, identifying an optimal "Warm & Dry" synthesis recipe that achieves the perfect achromatic point (x = 0.33, y = 0.33). To bridge the gap between simulation and the laboratory, we implement a three-tiered validation suite addressing geometric fit, color gamut reachability, and process robustness via Monte Carlo simulations. Results demonstrate that this simulation-aided approach reduces experimental trial-and-error by over 90%. By proving that the structural similarity of Yttrium to lanthanides provides a superior "sticking coefficient" over Zn-based alternatives, this methodology offers a rigorous, translatable roadmap for the rapid discovery of stable, multi-functional luminescent materials for next-generation solid-state lighting

Keywords: Metal-Organic Frameworks, White Light Emission, Machine Learning Optimization, Lanthanide Luminescence, Energy Transfer Kinetics, Materials Discovery.

CM-050

Mechanical and Optical Properties of SnO_2 Ceramic (Sintered At 200°C, 800°C,1000°C) Calculated by Using VASP

B.Subha[1], R. Saravanan[2], N.Srinivasan[1]

[1]*Research Centre and PG Department of Physics, Thiagarajar College, Affiliated to Madurai Kamaraj University, Madurai – 625009, Tamil Nadu, India.*

[2]*Research Centre and PG Department of Physics, The Madura College, Affiliated to Madurai Kamaraj University, Madurai – 625011, Tamil Nadu, India.*

ABSTRACT

A key innovation of this work is the use of a comprehensive multi-technique characterization strategy to assess the impact of sintering on the mechanical and optical properties of tin oxide (SnO_2) ceramics. Powder X-ray diffraction (PXRD) shown that the phase observed in SnO_2 has tetragonal rutile structure and is stable at all sintering temperatures (200°C, 800°C, and 1000°C). The mechanical and optical behaviour of sintered SnO_2 samples, were investigated by performing density functional theory (DFT) calculations using the generalized gradient approximation (GGA). Key mechanical parameters such as bulk modulus, Young's modulus, shear modulus, and Poisson's ratio were determined and compared with existing literature data. The computed elastic constants satisfy the Born-Huang stability criteria, confirming mechanical stability. In addition, optical characteristics were computed, including the refractive index $n(\omega)$, the real and imaginary portions of the dielectric constant $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, the extinction coefficient $k(\omega)$, the absorption coefficient $\alpha(\omega)$, the energy loss function $L(\omega)$, and reflectivity $R(\omega)$. The acquired DFT results offer a complete understanding of the optical response of sintered SnO_2 samples and were comparable to the previous studies. Overall, this integrated multi-technique study offers a comprehensive understanding of the influence of sintering on SnO_2 ceramics, on mechanical and optical properties.

Keywords: SnO_2, sintering, DFT, GGA, VASP, Mechanical properties, Optical properties.

CM-051

Multipole Plasmonic Peaks in Metal-dielectric Nanospheres-Modelling, Tuning and Analysis

Aswathy P. Vijayan*, A.P. Jayadevan, Bindu Krishnan

P. G and Research Department of Physics, Sree Kerala Varma College, University of Calicut, Thrissur-680011, Kerala, India

***Corresponding author e-mail:** aswathy27vijayan@gmail.com

ABSTRACT

Metal core-dielectric shell nanoparticles have attracted a great amount of interest in plasmonics due to the wide tunability of the plasmon resonances. In this paper, we have investigated the optical properties of Silver-TiO_2 and Aluminium-TiO_2 core-shell nanoparticles by simulations. It is observed that as the size of the core increases, besides the dipolar contribution, other multipolar peaks begin to appear. The resonance wavelength of these multipolar peaks, as well as their full width at half maximum and relative intensity, depend on shell thickness, the size of the core, and the surrounding medium. A wide size regime of core-shell nanoparticle structure was studied. The resonance wavelength dependence on core size follows opposite trends in different size regimes and attempted theoretical explanation for the observed pattern. This is significant in understanding the underlying physical processes as well as for engineering the plasmonic peak for precisely desired applications.

References:

1. Siavash Moakhar R, Gholipour S, Masudy-Panah S, Seza A, Mehdikhani A, Riahi-Noori N, Tafazoli S, Timasi N, Lim YF, Saliba M, Advanced science, 7(2020) 1902448.
2. Li S, Miao P, Zhang Y, Wu J, Zhang B, Du Y, Han X, Sun J, Xu P, Advanced Materials, 33(2021) 2000086.
3. Al-Qadi B, AIP Adv., 14(2024) 065207.

CM-052

Electronic Structure–Driven Design of Dual-Atom Active Sites on Iridagraphene for Efficient Electrochemical CO_2 Reduction: A First-Principles Study

Smruti Mishra, Chockalingam Gopalakrishnan, Muthuramalingam Prakash*

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail:** prakashm4@srmist.edu.in

ABSTRACT

The electrochemical CO_2 reduction reaction (CO_2RR) is a promising method for transforming greenhouse gases into valuable fuels and chemicals; however, attaining high selectivity for carbon products with atomically dispersed catalysts is difficult due to scaling relationships and the competing hydrogen evolution reaction (HER). This study comprehensively examines homonuclear dual-atom catalysts (DACs) anchored on Irida-graphene, an innovative two-dimensional carbon framework consisting of 3-, 6-, and 8-membered carbon rings, utilising density functional theory (DFT). Transition metal dimers from Mn to Zn were positioned at neighbouring nitrogen-coordinated sites to assess their structural stability, adsorption characteristics, and catalytic efficacy for CO_2 reduction reactions (CO_2RR) for highly valuable products . The reaction mechanism was analysed by calculating Gibbs free energy profiles for CO_2 reduction pathways leading to HCOOH and CO formation. The dual-atom configuration induces synergistic electronic interactions between neighbouring metal centres, enabling optimised adsorption and activation of CO_2 and stabilization of key intermediates such as *COOH and *OCHO. Free energy analysis identifies the potential-determining steps and reveals reduced limiting potentials for selected DAC systems, along with suppressed hydrogen evolution reaction (HER) activity. Bader charge analysis and charge density difference (CDD) calculations demonstrate significant interfacial charge redistribution between the metal dimers and the N-coordinated Irida-graphene support, confirming strong metal–support coupling and cooperative adsorption behaviour. The balanced electron donation and back-donation mechanisms facilitate efficient CO_2 activation and intermediate stabilisation.

References:

1. Y. Ding, D. Duan, M. Wu, C. Zhang, X. Liu, Q. Liu, and Y. Zhao, Langmuir, 41 (2025) 33988–34000.
2. L. Yu, F. Li, J. Huang, B. G. Sumpter, W. E. Mustain, and Z. Chen, ACS Catal., 13 (2023) 9616–9628.

CM-053

First-principles study on structural, electronic and optical properties of mixed halide perovskites $CsPbBr_{3-y}X_y$ (X = I, Cl, F; y = 0,1,2,3) using GGA, mBJ and HSE functionals

P Mahalaxmi[1], Vasu Veerapandy[1], and Ponniah Vajeeston[2]*

[1]*School of Physics, Madurai Kamaraj University, Madurai 625021, India.*

[2]*Department of Chemistry, Center for Materials Science and Nanotechnology, University of Oslo, Oslo 0371, Norway.*

***Corresponding author e-mail:** vajeeston.ponniah@kjemi.uio.no

ABSTRACT

This study presents a comprehensive density functional theory (DFT) investigation into the structural, electronic, and optical properties of inorganic halide perovskites with the general formula $CsPbBr_{3-y}X_y$ (where X = I, Cl, F; y = 0,1,2,3). Using the Vienna Ab initio Simulation Package (VASP), electronic band structures were calculated employing several functionals: the generalized gradient approximation (GGA), Tran-Blaha modified Becke-Johnson (TB-mBJ), TB-mBJ combined with spin-orbit coupling (SOC), and the hybrid HSE06 functional. Investigated the structural and optoelectronic properties of $CsPbBr_3$ upon halide substitution with F^-, Cl^- and I^-. Structural analysis shows that the substitution of bromine with smaller halides such as fluorine (F) and chlorine (Cl) contracts the lattice, whereas iodine (I) incorporation leads to lattice expansion, consistent with relative ionic radii. The results reveal systematic trends in bandgap tuning correlating with halide substitution and composition. Incorporation of F and Cl widens the bandgap; while substituting I narrows it. These changes are attributed to differences in orbital interactions and electronegativity. Optical results indicate that F and Cl enhance dielectric stability and are suitable for UV and wide-bandgap applications, whereas substitution of iodine improves absorption and refractive index, optimizing visible-light and photovoltaic performance. These findings demonstrate that halide composition is an effective parameter for engineering the optoelectronic behaviour of $CsPbBr_3$-based perovskites.

References:

1. Selmani, Y. & Bahmad, L. *Materials Science and Engineering: B* **319** (2025) 118373.
2. Kumari, A., Nag, A. & Kumar, J. *Journal of Physics and Chemistry of Solids* **161** (2022) 110430.
3. Song, Y. & Park, *Current Applied Physics* **36** (2022) 93–96.

CM-054

Effect of Metal Based Anion in Ionic Liquid@Uio-66 MOF for Selective CO_2 Capture and Separation: A Computational Study

Mohandas Sanjay Kumar, Muthuramalingam Prakash*

Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603 203, Chengalpattu, Tamil Nadu, India.

***Corresponding author e-mail:** prakashm4@srmist.edu.in

ABSTRACT

The carbon capture from flue gases is an important step to fight global warming and climate issues due to the fact that CO_2 is consider to be a main cause for global warming [1]. In past decade researches were carried out to identify a potential candidate for CO_2 capture and separation from the flue gas. Ionic Liquids (ILs) and metal organic framework (MOF) are two well-known materials in the field of CO_2 capture [2,3]. In this work we have selected UiO-66, a Zirconium based MOF with several ILs which has common cation as $[EMIM]^+$ and various anions such as $[Cl]^-$, $[AlCl_4]^-$ and $[FeCl_4]^-$. To understand the effect of metal-based anion in CO_2 capture and its selectivity over other gases, selected ILs were impregnated in *Octahedral* (*Oh*) and *Tetrahedral* (*Td*) pores of UiO-66 [4]. It is found from calculations that the selectivity of CO_2 increases with increase in spatial confinement. Heat of adsorption of CO_2 is relatively higher for $[EMIM]^+$ $[AlCl_4]^-$ @ UiO-66 composite. Selectivity of CO_2/CH_4 and CO_2/N_2 was evaluated for selected ILs@UiO-66 composites. Our study will depict a molecular level understanding towards effective CO_2 capture and its separation.

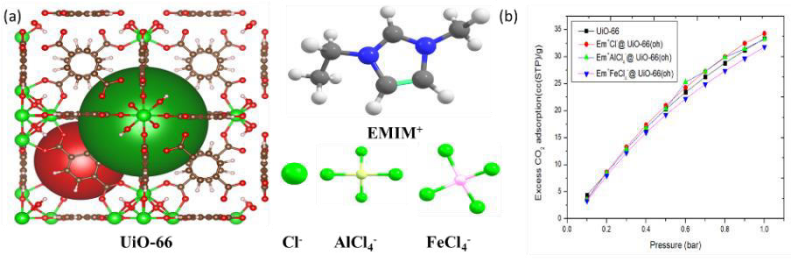


Figure 1 (a) UiO-66 with two different pores and Selected ILs, (b) Single adsorption isotherm of CO_2 on selected materials.

References:

1. X. Xia, G. Hu, W. Li, S. Li, *ACS Appl. Nano Mater.*, *2* (**2019**), 6022–6029.
2. A. Thomas, M. Prakash, *Appl. Surf. Science, 491* ***(*2019) *491***, 633-639.
3. A. Thomas, M. Prakash, *J. Phys. Chem. C*, *124* **(2020),** 26203–26213.
4. L. Valenzano, B. Civalleri, S. Chavan, S. Bordiga, M. H. Nilsen, S. Jakobsen, K. P. Lillerud, C. Lamberti, *Chem. Mater.*, *23* (**2011**), 1700–1718.

CM-055

Tuning CO_2 Activation via Choline–Amino Acid Ionic Liquids on Au (111): A First-Principles Study

Chockalingam Gopalakrishnan,[1] Mohandas Sanjay Kumar[1] and Muthuramalingam Prakash[1,2]

[1]*Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603 203, Tamil Nadu, India.*

[1,2]*Centre for Advanced Computational and Theoretical Sciences (ACTS), SRM Institute of Science and Technology, Kattankulathur - 603 203, Tamil Nadu, India.*

***Corresponding author e-mail:** prakashm4@srmist.edu.in

ABSTRACT

The efficient transformation of CO_2 into value-added chemicals is a key strategy in the pursuit of carbon-neutral technologies. Realizing this goal requires the development of sustainable and environmentally benign catalytic systems, especially within the fields of green chemistry and materials science. The biocompatible nature of ionic liquids has gained attention because of their tunable physicochemical properties, environmental compatibility, excellent recyclability, and eco-friendly character, making them suitable for CO_2 conversion into value-added products utilizing renewable energy sources. Reaction intermediates such as *COOH and *HCOO were examined, and the energy landscape was mapped using nudged elastic band (NEB) analysis. The results reveal that the interfacial environment significantly influences both the activation barriers and the stability of the transition states. This study provides a molecular-level understanding of amino acid-based ionic liquids (AA-ILs) in CO_2 conversion using first-principles approaches.

(a) (b)

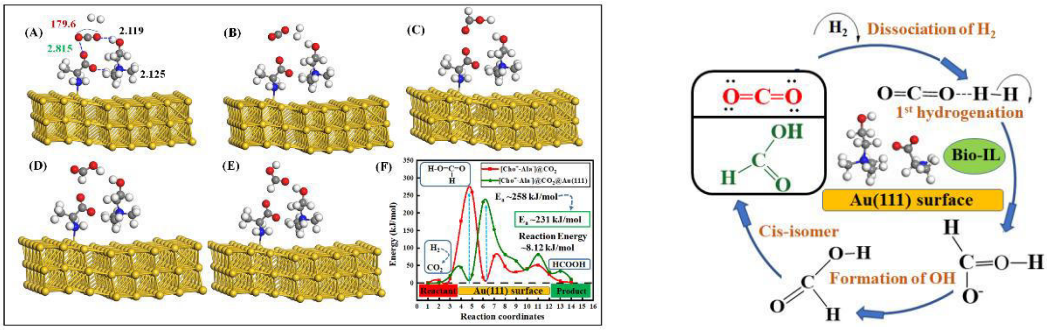


Fig. 1 (a) Simulation of the reaction mechanism between H_2 and CO_2 to form HCOOH at the Bio-IL@Au (b) Schematic diagram of the catalytic reaction mechanism.

References:

1. N. noleyy, R. Long, C. Gao and Y. Xiong, *Science China Press*, 2018, 61, 771–805.
2. N. Noorani and A. Mehrdad, *Sep. Purif. Technol*., 2021, 254, 117609.

CM-056

PEG-Functionalized Janus TiSSe Nanosheets as an Enhanced Nanoplatform for Targeted Drug Delivery

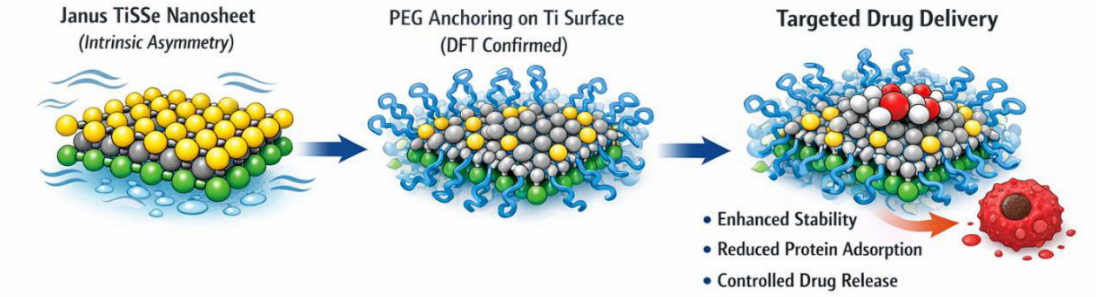
P. Sanjay[1], R. Mugunthini[1], P. Rooban[1], G. Madhumitha[1], K. Janani Sivasankar[1]*.

[1] *Computational Material Science and Nano Devices Simulation Laboratory, Department of Physics and Nano technology, SRM University, Kattankulathur, Chennai – 603 203, India.*

***Corresponding author e-mail:** jananik@srmist.edu.in

ABSTRACT

Janus transition metal dichalcogenides (JTMDs) have emerged as promising nanoplatforms for biomedical applications due to their intrinsic out-of-plane asymmetry, tunable surface chemistry, and strong drug–carrier interactions. Among them, Janus TiSSe has recently been reported as a potential drug delivery material; however, its practical translation is limited by issues related to colloidal stability, non-specific protein adsorption, and rapid clearance under physiological conditions. In this work, we present a polyethylene glycol (PEG) functionalized Janus TiSSe nanosheet system (PEG-TiSSe) designed to enhance biocompatibility, circulation stability, and drug delivery performance while preserving the inherent asymmetric properties of the Janus structure. Density Functional Theory (DFT) calculations are employed to investigate the binding energetics, charge redistribution, and electronic stability of PEG chains on Ti, S, and Se terminated surfaces, confirming preferential PEG anchoring on the Ti-rich side and enhanced surface passivation. Drug adsorption studies using a model anticancer molecule reveal that PEG functionalization maintains strong drug loading capacity while providing steric stabilization and reduced aggregation in aqueous environments. This study establishes PEG-TiSSe as an advanced Janus nanocarrier platform that overcomes key limitations of previously reported TiSSe-based drug delivery systems. The proposed functionalization strategy provides a rational pathway for tuning biocompatibility and therapeutic performance, offering new insights into the design of next-generation Janus nanomaterials for precision drug delivery.



Keywords: Janus, drug delivery, Density Functional Theory (DFT), TiSSe, polyethylene glycol (PEG).

References:

1. A.-Y. Lu et al., Nat. Nanotechnol., 12 (2017) 744–749.
2. J. Zhang et al., ACS Nano, 11 (2017) 8192–8198.
3. K. Knop et al., Angew. Chem. Int. Ed., 49 (2010) 6288–6308.

CM-057

First-Principle Investigation of NbS_2 TMDs for Two-Dimensional Drug Delivery Nanocarriers

Ragavi S[1] , Madhumitha G[1], Rooban P[1], Hariharan R M[1]*, Janani Sivasankar K[1], Preferencial Kala C[1]

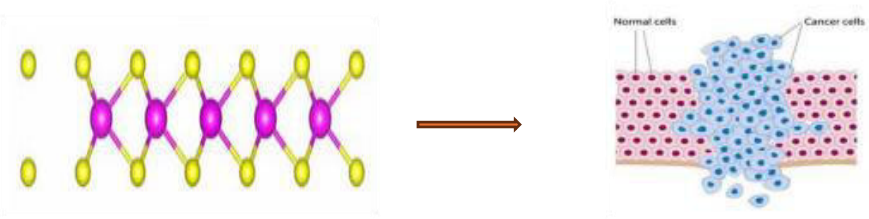
[1]*Computational Material Science and Nano Devices Simulation Laboratory, Department of Physics and Nano technology, SRM University, Kattankulathur, Chennai – 603 203, India.*

***Corresponding author e-mail:** hariharr@srmist.edu.in

ABSTRACT

Two-dimensional (2D) transition metal dichalcogenides have attracted growing interest as nanocarriers for drug delivery due to their large surface area, ultrathin structure, and versatile surface chemistry. Among them, niobium disulfide (NbS_2), a metallic 2D material, has emerged as a promising platform for biomedical applications owing to its strong near-infrared absorption and high photothermal conversion efficiency. Pristine NbS_2 nanosheets exhibit high drug-loading capacity through surface adsorption and noncovalent interactions, enabling efficient photothermally triggered drug release. However, their direct biomedical application is often hindered by limited colloidal stability and potential biocompatibility concerns in physiological environments. To overcome these challenges, functionalized NbS_2 nanocarriers, achieved via surface modification with polymers, biomolecules, or targeting ligands, demonstrate improved aqueous stability, reduced cytotoxicity, prolonged circulation time, and enhanced cellular uptake. Functionalization further enables targeted drug delivery, facilitating synergistic chemo-photothermal therapeutic strategies. While pristine NbS_2 offers simplicity and strong intrinsic photothermal performance, functionalized NbS_2 provides superior biological performance and controlled drug release. Continued investigations into long-term biosafety, biodegradation, and in vivo pharmacokinetics are essential to advance NbS_2-based nanocarriers toward effective and safe drug delivery applications.

Keywords: NbS_2,Transition metal dichalcogenides, Drug delivery.



References:

1. Q. Xu, J. Ma, W. Khan et al., Chem. Commun., 56 (2020) 6648–6651.
2. M. A. S. Sakr, H. Abdelsalam, N. H. Teleb, M. A. Saad, O. H. Abd-Elkader, Y. Liu, and Q. Zhang, J. Mol. Graph. Model., 136 (2025) 108937.

CM-058

Electro-Thermal and Process-Induced Analysis of Nanosheet FET-based Hydrogen Gas Sensors

Aravind Balaji[1], Sandeep Kumar[2], Chithraja Rajan[3], Navjeet Bagga[2], Sunil Rathore*[1]

[1]*Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India*

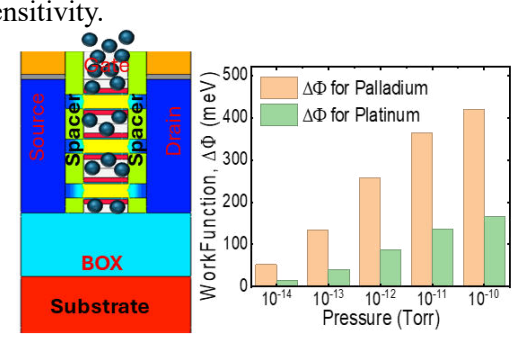
[2]*School of Electrical and Computer Sciences, Indian Institute of Technology Bhubaneswar, India*

[3]*School of Electrical and Electronics Engineering, Ramdeobaba University Nagpur, 440013 Maharashtra*

***Corresponding author:** sunil.rathore@manipal.edu

ABSTRACT

The self-heating and process variability has emerged as critical challenges in sub-5nm technology nodes, as they significantly affect the device electrical characteristics and overall sensing performance. We have investigated the combine effect of self-heating effect (SHE), interface traps concentration (ITC), and metal grain granularities (MGG) on p-Nanosheet FET (pNSFET) based hydrogen sensor. In our work, a palladium and platinum are used as a catalytic gate enables hydrogen diffusion, leading to the formation of an interfacial dipole layer that modulates the gate work function and consequently alters the sensor response. Changes in hydrogen gas concentration modify the pressure exerted on the catalytic gate, leading to a corresponding variation in the gate metal work function. Using well-calibrated TCAD models, due to consideration of self-heating effect, the lattice temperature increases to 347K, results in 5.9% drain current reduction. The sensitivity analysis i.e., V_{th}, I_{OFF}, I_{ON}, SS is investigated under different pressure conditions. Our analysis reveals that the acceptor interface trap concentration is highly susceptible to threshold voltage variations. In addition, palladium and platinum catalytic gate metals are employed to determine the most suitable material for achieving improved sensor sensitivity.



References:

1. N. Loubet et al., Proc. Symp. VLSI Technol., (2017) T230–T231.
2. S. Rathore, N. Bagga, and S. Dasgupta, Proc. IEEE Int. Reliab. Phys. Symp. (IRPS), (2024) P65.TX-1–P65.TX-4.
3. H. D. Sehgal, Y. Pratap, M. Gupta, and S. Kabra, IEEE Sens. J., 21 (2021) 13356–13363.
4. R. Lamba, R. Chaujar, and M. J. Deen, Proc. Devices Integr. Circuit (DevIC), (2025) 713–718.

CM-059

DFT Investigation on Highly Efficient Nanostructures for Bio Sensing Application

Azhagarsami T[1] , Surya S[1], Madhumitha G[1], Rooban P[1], Hariharan R M[1]*, Janani Sivasankar K[1], Preferencial Kala C[1], D. John Thiruvadigal[1]

[1]*Computational Material Science and Nano Devices Simulation Laboratory, Department of Physics and Nano technology, SRM University, Kattankulathur, Chennai – 603 203, India.*

***Corresponding Author**: hariharr@srmist.edu.in

ABSTRACT

Early diagnosis of neurodegenerative disorders such as Alzheimer's disease and Parkinson's disease remains a major clinical challenge due to the lack of non-invasive, cost-effective screening techniques. Volatile organic compounds (VOCs) present in exhaled breath have emerged as promising biomarkers reflecting metabolic alterations associated with these disorders. In this work, I propose a two-dimensional borophene based sensing platform for the selective detection of neurodegeneration-related VOCs using first-principles calculations. Density Functional Theory (DFT) simulations are performed within the framework of the Vienna Ab initio Simulation Package (VASP) to investigate borophene interaction with representative VOC biomarkers such as Styrene, 2-ethyltoluene, 3-octanone, 2-methylfuran, Carbamic acid (monoammonium salt) and Phosphonic acid, (p-hydroxyphenyl). Adsorption energies, density of states (DOS), charge density difference, and work function variations are systematically analyzed to evaluate sensitivity and selectivity. Our results are reveal strong surface reactivity and significant electronic response of borophene due to its anisotropic metallic nature and high carrier mobility. This study aims to establish borophene as a novel, highly responsive, and theoretically optimized 2D material for non-invasive breath-based detection of neurodegenerative diseases.

Keywords: Borophene, Volatile organic compounds, Neurodegenerative disorders, Non-invasive diagnostics, Biosensors

Reference:

1. N. Taşaltın, C. Taşaltın, S. Güngör, S. Karakuş, İ. Gürol, and M. Teker, J. Mater. Sci.: Mater. Electron., 33 (2022) 24173–24181.
2. N. Kumar, K. Thakur, P. Ranjan, A. Kumar, and N. Tit, Surf. Interfaces, 60 (2025) 106072.

CM-060

Ag-Doped Germanene as a High-Performance Platform for Breath-Based Detection of Lung Cancer Biomarkers: A DFT and Device-Level Investigation

Debadrita Chakraborty[1], R. Mugunthini[1], K.A. Jeeva Vergin Raj [1], B. Anitha [1], J. Sneha [1], V. Abinaya [1], U Sakthi [2], K. Santhi [3]*, R.M. Hariharan [1]*, K. Janani Sivasankar [1]*

[1] *Computational Materials Science and Nano Devices Simulation Laboratory, Department of Physics and Nanotechnology, SRM University, Kattankulathur, Chennai-603 203, India.*

[2] *Centre for AI in Health Science, School of Computing, SRM University, Kattankulathur, Chengalpattu, Chennai, TN, India,603203.*

[3] *Functional Materials and Energy Devices Laboratory, Department of Physics and Nanotechnology, SRM University, Kattankulathur, Chennai 603203, Tamil Nadu, India*

***Corresponding author e-mail**: jananik@srmist.edu.in, hariharr@srmist.edu.in, santhik@srmist.edu.in

ABSTRACT

Biosensors that translate molecular interactions into measurable electrical signals offer a promising route for non-invasive disease diagnostics. Lung cancer, a leading cause of global cancer mortality, is associated with specific volatile organic compounds (VOCs) detectable in exhaled breath. Among these biomarkers, 2-butanone and 3-hydroxy-2-butanone have been consistently reported in lung cancer patients and were selected here as target analytes. In this work, Density Functional Theory (DFT) simulations were employed to explore the structural stability, electronic properties, and adsorption behavior of transition-metal-doped germanene as a potential sensing platform. A buckled two-dimensional germanene monolayer was doped with Cu, Ag, and Au atoms to enhance its reactivity and sensing performance. Formation energy calculations confirmed the thermodynamic stability of all doped systems, with values of −5.765 eV (Ge–Cu), −5.765 eV (Ge–Ag), and −5.690 eV (Ge–Au). Adsorption studies revealed distinct interaction strengths for the selected VOCs. Notably, Ag-doped germanene interacting with 2-butanone exhibited the most favorable adsorption energy (−1.289 eV), indicating strong binding affinity and significant charge transfer, which are critical parameters for enhanced sensing sensitivity. Comparative analysis of the electronic structure further supports its superior sensing response. Based on these findings, Ag-doped germanene was selected for device-level feasibility evaluation. The integrated computational and device-oriented study highlights Ag-doped germanene as a promising candidate for selective, highly sensitive, and non-invasive breath-based lung cancer detection.

Keywords: Germanene, Metal Doping, DFT, VOC Gas Sensing, Lung Cancer Detection

References:

1. Acun *et al.*, “Germanene: The germanium analogue of graphene,” *J. Phys.: Condens. Matter*, 27, 443002, 2015.
2. K. P. Devi *et al.*, “Exploring transition metal doped germanene for enhanced glucose sensing: A DFT study on adsorption mechanisms,” *Proc. IEEE MoSICom*, 2024

CM-061

Thickness Driven Modulation of Structural, Electronic, Mechanical, Thermodynamic, and Thermoelectric Properties of 2D-Zrnisn Nanosheets

Monika S[1], Kalpana G[1]*

[1]*Department of Physics, Anna University,Chennai, Tamilnadu, India, 600025*

***Corresponding author e-mail:** gkalpa@yahoo.com

ABSTRACT

The properties of 2D materials highly depends on the thickness of the nanosheets and yet only few studies have highlighted their importance [1.2]. Here we have modulated 2D ZrNiSn nanosheets with different layer thicknesses of 0.55 Å, 0.85 Å, 1.34 Å and 1.63 Å through first-principles calculations within the frame work of Density Functional Theory as implemented in Quantum Espresso. 2D-ZrNiSn nanosheet exhibits hexagonal lattice with a space group of P-3m1.The lattice constants of 2D ZrNiSn nanosheets with different layer thicknesses are obtained by relaxing the atomic positions and lattice constants. The calculated lattice constants are found to decrease as the layer thickness increases. Studies have revealed that the mechanical and thermodynamic properties change with different layer thicknesses of nanosheets. Electronic band structure analysis demonstrate the band gap of 2D ZrNiSn nanosheets changes with layer thickness accompanied by variation in effective mass and density of states near Fermi level. Further thermoelectric properties of 2D ZrNiSn nanosheets with different layer thicknesses were calculated using the BoltzTrap code over the temperature range of 100 K to 800 K. 2D nanosheets with specific layer thicknesses have resulted in high Seebeck coefficient, power factor and ZT values. Overall, our findings provide comprehensive insight into how layer thickness governs the multifunctional properties of 2D ZrNiSn and offer guidance for designing thickness-optimized nano-electronic and thermoelectric devices.

Keyword-Layer thickness, 2D-ZrNiSn, DFT, nanosheet, Quantum Espresso.

References:

1. Hess, Peter, Nanoscale Horizons 5, no. 3 (2020): 385-399.
2. Chen, Lanli, Hongduo Hu, Aiping Wang, Yuanyuan Cui, and Zhihua Xiong, Applied Surface Science 661 (2024): 160045.

CM-062

Negative Capacitance Gate-Overlap Tunnel FET With Source Pocket Using KNN-Based Ferroelectric Parameter Extraction for Low-Power RF Applications

Sujaya Grace Ch[1], Anshul Awasthi[2], Surya Shankar Dan[2], Ramakant Yadav[1]*, Pooran Singh[1]

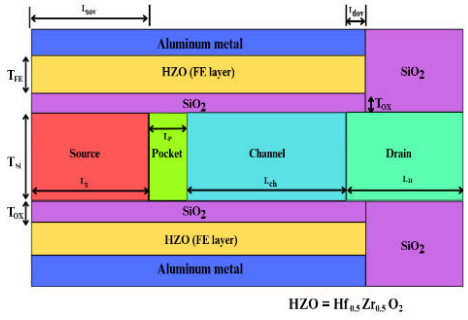
[1]*École Centrale School of Engineering, Mahindra University, Hyderabad, 500043 India,*

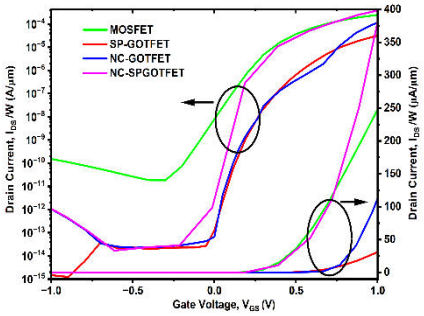
[2] *BITS Pilani, Hyderabad Campus, Hyderabad, 500078 India*

***Corresponding author e-mail:** ramakant@mahindrauniversity.edu.in

ABSTRACT

This paper presents a novel negative capacitance source-pocket gate-overlap tunnel FET (NC-SPGOTFET) for low-power RF applications. The device integrates a ferroelectric layer in the gate stack and a 3 nm source-side pocket within the channel. The source-side gate overlap enhances vertical band-to-band (BtB) tunneling, while the pocket strengthens lateral BtB tunneling at the source-channel junction, significantly improving ON-current. A fully data-driven, nonparametric modeling approach based on K-Nearest Neighbors (KNN) regression is employed to accurately capture the ferroelectric behavior of the $Hf_{0.5}Zr_{0.5}O_2$ layer integrated between the gate electrode and the SiO_2. A 3 nm drain-side gate overlap is introduced to suppress ambipolar current under negative gate bias. Using Synopsys® *Sentaurus* TCAD simulations, the results show that the NC-SPGOTFET achieves an ON-state current I_{on} of 383.4 µA, compared to 114 µA for NC-GOTFET (without a pocket) and 31.7 µA for SPGOTFET (without an NC layer), corresponding to ~3.3× and ~12× enhancements, respectively. The subthreshold swing is reduced to 44.6 mV/dec, outperforming NC-GOTFET (86.17 mV/dec) and SPGOTFET (65.38 mV/dec). The device also demonstrates strong RF performance, with a peak transconductance g_m of 1165.219 µS and a maximum unity gain frequency f_T of 588.64 GHz. In terms of ambipolar conduction, the NC-SPGOTFET exhibits an ambipolar current of (1.08×10^{-12} A), comparable to NC-GOTFET (1.04×10^{-12} A) and SPGOTFET (1.536×10^{-15} A), indicating that ambipolar conduction is effectively suppressed in the proposed NC-SPGOTFET. Overall, the NC-SPGOTFET outperforms NC-GOTFET, SPGOTFET, and conventional MOSFETs at the 32 nm technology node, highlighting its suitability for next-generation low-power RF applications.





CM-063

Design and Analysis of Dielectric Modulated Hetero-Dielectric Tunnel FET-Based Label-Free Biosensor with Enhanced Sensitivity

Jitesh Reddy R[1], Sri Sai Deep Duduka[1], Sujaya Grace[1], Sunil Rathore[2], Ramakant Yadav[1*]

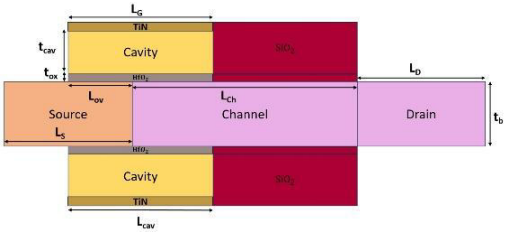
[1]*École Centrale School of Engineering, Mahindra University, Hyderabad, 500043 India,*

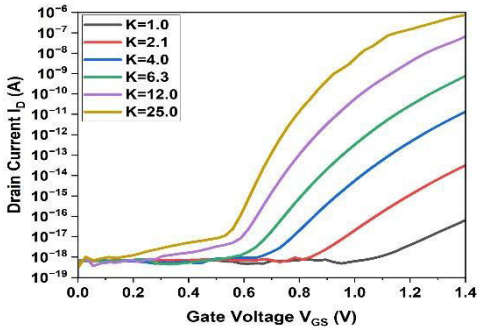
[2] *BITS Pilani, Hyderabad Campus, Hyderabad, 500078 India*

***Corresponding author e-mail:** ramakant@mahindrauniversity.edu.in

ABSTRACT

This paper presents a comprehensive investigation of a dielectric-modulated hetero-dielectric tunnel FET (DM-HD-TFET) and demonstrates enhanced sensitivity for biomolecule detection. To increase ON-state current, reduce leakage current, improve sensitivity, and enhance overall device performance, the design incorporates dual insulators—high-κ HfO_2 on the source-channel side and low-κ SiO_2 on the channel-drain side. The proposed structure enhances band-to-band tunnelling at the source–channel junction in the ON-state while suppressing it at the drain–channel junction in the OFF-state, leading to higher I_{ON} and lower I_{OFF}. A critical aspect of this study is the analysis of the gate overlap on the source side and hetero-dielectric in the oxide region to improve the performance of the proposed sensor. The use of titanium nitride (TiN) as a gate metal optimizes energy band bending at the tunnelling junction, thereby increasing the I_{ON}/I_{OFF} ratio and enhancing device sensitivity. Using the Synopsys® *Sentaurus* TCAD tools, the device characteristics and sensing capabilities of the DM-HD-TFET were evaluated via dielectric modulation for the detection of various charged and neutral biomolecules. The simulation results indicate exceptional sensing performance: when detecting Gelatine (K = 12), the DM-HD-TFET achieves a current sensitivity of 1.05×10^{9}. Furthermore, for charged amino acids such as Lysine or Arginine (K = 25), the device demonstrates a superior current sensitivity of 1.16×10^{10}. The device also exhibits a high I_{ON} /I_{OFF} switching ratio of 1.04×10^{12}, making the proposed DM-HD-TFET an excellent candidate for high-sensitivity, label-free biosensing applications.





References:

1. P. Harika, G. G. Sravani, S. S. Rao, and A. L.-E. Kille, IEEE Trans. Nanobiosci., 24 (2025) 25–36.
2. B. V. Krishna et al., Silicon, 14 (2022) 10893–10899.

CM-064

Size-Dependent Π-Metal Interactions on Gold Nanoclusters: A DFT Study of Aromatic Adsorption from Benzene to Graphene

Masiyappan Karuppusamy[1] and Muthuramalingam Prakash[1,2*]

[1]*Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603 203, Tamil Nadu, India.*

[2]*Centre for Advanced Computational and Theoretical Sciences (ACTS), SRM Institute of Science and Technology, Kattankulathur – 603 203, Tamil Nadu, India.*

***Corresponding author e-mail:** prakashm4@srmist.edu.in

ABSTRACT

Understanding interfacial interactions between π-conjugated systems and metal nanostructures is essential for designing advanced functional materials for sensing, catalysis, nanoelectronics, and optoelectronic applications. In this work, density functional theory (DFT) simulations implemented in the CP2K package were used to investigate the adsorption behavior of representative aromatic molecules-benzene, naphthalene, anthracene, and phenanthrene on Au_{144} nanoclusters. To examine trends associated with increasing π-surface area, additional calculations were performed for benzene, coronene, dodecacoronene, and graphene fragments interacting with the same gold cluster model. Geometry optimizations and adsorption energy analyses reveal a systematic increase in binding strength with increasing molecular size and planarity, highlighting the dominant roles of dispersion and π-metal coupling interactions. Larger polyaromatic systems show stronger stabilization due to increased contact area and cooperative van der Waals interactions with the cluster surface, whereas smaller aromatics exhibit comparatively weaker but stable physisorption. Electronic structure analysis indicates minimal charge transfer between the adsorbates and the gold cluster, confirming that adsorption is governed primarily by noncovalent interactions rather than chemisorption. Comparative trends across molecular and extended π-systems reveal a gradual transition from localized adsorption behaviour to surface-like interaction regimes as conjugation length increases. These findings provide atomistic-level insight into how molecular size, conjugation, and interfacial contact govern adsorption on noble metal nanoclusters. The results establish predictive design guidelines for tailoring metal-organic hybrid interfaces relevant to functional nanomaterials and device architectures. Overall, this study demonstrates the effectiveness of CP2K-based first-principles simulations for accurately describing weak interfacial interactions that are critical to next-generation advanced functional materials.

References:

1. M. Prakash et al., Phys. Chem. Chem. Phys., 26 (2024) 17489-17503.
2. Alvaro Munnoz-Castro et al., J. Phys. Chem. C, 120, (2016) 7358-7364.

CM-065

Selective Detection of Ovarian Cancer Biomarkers Using Atomically Engineered Black Phosphorene Nanosheets

Ramkumar D[1], Jeeva vergin raj K A, C. Preferencial Kala[1, *], Hariharan R M,

[1]*Centre for Materials Sciences and Nanodevices, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203, India.*

***Corresponding author e-mail:** *preferec@srmist.edu.in*

ABSTRACT

Early-stage diagnosis of ovarian cancer is critically limited by the absence of sensitive, non-invasive screening technologies. The analysis of disease-associated VOCs in exhaled breath is a promising diagnostic route; however, success depends on sensor materials that can differentiate chemically similar analytes with high precision. This work focuses on developing a nanoscale sensing platform with enhanced sensitivity and reliable selectivity for key ovarian cancer VOC biomarkers, including 2-butanone, decanal, and nonanal. To uncover the sensing mechanism and assess stability against interfering gases (H_2O and CO_2), we used van der Waals corrected DFT + NEGF transport calculations to analyse adsorption behavior and electronic response on metal-functionalized black phosphorene. We found that pristine black phosphorene interacts only weakly with the VOCs, exhibiting low adsorption energies (E_{ads}) that limit its practical sensing capability. In contrast, metal functionalization with Au, Ag, and Cu markedly enhances molecular binding. Among all configurations, Cu@BP shows the strongest affinity, with adsorption energies of -0.82 eV for 2-butanone, -0.68 eV for decanal, and -0.65 eV for nonanal, respectively. Charge-transport analysis demonstrates that Cu-decorated black phosphorene exhibits a markedly enhanced sensing response, with conductance modulation reaching 84 - 100%, whereas pristine black phosphorene shows only modest variations in the range of 4 - 48%, while rapid recovery at room temperature further confirms excellent reversibility and reusability of the sensor. Overall, these results establish Cu-decorated black phosphorene as a promising nano sensing platform for the selective and non-invasive detection of ovarian cancer-related VOC biomarkers.

Keywords: DFT+NEGF, Black phosphorene, ovarian cancer, adsorption energy

CM-066

Decoupling Thermal and Electronic Transport in a Monolayer Mg-Based Ternary chalcogenides for Enhanced Thermoelectric Performance

Shamiyubtha Shiri R[1], Kathirvel V[1*]

[1]*SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** kathirvv@srmist.edu.in

ABSTRACT

Two-dimensional (2D) materials have emerged as promising candidates for high-performance thermoelectrics due to their ability to decouple electrical and thermal transport, thereby enhancing the thermoelectric figure of merit (zT). Unlike conventional three-dimensional (3D) bulk materials such as Bi_2Te_3, whose performance is constrained by intrinsically coupled transport properties, 2D systems enable nanoscale engineering strategies that significantly suppress lattice thermal conductivity (κ_l) without degrading electronic transport. Enhanced phonon scattering at surfaces and interfaces, combined with strong out-of-plane anisotropy, reduces κ_l to values approaching ~1 $Wm^{-1} K^{-1}$ while preserving favourable Seebeck coefficients and electrical conductivity. Among emerging 2D thermoelectric materials, chalcogenide-based systems are particularly attractive due to their tunable electronic structure, bond heterogeneity, and the presence of lone-pair electrons, which promote strong anharmonic phonon scattering and ultralow lattice thermal conductivity. We perform a comprehensive first-principles investigation of Mg-based ternary 2D chalcogenide materials (MgX_2Se_4) to evaluate and optimize their thermoelectric performance. The electronic transport properties were calculated using the Boltzmann transport formalism as implemented in BoltzTraP2, while phonon dispersion and lattice thermal conductivity were obtained from third-order anharmonic force constant calculations using Phono3py. The absence of imaginary modes in the phonon dispersion confirms the dynamical stability of the material. These chalcogenides are narrow-bandgap semiconductors exhibiting favourable electronic transport properties for thermoelectric applications. The elastic properties were evaluated using the ElaStic code, and the results indicate mechanical stability. The low lattice thermal conductivity of MgX_2Se_4 suggests that these materials are promising thermoelectric candidates and motivates further experimental investigation.

References:

1. Shuwei Tang, Journal of Materiomics 10 (2024) 1004e1016.
2. Mingkai Li, Journal of Alloys and Compounds 931 (2023) 167586.

CM-067

Solvation-Driven Tuning of Electronic Structure and Photovoltaic Performance in Purpurin Isolated from *Rubia cordifolia* for Dye-Sensitized Solar Cells: An Integrated Experimental and DFT/TD-DFT Study

Buvaneswari.V[1], S. Begam Elavarasi[1*]

[1]*Anna University, Chennai, Tamilnadu, India - 600 025*

[*]**Corresponding author e-mail:** elavarasi.begam@gmail.com

ABSTRACT

Natural anthraquinone dyes have attracted considerable attention as environmentally benign sensitizers for dye-sensitized solar cells (DSSCs). In this work, purpurin isolated from *Rubia cordifolia* was systematically investigated to elucidate the solvation-driven tuning of its electronic structure and photovoltaic performance. The molecular structure and optical characteristics were experimentally validated using UV–Vis and FTIR spectroscopy, and the results were correlated with density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations. A comprehensive computational analysis was performed under various protic and aprotic solvent environments employing the polarizable continuum model (PCM) to understand solvent-induced modulation of frontier molecular orbitals, energy gap, dipole moment, and excited-state transitions. Key photovoltaic descriptors, including light-harvesting efficiency (LHE), reorganization energy (λ), electron injection free energy (ΔG_{inject}), dye regeneration energy (ΔG_{reg}), and open-circuit voltage (V_{oc}), were calculated to predict photo-conversion efficiency trends. The results reveal that solvent polarity significantly influences HOMO–LUMO alignment relative to the conduction band edge of TiO_2, thereby modulating charge injection dynamics and recombination probability. Aprotic solvents demonstrate improved energetic alignment and reduced reorganization energy, indicating enhanced electron-transfer characteristics. This integrated experimental and theoretical investigation provides molecular-level insight into solvent-assisted charge-transfer mechanisms and establishes rational guidelines for optimizing bio-derived sensitizers in DSSC applications.

References:

1. Zorgani, R. N. E. H., Lebsir, F., Reguig, F. H., Zorgani, M. A., Adda, A., Bounaceur, B., & Rérat, M. (2026). DFT and TD-DFT Investigation of π-Conjugated Organic Donors for Solar Cells: Electronic, Optical, and Photovoltaic Properties. *ChemistrySelect*, *11*(2), e05771.
2. Singh, R., Sharma, K., Elavarasi, S. B., & Guin, M. (2024). Exploring the impact of tailored π-linkers on perovskite solar cell efficiency: a computational study in triphenylamine-based hole transport material design. *Optical and Quantum Electronics*, *56*(6), 1002.
3. Abdelaaziz, A., Bouzzine, S. M., & Hamidi, M. (2024). Computational investigation of dyes-sensitized solar cells containing various π-bridges achieving high photovoltaic performance with triazatruxene-based dyes. *Journal of Photochemistry and Photobiology A: Chemistry*, *447*, 115192.

CM-068

Transforming Waste into Infrastructure: Evaluation of High Temperature Strength and Structural Stability of Fully Waste Pavement Blocks

Ananya Pal[1*], Jajneswar Biswal[2], Tushar Gupta[2].

[1]*Department of Chemical Engineering, National Institute of Technology Rourkela, India*

[2]*Department of Mining Engineering, National Institute of Technology Rourkela, India.*

***Corresponding author e-mail:** pal.ananya17@gmail.com, 224ch3001@nitrkl.ac.in)

ABSTRACT

This experimental study investigates the thermal performance and strength characteristics of plastic modified pavement blocks prepared using fly ash, slag, lime, sand, and varying percentages of plastic waste. The primary focus of the investigation was to determine the residual compressive strength of the pavement blocks after heat treatment. Pavement block specimens were produced by incorporating plastic at three different content levels such as 3%, 5%, and 7% by weight, while maintaining consistent proportions of the other constituents. The materials were thoroughly mixed, moulded into block specimens, and allowed to cure under controlled conditions for a fixed period of 14 days before thermal exposure to ensure adequate strength development and matrix stabilization. To evaluate the influence of elevated temperatures on structural integrity, the manufactured blocks were subjected to heat treatments at 130^0C, 160^0C, and 190^0C for exposure durations of 1, 3, 6, 12, and 24 hours. The variation in plastic content was designed to assess its role in thermal stability and bonding behaviour within the composite matrix. At the same time, the different temperature and time combinations simulated potential high temperature service or environmental conditions. Strength testing was conducted to identify any degradation, deformation, or performance changes resulting from thermal exposure. The results provide insight into the relationships among plastic percentage, heat exposure conditions, and post-treatment strength performance, thereby evaluating the feasibility of using plastic-modified materials in durable, thermally stable pavement applications.

Keyword: Sustainable pavement material, Durability assessment, Optimization, Green building materials, Waste plastic utilization, High-temperature exposure.

CM-069

Optimizing FFD 3D Printer Parameters for Printing of Bio-inspired Xylotus Lattice Structure using Taguchi Approach

Radhika Chada*, Ranjith Kumar A

Department of Mechanical Engineering, Kakatiya University, Telangana, 506009

***Corresponding author e-mail:** radhikareddy.chada@gmail.com

ABSTRACT

The growing demand for lightweight and energy-efficient polymer components has stimulated attention in bio-inspired lattice structures drawn from natural systems[1]. In this study, a novel hybrid lattice structure, labelled Xylotus as shown in Fig.1., stimulated by the tubular architecture of xylem and the cellular skeleton of lotus, was designed and built using Fused Filament Deposition (FFD). A Taguchi L27 design was employed to assess the effects of influenced parameters such as raster angle, layer thickness, infill density, and printing orientation at three levels on compressive performance of printed component. Quasi-static compression tests were performed as per ASTM D1621 standards to study deformation mechanisms and energy absorption behaviour [2]. The results show that energy absorption is varied not only by architectural design but also by manufacturing- induced parameters such as interlayer bonding quality, porosity, and defect distribution result from process parameter adoption. The optimized Xylotus configuration exhibited progressive buckling and enhanced specific energy absorption of 50.06J/kg, demonstrating the effectiveness of hybrid bio-inspired designs for lightweight, high-performance structural applications.

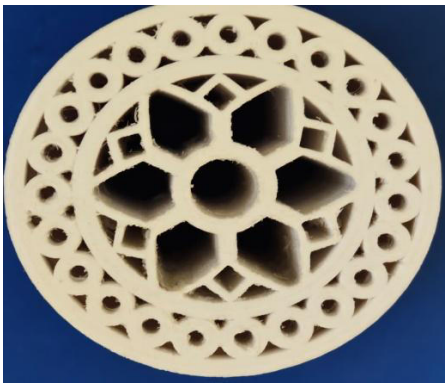


Figure.1. Bio Inspired Xylotus Structure for Compression Test Sample

References:

1. G. Chouhan, B. M. Gunji, P. Bidare, D. Ramakrishna, R. Kumar, *Experimental and numerical investigation of 3D printed bio-inspired lattice structures under quasi-static loading,* Materials Today Communications, 35 (2023) 105658.
2. O. A. Calleja, B. H. Gonzalez, N. L. Lacalle, S. Martinez, J. Albizuri, A. Lamikiz, A new approach in the design of microstructured ultralight components to achieve maximum functional performance,Materials, 14 (2021) 1588.

CM-070

Electron Spin Resonance-shift of Gadolinium ion in p-type $Sn_{1-x}Gd_xTe$ ($0.0005 \leq x \leq 0.01$) Diluted Magnetic Semiconductor

Satya Bishnu Panigrahi, Sashi S. Behera*

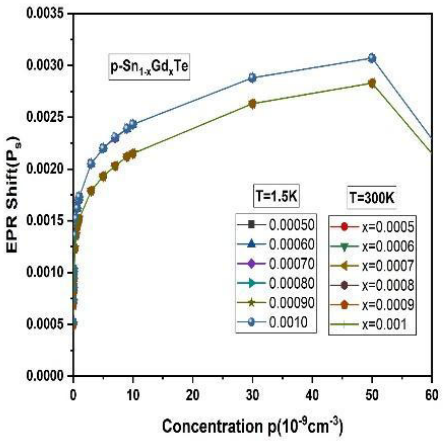
Department of Physics, Berhampur University, Bhanja Bihar, Berhampur, 760007

Corresponding author e-mail:- sashisekhar10@gmail.com

ABSTRACT

In this communication, we calculate the band dispersion and related parameters in p-type $Sn_{1-x}Gd_xTe$ by taking into account the 6-level energy band structure and simulated energy band gap as a function of Gadolinium impurity from T=1.5K to T=300K. The energy dispersion is parabolic at $k \rightarrow 0$ and away from k it could be describable by a non-parabolic band dispersion of 4^{th} order in k. Under effective mass representation, an equation of motion is derived in the presence of spin-orbit interaction, an external magnetic field, and a magnetic impurity. The hybridized exchange interaction between magnetic impurity and carrier and that of the external magnetic field and the carrier is used in the $\vec{k}.\vec{\pi}$ perturbation approach. Here, we derive the expression for (EPR) shift (Ps) by using Green's function perturbation expansion in the presence of spin-orbit interaction and external magnetic field in effective mass representation. To get around the problem of loss of translational symmetry in magnetic vector potential in the presence of the magnetic field Green's function is redefined in terms of Peierl' phase factor. Here we have made an extensive study of the spin EPR shift of Gd^{+3} ion in p-type $Sn_{1-x}Gd_xTe$ for several impurity concentrations from x = 0.0005 to x = 0.01 from temperature T=1.4K to T=300K. Lastly, we analyze the EPR shift and other electronic parameters and their anisotropies in p-type $Sn_{1-x}Gd_xTe$ as functions of carrier concentration and Gd impurity from T=1.5K to T=300K. We report the EPR shift is 3.0×10^{-3} for $p=5\times10^{20}cm^{-3}$ in contrast to the experimental observation 4.6×10^{-3} in the system. The discrepancy might be due to the decrease in the density of states at Fermi energy at L-band which results from the increase in density of states at Σ−band for high hole concentrations $p \geq 5 \times 10^{20}cm^{-3}$. The calculated EPR shift shows considerable anisotropy due mainly to the spin-orbit interaction.

Keywords: *$\vec{k}.\vec{\pi}$ method, spin-orbit interaction, 6-level band structure, Bumped band edge structure, Green's function, Effective g factor, spin-EPR shift*



CM-071

Magnetization Reversal in the Presence of Spin Textures in a Synthetic Antiferromagnet

Mani Bharathi Manickavasagam[1], T. Perarasan[1], Priyanka Babu[1], Jaivardhan Sinha[1]*

[1]*Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** jaivardr@srmist.edu.in

ABSTRACT

Chiral magnetic spin textures in the synthetic antiferromagnet (SAF) attract the interest of spintronics and magnetism communities for their robustness and the low-power requirement for data processing [1]. In our work, we present the magnetization reversal of typically designed SAF nanotrack with a narrow track on the left and a wider track on the right. For this, we study the hysteresis behaviour in the presence as well as absence of spin textures in SAF along the easy axis of the system using the micromagnetic simulation tool, UBERMAG integrated with the Object Oriented Micromagnetic Framework (OOMMF) [2]. The material parameters of the system we considered are similar to that of Co/Pt. Interestingly, we notice that the nucleation field for the magnetization reversal is relatively higher when the system contains no spin textures in it and this field decreases rapidly when the spin textures are present in it. The reversal occurs at a faster rate in the order of: presence of skyrmions > presence of domain wall pair > absence of any spin textures in SAF. Further, we explore the conversion of a domain wall pair to a skyrmion in the SAF system, in the absence of external magnetic bias field. We find that this conversion mechanism is different from the one observed in ferromagnet because of the RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction between the ferromagnetic layers of SAF. The stabilized skyrmion has the diameter of ~25 nm and the net topological charge estimated for whole nano track remain zero. Our findings and analysis offer comprehensive insight into the current understanding of spin textures as information carriers in many spintronic applications.

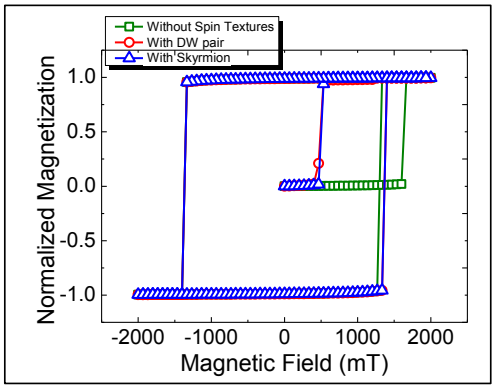


Fig. 1. represents the hysteresis behavior of SAF in the absence and presence of spin textures

Keywords: Magnetization reversal; Synthetic Antiferromagnet; Domain Wall; Skyrmion

References:

1. T. Dohi, *et al.*, *Nat Commun*., 10, 5153 (2019)
2. H. Fangohr, *et al., AIP Adv*., 14, 1 (2024)

CM-072

DFT study on the Structural and Electronic Properties of $Mg_xCa_{1-x}FeSiO_4$ as a Cathode for Magnesium–Ion Battery

Astha. E[1], V. Sudha[1*]

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India.*

***Corresponding author e-mail:** sudhav1@srmist.edu.in

ABSTRACT

The pursuit of high energy density, cost-effectiveness, and superior safety features renders the rechargeable magnesium ion battery (RMI) an enticing prospect for the next era of battery technology. The concept of providing higher energy density from the divalent charge of the magnesium ion has brought a desire for the development of magnesium ion batteries. Nevertheless, the observed low energy density in MIBs can be enhanced by improving the structure of cathode materials to overcome the limited diffusivity of Mg^{2+} ions in the electrode. This can be achieved through approaches such as modifying the material morphology, doping, and substituting heteroatoms into the materials. In the current study, we considered the olivine structured $MgFeSiO_4$ and intermixing of non-transition metal cation viz. $Mg_xCa_{1-x}FeSiO_4$ as a cathodic candidate. The suitability of these materials was analysed by carrying out their structural optimization, electronic properties, and charge transfer studies. Also, Molecular Dynamics simulations were performed to investigate the thermal stability and the dynamical behaviour of the system at finite temperature.

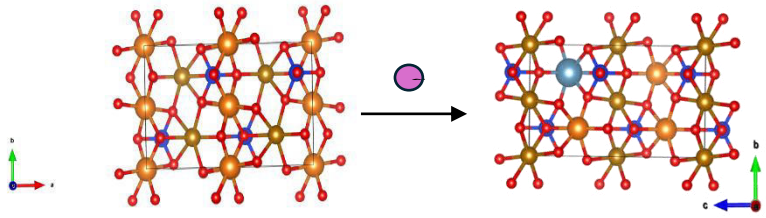


Figure: Olivine-type structure of $MgFeSiO_4$, where orange, Silver, brown, blue, and red spheres indicate Mg, Ca, Fe, Si, and O atoms, respectively.

References:

1. Jennifer Heath, Hungru Chen, M. Saiful Islam, $MgFeSiO_4$ as a potential cathode material for magnesium batteries: ion diffusion rates and voltage trends, *J. Mater. Chem. A*, 2017, 5, 13161
2. Yuki Orikasa, Titus Masese, Yukinori Koyama, Takuya Mori, Masashi Hattori, Kentaro Yamamoto, Tetsuya Okado, Zhen-Dong Huang, Taketoshi Minato, Ce´dric Tassel, Jungeun Kim, Yoji Kobayashi, Takeshi Abe, Hiroshi Kageyama & Yoshiharu Uchimoto, High energy density rechargeable magnesium battery using earth-abundant and non-toxic elements, *Sci. Rep*, 2014, 4, 5622.

CM-073

Molecular Dynamics Insights into Microstructure and Mechanical Behavior of PBSA/PHBH Biopolymer Blends for Sustainable Packaging

Vaishnu Suresh Kumar[1,2], Fugen Daver[2], Mohit Garg*[1]

[1]*Department of Chemical Engineering, Birla Institute of Technology and Science (BITS), Pilani Campus, Vidya Vihar, Pilani, 333031, Rajasthan, India*

[2]*School of Science, RMIT University, Bundoora, Victoria 3083, Australia*

***Corresponding author e-mail:** mohit.garg@pilani.bits-pilani.ac.in

ABSTRACT

Blending biopolymers is an economical and practical strategy to tailor the properties of biodegradable materials for sustainable packaging applications. The performance of polymer blends is governed by their phase microstructure and interfacial characteristics[1], whose detailed characterization often requires sophisticated experimental techniques and costly instrumentation. Experimental approaches such as electron microscopy, scattering techniques, and advanced spectroscopy can provide valuable information on blend microstructure, but these methods may be limited in their ability to directly probe molecular-scale interactions and phase evolution. In this context, molecular dynamics (MD) simulations can serve as a computational microscope to directly observe the microstructures formed during polymer blending and relate them to macroscopic properties, providing complementary molecular-level insight that is difficult to obtain experimentally[2,3]. In this study, MD simulations were employed to investigate blends of poly(butylene succinate-co-butylene adipate) (PBSA) and poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (PHBH) at different compositions. These biodegradable polyesters are widely considered promising materials for sustainable packaging applications due to their favourable mechanical performance and biodegradability. The simulations successfully reproduced experimentally observed blend microstructure, revealing an immiscible system characterized by droplet–matrix structures across the composition range investigated. PBSA exhibited partial miscibility in PHBH-rich compositions, consistent with experimental observations reported for related biopolymer blends. The simulations further indicate that the interfacial surface area between PBSA and PHBH domains plays an important role in determining the mechanical and viscoelastic behaviour of the blends. In particular, the Young's modulus increased with increasing PHBH content, indicating a strong composition dependence of the mechanical response. These findings highlight the capability of MD simulations to capture realistic blend microstructure and establish structure–property relationships in biodegradable polymer blends, providing molecular-level insight that can support the design and optimization of next-generation sustainable packaging materials.

References:

1. Righetti, M.C., Cinelli, P., Aliotta, L., Bianchi, E., Tricoli, F., Seggiani, M. and Lazzeri, A.. *Polymer International*, *71*(1) (2022), pp.47-56.
2. Bejagam, K.K., Iverson, C.N., Marrone, B.L. and Pilania, G., 2020. *Physical Chemistry Chemical Physics*, *22*(32), pp.17880-17889.
3. Jena, S.S., Suneesh, S., Kumar, V.S., Garg, M. and Ghosh, S, *ACS Applied Polymer Materials*, *7*(19)(2025), pp.12897-12911.

CM-074

Effect of Clay Nanomaterials on the Nanoscale Morphology of poly(benzimidazobenzophenanthroline) BBL: A Molecular Dynamics Study

Isha Chauhan[1], Sarbani Ghosh[1], Mohit Garg[1]*

[1]*Department of Chemical Engineering, Birla Institute of Technology and Science (BITS), Pilani, Rajasthan 333031, India*

***Corresponding author e-mail:** mohit.garg@pilani.bits-pilani.ac.in

ABSTRACT

Conducting polymers are an important class of materials that find applications in a variety of electronic and energy devices such as printed electronics, batteries, neuromorphic systems, solar cells, and flexible organic electronics. The performance of these devices strongly depends on the nanoscale morphology and molecular orientation of polymer chains, which is strongly influenced by the surrounding environment. Layered materials such as clays can act as confining surfaces that regulate polymer packing and ordering, leading to different structural arrangements such as intercalated, exfoliated, or stacked morphologies. In the present study, we investigate the nanoscale morphology of the n-type conducting polymer poly(benzimidazobenzophenanthroline) (BBL) in the presence of tallow-modified functional clay nanoparticles. The introduction of lamellar layered clays into the conjugated polymer system creates a nanoscale confinement that regulates polymer packing, backbone orientation, and interfacial interactions. We performed molecular dynamics (MD) simulations to study how the nature of the clay surface influences polymer packing and orientation. Cloisite-Na promotes stronger interfacial interactions that favor more ordered arrangements of BBL chains, whereas the organically modified Cloisite-15A provides a relatively flexible environment that allows different stacking configurations. The degree of functionalization further modulates the transition between the orientations of the polymer backbone relative to the clay surface. Such confinement-induced structural changes directly influence the stacking and orientation of the polymer chains, thereby affecting the potential charge transport pathways within the system. This work gives a molecular-level insight into how clay chemistry and functionalization regulate the polymer orientation and nanoscale morphology under confinement, offering design principles to tailor charge transport in BBL-based hybrid materials.

Keywords: Conducting polymers; poly(benzimidazobenzophenanthroline) (BBL); molecular dynamics (MD); nanoscale morphology.

CM-075

Functional $CuMoO_4$/f-CNF Nanocomposites for Machine Learning–Assisted Electrochemical Pesticide Monitoring

Balaji Ramachandran[1]*, Saranvignesh Alagarsamy[2], Kommuru Bhargava Venkata Sai Arun Kumar[1] and Ying-Chih Liao[2]*

[1]*Department of Electronics and Communication Engineering, Koneru Lakshmaiah Education Foundation, Andhra Pradesh, 522302, India*

[2]*Department of Chemical Engineering, National Taiwan University, Taiwan*

ABSTRACT

A machine learning–assisted electrochemical sensing platform was developed using a $CuMoO_4$/f-CNF (copper molybdate/functionalized carbon nanofiber) nanocomposite for the detection of the fungicide carbendazim (CBZ). $CuMoO_4$ was integrated with a conductive f-CNF matrix to combine redox activity with efficient electron transport. The nanocomposite was systematically characterized to confirm its structural integrity and interfacial compatibility. Electrochemical properties of the modified electrode were evaluated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), revealing enhanced charge-transfer behavior and improved electroactive surface characteristics. Electrode optimization for CBZ detection was performed using CV to achieve stable and sensitive electrochemical responses.

To improve concentration prediction and analytical reliability, machine learning models including k-nearest neighbours (KNN), linear regression, random forest, and support vector machine (SVM) were applied to correlate electrochemical signals with CBZ concentration. The optimized sensing platform achieved a low limit of detection of 0.0027 µM with a sensitivity of 0.564 µA μM^{-1}. The practical applicability of the sensor was demonstrated through successful analysis of environmental samples with satisfactory recovery. This study demonstrates the effectiveness of combining functional metal–carbon nanocomposites with data-driven machine learning approaches for accurate and reliable pesticide detection in environmental monitoring applications.

Key Words: $CuMoO_4$/f-CNF; Electrochemical sensor; carbendazim; machine learning models; environmental monitoring.

BM-001

Mechanical properties of polymer/natural infill composite fabrication by FDM process

Akthar H, Susindharan N, Vijay B, Ravi Kumar K*

Karpagam College of Engineering, Coimbatore, Tamilnadu, India, 641032

***Corresponding author e-mail:** hod.mech@kce.ac.in

ABSTRACT

Fused deposition modelling is an additive manufacturing technology for fabricating parts using thermoplastic filaments. PLA is popular because it is easy to print and biodegradable. Compositing wood dusts to PLA also economical and is environmental-friendly. The application of wood dust on the reinforcement of PLA filament is the subject matter presented herein. It includes single screw extrusion, compounding, drying and mixing. The pressure command also considers handling, diameter control and filament drawing. Process factors that affect quality: the Z value, cooling, print speed, nozzle temperature. Element surface modifications and polymer choice improve particle adhesion. Wettability and strength as printing parameters are based on dispersion, the loading, and particle size. Tests that reflect mechanical trends are tensile, flexural and impact tests. Test procedures that are transparent, controlled compounding and regular drying are one of the proposals. Standards, life cycle information and industrial trials should be the primary areas of investigation.

Keywords: Natural Fibers, Woven Composites, Hygrothermal Aging, Durability, Kenaf, Banana, Sisal, Mechanical Properties.

References:

1. M. M. Hanon, L. Zsidai, and Q. Ma, Materials Today: Proceedings (2021) 3089–3096.
2. D. Rahmatabadi, I. Ghasemi, M. Baniassadi, K. Abrinia, and M. Baghani, Journal of Materials Research and Technology 21 (2022) 3970–3981.
3. G. Gamon, Ph. Evon, and L. Rigal, Industrial Crops and Products 46 (2013) 173–185.
4. S. Bhagia, et al., Applied Materials Today 21 (2020) 100832.
5. A. Boucherit, M.-N. Avettand-Fènoël, and R. Taillard, Materials & Design 124 (2017) 87–99.

BM-002

Enabling Visible Light Driven Chemo-Photodynamic Therapy and Imaging of Cancer Cells by pH-sensitive CD-Metal Organic Gel

Sayani Maiti[1], Susanta Banerjee[2]*, Narayan Ch. Das[3]*

[1]*School of Nano Science and Technology, Indian Institute of Technology Kharagpur, Kharagpur 721302, India*

[2]*Materials Science Centre, Indian Institute of Technology Kharagpur, Kharagpur 721302, India*

[3]*Rubber Technology Centre, Indian Institute of Technology Kharagpur, Kharagpur 721302, India*

***Corresponding author e-mail:** susanta@matsc.iitkgp.ac.in

ABSTRACT

This work introduces a stimulus-responsive, biodegradable drug delivery platform designed to achieve targeted cancer therapy with reduced side effects. The system is built around a Fe-based metal–organic coordination gel (MOG) featuring a highly porous structure that enables efficient drug loading and promotes Fenton-type reactions for cancer cell elimination. Synthesized through a simple, eco-friendly process, the MOG exhibits peroxidase-like catalytic behaviour under visible light, enhancing its therapeutic efficacy. Carbon dots (CDs), prepared hydrothermally, are incorporated to provide fluorescence imaging and facilitate real-time cellular tracking. The anti-cancer drug 5 fluorouracil (5 FU) is encapsulated with an excellent loading capacity of 72.9%. The platform ensures controlled, pH-responsive drug release, minimizing premature leakage and lowering toxicity to healthy cells. Under 450 nm visible light, Fe^{3+} ions released in acidic tumor environments are photo reduced to Fe^{2+}, which reacts with intracellular H_2O_2 to produce hydroxyl radicals (HO•). These reactive species induce oxidative damage to vital biomolecules, suppressing cancer cell growth. Cellular uptake and MTT assays confirm selective cytotoxicity toward folate-positive HeLa cells, with reduced effects on less folate-expressing MDA-MB-231 cells and non-cancerous L929 cells. Overall, this multifunctional system synergistically combines pH-responsive chemotherapy, light-triggered photodynamic activity, and imaging capability, highlighting its strong potential for advanced cancer treatment.

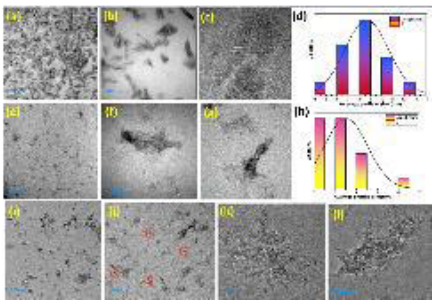


Fig. 1 [(a), (b), (c)] are the TEM image of CD (d) average particle size distribution curve for CD, [(e), (f), (g)] are the TEM image of MOG, (h) average particle size distribution curve for MOG, [(i), (j), (k), (l)] are the TEM image of CD-MOG.

Keywords: carbon dot (CD), metal organic gel (MOG), photo dynamic therapy (PDT).

References:

1. Wei, Qiang, and S. L. James. Chemical communications, 12 (2005): 1555-1556.
2. Lin, Haitao, et al, Royal Society open science, 5.5 (2018): 172149.

BM-003

A Review on Antibacterial Growth Control in Additive Manufacturing Using Chromium–Cobalt Materials

K Arun Kumar[1], Arvind Krishnan V[1], Jeevansri G[1], Arun S[1]*

[1]*Karpagam College of Engineering Coimbatore-641032*

***Corresponding author e-mail:** arunkumar.k@kce.ac.in

ABSTRACT

Modern production has changed significantly due to additive manufacturing (AM), enabling the fabrication of complex geometries and customized components for engineering and biomedical applications. However, the inherent surface porosity and layer-by-layer deposition in AM parts promote bacterial adhesion and biofilm formation, posing challenges to hygiene and long-term performance. To mitigate this issue, the incorporation of antibacterial agents into AM materials has gained increasing research attention. Among various metallic additives, chromium (Cr) and cobalt (Co) exhibit strong potential owing to their high mechanical strength, corrosion resistance, and intrinsic antibacterial properties. This review investigates the antibacterial mechanisms of chromium–cobalt systems, including metal ion release, oxidative stress induction, and surface energy modulation. Recent advancements in material synthesis strategies—such as nanoparticle incorporation, alloy reinforcement, and surface functionalization are discussed to highlight their role in enhancing antimicrobial efficiency. Comparative analysis with silver-, copper-, and zinc-based antibacterial additives demonstrates the superior durability, thermal stability, and controlled cytotoxicity of Cr–Co composites. Furthermore, key challenges such as nanoparticle agglomeration, cytotoxicity management, and preservation of printability are addressed. Overall, chromium–cobalt-based additive manufacturing materials show strong promise for next-generation biomedical implants, surgical instruments, and hygienic engineering components with improved safety, durability, and sustainability.

References:

1. S. Acharya, R. Soni, S. Suwas, and K. Chatterjee, Journal of Materials Research (2021).
2. B. AlMangour, M. Luqman, D. Grzesiak, H. Alharbi, and F. Ijaz, Mater. Sci. Eng. A (2020).
3. T. A. Alwattar, H. Abdulhadi, A. Al-Yasari, and A. Mian, Journal of Elastomers & Plastics (2025).
4. S. F. Anderabi, et al., Studia Universitatis Babeș-Bolyai Chemia (2025).
5. A. Arjunan, J. Robinson, A. Baroutaji, M. Martí, A. Tuñón-Molina, and Á. Serrano-Aroca, bioRxiv (2021).

BM-004

Modeling and Analysis of Dielectric Elastomer Actuator for Underwater Propulsion

Vinod Kumar[1] and Sujoy Mukherjee[1]*

[1]*PDPM IIITDMJ, Jabalpur, Madhya Pradesh, India, 482005*

***Corresponding author:** sujoy@iiitdmj.ac.in

ABSTRACT

Electroactive polymers are the material that demonstrates large strain in response to electric field. Actuator made from the electroactive polymer shows the capacities like an animal muscle so they are called as artificial muscles. Use of dielectric elastomer actuator for underwater propulsion can be used for different purposes. It can be seen from the literature that the previous works have been done on body and caudal fin for a fish. Therefore, the current work focuses on the modelling and fabrication of a pectoral fin-based propulsion actuated by a dielectric elastomer actuator. This is because of the fact that pectoral fins can be used for up and down movement, side to side movement etc. A dielectric elastomer made from an acrylic foam tape (VHB 4910 by 3M) used as main constitute material and conductive carbon grease 846 used as compliant materials. Copper tape used for electrical wiring connection. Flexible PET plastic substrate used for giving proper shape and size. A scotch magic tape used for giving stiffness to the actuator as pre-stretching is required for VHB tape for obtaining high actuation pressure. The CAD model of pectoral fins and caudal fin are drawn and designed in SOLIDWORKS software and two prototype one with only pectoral fins and in other prototype pectoral fins equipped with caudal fin.

Keywords: Electroactive Polymer, Actuator, Artificial Muscle, Dielectric Elastomer, Propulsion, Pectoral Fin

References:

1. Yaguang Guo, Liwu Liu,Yanju Liu, and Jinsong Leng, Advanced Intelligent Systems, 3 (2021) 2000282
2. Jun Shintake, Vito Cacucciolo, Herbert Shea, and Dario Floreano, Soft Robotics, 5 (2018) 466-474.
3. Bangyuan Liu, Feiyu Chen, Sukai Wang, Zhiqiang Fu, Tingyu Cheng, Tiefeng Li, J. Appl. Mech, 84 (2017) 091005.

BM-005

Optimizing Chitosan Extraction from *Squid Gladius* for Advanced Biomaterials in Cartilage Regeneration

Faraaz Ahamed[1], Saranya Srinivasan[1], Lokesh Saravanan[1], Ashwathi Vijayalekha[1], Ashok Kumar Pandurangan[1]*

[1]*School of Life Sciences, B.S. Abdur Rahman Crescent Institute of Science and Technology, Vandalur, Chennai – 600 048*

***Corresponding author e-mail:** panduashokkumar@gmail.com

ABSTRACT

Cartilage damage resulting from trauma, degenerative diseases, or congenital defects remains a significant clinical challenge due to the limited regenerative capacity of the tissues. Existing treatments, including grafts and synthetic implants, often face issues such as immune rejection and poor integration with host tissue. This study aims to develop a novel composite scaffold for cartilage tissue engineering using chitosan extracted from *Squid gladius*, Hydroxyapatite (HAP), and the bioactive phytocompound *Diosgenin* (DN). Chitosan (CH), valued for its biocompatibility and biodegradability, was extracted through optimized processes and characterized using FTIR and XRD. HAP was incorporated to enhance structural stability and osteo-conductivity, while *Diosgenin* was selected for its chondroprotective and anti-inflammatory properties. The fabricated scaffold underwent biochemical characterization, including swelling analysis, porosity assessment, biodegradability studies and other physicochemical studies (FTIR, XRD, SEM and TGA). Furthermore, *in-vitro* biocompatibility assays were conducted to assess its potential for cartilage regeneration. A network pharmacology approach identified key target genes modulated by *Diosgenin*, and molecular docking studies were performed to analyse its interactions with inflammatory and cartilage-related proteins. The results suggest that this chitosan-based scaffold, reinforced with HAP and *Diosgenin*, holds significant promise for cartilage repair. By utilizing seafood waste, this study also offers a sustainable approach to regenerative medicine.

Keywords: Chitosan, *Squid Gladius*, *Diosgenin,* Cartilage Regeneration, MG-63 cells.

References:

1. J. C. Valdoz, et al., Int. J. Mol. Sci. 22 (2021) 12690.
2. M. Rahimi, et al., Int. J. Biol. Macromol. 215 (2022) 346–367.
3. A. R. Bastos, et al., Int. J. Biol. Macromol. 271 (2024) 132611.

BM-006

The effect of abrasives in Dynamic Chemical polishing of Additive Manufactured Features

Dhananjayulu Avula[1,2], Satyanarayana Maddilate[2], Ravi Sankar Mamilla[1]*

[1]*Department of Mechanical Engineering, Indian Institute of Technology Tirupati, Andhra Pradesh, India, 517619.*

[2]*Department of Mechanical Engineering, S V Government Polytechnic, Tirupati, India, 517501*

***Corresponding author e-mail**: evmrs@iittp.ac.in

ABSTRACT

Laser Powder Bed Fusion (LPBF) has emerged as one of the most advanced additive manufacturing techniques for producing stainless steel components with high geometric precision and design freedom. In this study, SS 316L samples were fabricated using LPBF to evaluate surface improvement strategies for as-built parts. A key limitation of the LPBF process is the inherently rough surface finish, which results from the solidification dynamics of the melt pool and the presence of partially melted or unmelted powder particles fused to the surface. These surface irregularities adversely affect the mechanical, and tribological performance of the fabricated components, making post-processing essential. To address this challenge, a dynamic chemical polishing technique was employed to enhance the surface quality of LPBF-produced SS 316L samples. The results demonstrated a substantial reduction in surface roughness (Sa) after chemical polishing compared to the as-built condition, confirming the effectiveness of the method in achieving a smoother and more uniform surface. However, extending the polishing duration beyond the optimized timeframe led to a gradual increase in roughness, likely caused by non-uniform etching or excessive material dissolution. These findings highlight the need for precise control and optimization of chemical polishing parameters to ensure consistent and high-quality surface refinement in LPBF-fabricated SS 316L components.

Keywords: Laser Powder Bed Fusion; Chemical Polishing; Surface finish.

BM-007

Effect of Hygrothermal Aging in Oil, Distilled Water, Saline Water and HCL Acid on the Mechanical Behaviour of Kenaf, Banana and Sisal Woven Fiber Composites

Adhiarumugam R, Kathir T, Manoj Kumar M, Arulmurugan R*

Karpagam College of Engineering, Coimbatore, Tamilnadu, India, 641032

***Corresponding author e-mail:** arulmuruganraju@gamil.com

ABSTRACT

Natural-fiber composites made from kenaf, banana, and sisal offer lightweight, low-cost, and eco-friendly alternatives to synthetic composites, but their durability in real environments is limited. This study examines their aging behaviour under hygrothermal exposure to distilled water, saline water, oil, and hydrochloric acid. Both Fickian and non-Fickian diffusion were observed, allowing moisture and chemicals to penetrate the matrix, causing swelling, fiber expansion, interfacial debonding, and in severe cases, hydrolysis. Degradation severity followed the order: HCl > saline > distilled water > oil. The fiber–matrix interface proved most vulnerable, leading to major reductions in tensile, flexural, and impact properties. Dynamic mechanical analysis showed decreased storage modulus, increased damping, and shifts in glass transition temperature. Although water-aged specimens regained some strength after drying, microcracking limited full recovery. Durability can be enhanced through fiber treatments, compatibilizers, matrix modification, hybridization, and reduced void content. These findings support the development of more resilient woven natural-fiber composites for practical applications.

Keywords: Natural Fibers, Woven Composites, Hygrothermal Aging, Durability, Kenaf, Banana, Sisal, Mechanical Properties.

References:

1. A. Bachchan, P. P. Das, and V. Chaudhary, Mater. Today: Proc., 49 (2022) 3403–3408.
2. M. R. M. Asyraf et al., Cellulose, 28 (2021) 2675–2695.
3. S. O. Amiandamhen, M. Meincken, and L. Tyhoda, Fibers Polym., 21 (2020) 677–689.
4. M. Assarar et al., Mater. Des., 32 (2011) 788–795.
5. H. A. Aisyah et al., Polymers, 13 (2021) 471.

BM-008

Comparative Biomechanical Study of Natural and Synthetic Materials in Femoral Analysis Using FEA

Naveen Kumar[1]*, M Muruganandam[2], Balasa Munesh[1], R Bharath[1], P Rajesh[1]

[1]*Kuppam Engineering College, Kuppam, Andhra Pradesh, India, 517425*

[2]*Karpaga Vinayaga College of Engineering and Technology, Kolambakkam, Tamilnadu, India, 603308*

***Corresponding author e-mail:** naveenkumargulbarga@gmail.com

ABSTRACT

The femur is the longest and strongest bone of the human body and plays a critical role in weight-bearing and locomotion. Its biomechanical evaluation is therefore essential for advancing orthopedic implant design and reducing implant-related complications. In this study, a three-dimensional femur model was reconstructed in CATIA V5 and analyzed using finite element analysis (FEA) in ANSYS Workbench to investigate stress distribution, elastic strain, and total deformation under physiological loading conditions. Six materials were considered: cortical bone, trabecular bone, titanium alloy (Ti-6Al-4V), stainless steel (316L), polyether ether ketone (PEEK), and ultra-high molecular weight polyethylene (UHMWPE). A compressive load of 2100 N, approximating three times body weight during gait for a 70 kg subject, was applied at the femoral head while the distal condyles were constrained. Results revealed that metallic alloys, particularly Ti-6Al-4V, exhibited minimal deformation (<0.001 mm) and uniform stress transfer, confirming their suitability for load-bearing applications. However, the high stiffness of stainless steel posed risks of stress shielding. In contrast, polymers such as PEEK and UHMWPE demonstrated higher deformation (0.0001–0.0004 mm) but mechanical compatibility closer to natural bone, thereby reducing stiffness mismatch. Trabecular bone showed the greatest deformation (0.0007 mm) and strain (1.7×10^{-4}), consistent with its function as a shock absorber, while cortical bone exhibited minimal strain (5.0×10^{-6}). Unlike previous studies that primarily investigated bone tissues or individual implant materials, this work presents a consolidated comparative evaluation of natural and synthetic biomaterials, offering new insights into trade-offs between strength, flexibility, and long-term biomechanical compatibility. These findings emphasize the importance of material selection in femoral implants, balancing structural stability against the risk of stress shielding and long-term remodeling.

References:

1. D. R. Carter and W. C. Hayes, J. Bone Joint Surg., 59A (1977) 954–962.
2. R. Huiskes and E. Y. S. Chao, J. Biomech., 16 (1983) 385–409.
3. M. Viceconti, S. Olsen, L. P. Nolte, and K. Burton, Clin. Biomech., 20 (2005) 451–454.
4. B. Helgason, F. Taddei, H. Pálsson, E. Schileo, L. Cristofolini, M. Viceconti, and S. Brynjólfsson, Med. Eng. Phys., 30 (2008) 444–453.
5. L. Cristofolini, J. Biomech., 43 (2010) 314–320.

BM-009

Fabrication of Diglycolic Anhydride - Functionalized G-C_3N_4/PVA Hydrogel Incorporated with Selected Plant Extract and Silver Nanoparticles for Enhanced Antibacterial and Wound Healing Application

Harini A[1], Ilaiyaraja Perumal[2]

[1]*Department of Chemistry, School of Advanced Science, Vellore Institute of Technology Chennai Campus, Tamil Nadu, 600127, India*

[2]*Centre for Advanced Materials and Innovative Technologies (CAMIT), Vellore Institute of Technology Chennai Campus, Tamil Nadu, 600127, India*

ABSTRACT

Photocatalytic sterilization has proven to be an effective approach for eliminating harmful microorganisms, highlighting the importance of developing photocatalytic antibacterial hydrogels for skin wound treatment. This study introduces a novel hydrogel composed of PVA/ diglycolic anhydride- functionalized graphitic carbon nitride, enhanced with bioactive component and silver nanoparticles, which exhibits significant antibacterial activity against Escherichia coli (E.coli). The hydrogel was synthesized using a cyclic freeze-thaw method. X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, field emission scanning electron microscopy (FESEM), and other basic characterization were used to examine the structure and morphology of the synthesized hydrogels. The mechanical properties of the hydrogel, including its adhesion, tensile strength, and anti-fatigue strength, were evaluated. The hydrogels demonstrated strong antibacterial effects against non-pathogenic Escherichia coli (E.coli) bacteria. Furthermore, the hydrogel exhibited excellent wound-healing abilities, as evaluated by an in vitro scratch assay using the 3T3L1 cell line. The biocompatibility of the hydrogel was studied using MTT assay. In conclusion, the synthesized hydrogel exhibited effective bactericidal activity, wound healing potential, and exceptional mechanical properties, which could significantly improve wound healing. This study provides novel insights into the development of photocatalytic antibacterial hydrogel materials.

Keywords: Photocatalytic antibacterial hydrogel, wound healing, antibacterial, nano silver

BM-010

Drug-Loaded 3D-Printed Cellulose–Alginate Scaffolds Fabricated from Waste Cotton for Soft Tissue Engineering Applications

Jayendran Udaiappan[1], Krithika Sudhakar[2], Gobisarvanan Kaliaraj[1]*

[1]*Centre of Excellence for Additive Manufacturing, Sathyabama Institute of Science and Technology, Chennai – 600119.*

[2]*Prince Shri Venkateshwara Arts and Science College, Chennai – 600073.*

***Corresponding author e-mail:** gobisaravanan@sathyabama.ac.in

ABSTRACT

Cellulose nanoparticles (CNP) have gained attention in the field of biomedicine and healthcare applications because of their excellent biocompatibility, biodegradability, durability and outstanding mechanical properties. In the present study, composite scaffolds composed of sodium alginate and cotton waste–derived cellulose nanoparticles (CNP), incorporated with antibiotic salt, were fabricated using extrusion-based 3D printing. Scanning electron microscopy results revealed that the printed scaffolds exhibit interconnected porous structure. X-ray diffraction result confirms the crystalline phase of the synthesized CNP. Fourier transform infrared spectroscopy results confirms the intermolecular interactions between the polymer matrix and the antibiotics. The developed 3D scaffold exhibited excellent thermal stability confirmed by thermogravimetric analysis, which is due to the CNP. Antibacterial evaluation revealed effective microbial inhibition of 80% against both Staphylococcus aureus and Escherichia coli by the printed scaffolds and cytocompatibility assays confirmed the scaffolds were non-toxic and compatible with bone cells. The 3D-printed sodium alginate/CNP scaffolds integrate architectural precision with improved antibacterial and biological performance, making them promising candidates for soft tissue engineering.

Keywords: Cellulose nanoparticles, 3-D printed scaffolds, Biomaterials, Tissue engineering

BM-011

Synthesis and characterization of Chitosan/ strontium Titanate/PVA based Triboelectric Nanogenerator for Energy Harvesting Applications

Sanket A. Anandea, R. S. Gedam*

Department of Physics, Visvesvaraya National Institute of Technology, Nagpur- 440010, India

***Corresponding author e-mail:** rupesh_gedam@rediffmail.com

ABSTRACT

The global energy challenge and environmental concerns have groomed the TENG as a promising technology for grasping mechanical energy from the environment and to convert it into electrical energy. Enhancing the output performance of TENG is the key challenge due to the limited number of triboelectric materials. This study proposes an enhanced flexible TENG featuring a cubic and flower structure composed of strontium titanate/chitosan/polyvinyl chloride (Sr-chitosan/PVA) for wireless monitoring of human finger taping signals. Contact separation structure was constructed by varying morphology (cubic and flower) of strontium titanate, the surface of the positive triboelectric layer film, significantly increasing its contact area and surface roughness. Further incorporation of chitosan derived from crab shell enhanced the electrical output performance of the TENG through synergistic effects with a triboelectric effect. The corresponding TENG achieved electrical output performance of 228 V and 198 µA. The TENG based on this design can collect minute mechanical signals generated when a human hand taps.

References:

1. S. Wang, X. Mu, X. Wang, A. Y. Gu, Z. L. Wang, and Y. Yang, ACS Nano 9, 9554 (2015).
2. S. Hajra, M. Sahu, A. M. Padhan, J. Swain, B. K. Panigrahi, H. G. Kim, S. W. Bang, S. Park, R. Sahu, and H. J. Kim, J. Mater. Chem. C 9, 17319 (2021).

BM-012

Biological Assessment of Carboxymethyl Chitosan-based Scaffold for Pulp-Dentin Engineering Applications

Balasubramanian Saravana Karthikeyan[1]*, Sekar Mahalaxmi[1], M. Madhana Madhubala[1], G. Rajkumar[2], V. Dhivya[3], Anil Kishen[4]

[1]*Department of Conservative Dentistry and Endodontics, SRM Dental College, Bharathi Salai, Ramapuram, Chennai-600 089, SRM Institute of Science and Technology, Tamil Nadu, India.*

[2]*Department of Physics, Easwari Engineering College, Chennai-600 089, Tamil Nadu, India.*

[3]*Department of Biotechnology, Easwari Engineering College, Chennai-600 089, Tamil Nadu, India.*

[4]*Faculty of Dentistry, University of Toronto, Ontario M5G 1X3, Canada.*

***Corresponding author e-mail:** saravanb@srmist.edu.in

ABSTRACT

Traditional pulp biomaterials like calcium hydroxide and mineral trioxide aggregate (MTA) primarily control infection and inflammation, resulting in reparative dentin rather than complete regeneration, highlighting the need for advanced tissue-engineered scaffolds. This study aimed to synthesize and characterize a carboxymethyl chitosan (CMC) biopolymeric scaffold and evaluate its biological response in-vivo and pulp capping efficacy in in-vivo animal model. CMC scaffolds fabricated by freeze-drying were characterized using SEM-EDX, XRD, and FTIR, while cytocompatibility (MTT assay) and biomineralization potential (ALP, OPN, DSPP, and DMP-1 expression by RT-qPCR over 21 days) were assessed using dental pulp stem cells. In vivo efficacy was evaluated by orthotopic placement in Wistar rat molars, with histological assessment of dentin bridge formation over three months and MTA as a positive control, followed by statistical analysis using one-way ANOVA and Tukey's post-hoc test ($p < 0.05$). The CMC scaffold exhibited a porous amorphous structure with characteristic functional groups, high cytocompatibility, significant upregulation of dentin-specific genes, and formation of a well-organized odontoblastic layer with a thicker calcific bridge compared to MTA, indicating its potential as a promising alternative material for pulp–dentin regeneration.

Keywords: Carboxymethyl chitosan; scaffold; dentin regeneration; pulp capping

References:

1. B. Saravana Karthikeyan, and S. Mahalaxmi., Int. J. Biol.Macromol, 270 (2024) 132359.
2. B. Saravana Karthikeyan, M.M. Madhubala, G. Rajkumar, V. Dhivya, A. Kishen, N. Srinivasan, S. Mahalaxmi. Int J Biol Macromol, 271 (2024) 132620.

BM-013

Biocompatible Magnesium Ferrite Nanoparticles for Magnetic Fluid Hyperthermia Therapy

Dhanashri S. Kolte[1], Vishwajeet M. Khot[2], Atula U. Patil[1], Ashwini B. Salunkhe[1]*

[1]*Department of Physics, Rajaram College, Kolhapur, 416004, MS, India.*

[2]*Department of Medical Physics, Centre for Interdisciplinary Research, D. Y. Patil Education Society, Kolhapur, 416006, MS, India.*

***Corresponding author e-mail:** vasusalunkhe@gmail.com

ABSTRACT

A straightforward solid-state combustion approach has been used to synthesize magnesium iron oxide nanoparticles (MgF). In combustion synthesis, fuel and adiabatic flame temperature are the most scalable parameters. The effect of egg white fuel on structural and magnetic properties was studied in detail. In the present investigation, egg white shows interesting magneto–structural as well as thermal properties due to higher gas evolution, biogenic content in it, which assists the material towards biocompatibility, and shows rapid combustion as compared to reported conventional chemical fuels. The average crystallite size calculated with the plane (311) of MgF is 21.2±3.1 nm. High-resolution transmission electron microscope (HR-TEM) results confirm the formation of smaller particles with an average particle size of 19.2±2.1 nm. Saturation magnetization (Ms) values obtained from the vibrating sample magnetometer (VSM) are found to be 29.5 emu/g for Egg white. The specific absorption rate (SAR) for the sample prepared with egg white fuel is determined to be 216.63 W/g for 2 mg/mL. The hemolysis activity and antioxidant assay are carried out to study the physiologically safe administration of synthesized MgF to the human body in the near future. The anti-microbial activity was analyzed to study the functional property for their use in various biomedical and environmental applications.

References:

1. P. Heidari and S. M. Masoudpanah, J. Mater. Res. Technol., 9 (2020) 4469–4475.
2. S. E. Hassan, A. Fouda, E. Saied, M. M. Farag, A. M. Eid, M. G. Barghoth, M. A. Awad, M. F. Hamza, and M. F. Awad, J. Fungi, 7 (2021) 372.
3. A. Salunkhe, V. Khot, S. I. Patil, S. A. Tofail, J. Bauer, and N. D. Thorat, ACS Appl. Bio Mater., 3 (2020) 2305–2313.
4. V. M. Khot, A. B. Salunkhe, N. D. Thorat, R. S. Ningthoujam, and S. H. Pawar, Dalton Trans., 42 (2013) 1249–1258.
5. T. P. Patil, A. A. Vibhute, S. L. Patil, T. D. Dongale, and A. P. Tiwari, Appl. Surf. Sci. Adv., 13 (2023) 100372.

BM-014

Artificial Synaptic Functions and Resistive Switching in Al-Doped ZnO/Polymer Nanocomposite Based Transparent and Flexible Memristors

Kazi Md Jahirul Hassan[1], Pranab Kumar Sarkar[2], Tapas Mondal[1], Subhodeep Barman[3],Suranjan Sikdar[4], Rahul Das[1]*

[1]*Department of Physics, The University of Burdwan, West Bengal,India*

[2]*Department of Applied Science and Humanities, Assam University, Silchar, Assam*

[3]*Department of Physics, Gangarampur College, West Bengal, India*

[4]*Department of Chemistry, Ghani Khan Choudhury Institute of Engineering and Technology, Malda, India*

***Corresponding author e-mail:** rdas@phys.buruniv.ac.in

ABSTRACT

We demonstrate organic memristive devices fabricated using Azadirachta indica leaves extract-based green synthesized Al-doped ZnO nanoparticles embedded in a PMMA matrix. Spin-coated AZO:PMMA nanocomposite films exhibit stable bipolar resistive switching and synaptic functionality, strongly influenced by Al concentration and oxygen vacancy–assisted carrier trapping. Ag/5% AZO:PMMA/ITO devices show forming-free operation, low switching voltages, high ON/OFF ratio (~10^2), good uniformity, and long retention (>104 s). Pulse measurements confirm essential synaptic behaviors, including postsynaptic current, paired-pulse facilitation, and short- and long-term plasticity under flat and bending conditions, highlighting their suitability for flexible neuromorphic systems. Additionally, Z-scan studies reveal enhanced third-order nonlinear optical response in 5% Al-doped ZnO, indicating potential for nonlinear photonic applications.

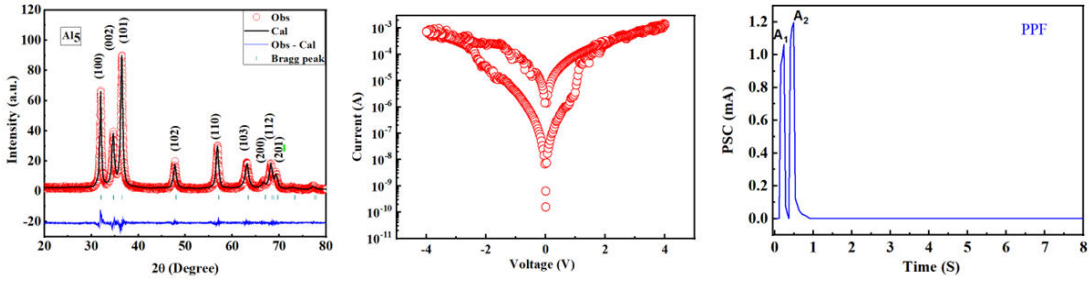


Fig. (a) The XRD pattern of 5% Al-doped ZnO nanoparticles (b) Resistive switching characteristics of the Ag/AZO:PMMA/ITO device (c) Synaptic behaviors of the device by applying Pair-pulse facilitation

Keywords: Resistive Memory device; synaptic functionalities; neuromorphic computing; nonlinear photonic

References:

1. Subhodeep Barman et al.Nano Ex. 1(2020)020003.
2. Snigdha Bhattacharjee et al. Microelectron Engg 164(2016) 53.
3. PK Sarkaret al. RSC Advances 5(2015)105661.

BM-015

Biocompatible ZnO–Biopolymer Nanofilms and Electrospun Nanofibers for Moisture-Responsive Wearable Biosensors

Siva Prasad TN [1], Akash Raj V [1], Aamir Mohamed [1], Harshiny M [2]*

[1]*Department of Biomedical Engineering, Easwari Engineering College, Ramapuram, Tamilnadu, India, 600089*

[2] *Department of Biotechnology, Easwari Engineering College, Ramapuram, Tamilnadu, India, 600089*

***Corresponding author e-mail:** harshiny.bio36@gmail.com

ABSTRACT

In this work, zinc oxide (ZnO) nanoparticles were synthesised using citrus peel extract as a green reducing and stabilising agent and subsequently incorporated into an optimised biopolymer matrix composed of chitosan (2% w/v), polyvinylpyrrolidone (PVP, 8–10% w/v), polyethylene glycol (PEG 400, 3–5% v/v), and glycerol (1–2% v/v). Systematic optimisation identified a ZnO loading of 0.5 wt% as optimal, providing homogeneous dispersion, improved elasticity, and enhanced mechanical integrity. The optimised formulation was fabricated into nano films using a solvent casting method and further processed into electrospun nanofibers using the same composition, demonstrating its versatility as a sensor base material. Electrospinning was performed at an applied voltage of 18+/- 2 kV, a tip-to-collector distance of 12 +/- 2 cm, and a flow rate of 0.4–0.8 mL h^{-1}.The films and nanofibers were characterised using analytical techniques. Morphological analysis confirmed uniform, bead-free nanofibers with effective polymer blending and nanoparticle dispersion. The nanofibers exhibited favourable porosity, mechanical stability, and tunable wettability, enabling efficient moisture handling and biofluid interaction for wearable biosensor applications.The electrospun nanofibers demonstrated effective antimicrobial activity against both Bacillus species and Escherichia coli as confirmed by the disc diffusion method, and exhibited low cytotoxicity toward human embryonic kidney (HEK 293) cells as evaluated by the MTT assay, confirming their biocompatibility and suitability for wearable biosensor applications.

BM-016

Sustainable CS-MWCNT doped Eutectogels synthesis via Rapid Frontal Polymerisation: High-Strength Conductive Composites.

Sayantika Kar*, Hemakesh Mohapatra

Materials Science Centre, IIT Kharagpur, Kharagpur, India

***Corresponding author e-mail:** karsayantika8@gmail.com

ABSTRACT

Frontal polymerisation (FP) offers a rapid, energy-efficient route to fabricate multifunctional eutectogels, yet integrating conductive nanofillers like multi-walled carbon nanotubes (MWCNTs) remains underexplored for electronic applications. Here, we report chitosan-functionalized MWCNTs (CS-MWCNTs) incorporated into a polymerisable deep eutectic solvent (DES) to form eutectogel composites. CS grafting onto oxidised MWCNTs via amide coupling enhances filler dispersion and interfacial hydrogen bonding within the DES matrix [1], enabling homogeneous nanocomposites. Thermal FP, initiated at localised hotspots, propagates self-sustaining fronts (<4 min) to yield robust CS-MWCNT/eutectogels with tunable MWCNT loadings (0.5–3 wt%). The resulting composites exhibit superior mechanical strength, ionic conductivity, and adhesiveness, attributed to percolated MWCNT networks reinforced by dynamic DES crosslinking. Self-healing efficiency exceeds 90% at 60 °C, driven by reversible H-bonding. For electronics, these eutectogels serve as flexible strain sensors (gauge factor ~2.5, 500% stretchability) and Joule-heatable actuators, withstanding >1000 cycles. FP scalability and waste-derived DES compatibility position CS-MWCNT eutectogels [2] as sustainable alternatives to conventional conductive polymers, advancing soft robotics and wearable devices.

Keywords: Frontal polymerisation, eutectogels, flexible electronics, deep eutectic solvent.

References:

1. H. Mahmoodian et al., J. Mol. Liq., 202 (2015) 189–198.
2. P. Lu et al., Nanomicro Lett., 16 (2024) 206.

BM-017

$ZnFe_2O_4$-gC_3N_4 /PVDF Composite Film-Based Self-Poled Piezoelectric Nanogenerator for Efficient Energy Harvesting Applications.

Nil Lohit Sengupta, Bhanu Bhusan Khatua

Materials Science Centre, IIT Kharagpur, Kharagpur, India

***Corresponding author e-mail:** nil1997sengupta@gmail.com

ABSTRACT

In the era of modern electronics, scientists are focused on developing flexible wearable devices1 that are capable of harvesting energy[2] without any use of external electrical sources. Here we developed $ZnFe_2O_4$-gC_3N_4 hybrid filler based pvdf composite to fabricate a self-poled flexible piezoelectric nanogenerator[3]. The g-C_3N_4 has a graphite-like layered 2D structure rich in nitrogen-containing functional groups with aromatic π-systems. While $ZnFe_2O_4$ has Spinel-type structure with active surface metal sites (Zn^{2+} and Fe^{3+}). Here gC_3N_4 act as a matrix for the $ZnFe_2O_4$ nanoparticle to prevent agglomeration. The positively charge metal site of $ZnFe_2O_4$ and the negative π-systems can interact with the PVDF polymer chain.The $ZnFe_2O_4$-gC_3N_4 can successfully stabilize the β-phase of the PVDF polymer up to ~90%. The $ZnFe_2O_4$-g-C_3N_4 /PVDF composite was subsequently moulded and positioned between the copper electrodes. Under a human finger pressure of around 20 kPa, the manufactured piezoelectric nanogenerator (PNG) can produce up to ~38 V of voltage and 0.8 μA of current. Furthermore, small electronic devices such as calculators, speakers, and wristwatches can be operated by the PNG. The fabricated nanogenerator also retains nearly identical output performance even after four weeks, confirming its long-term stability.

References:

1. X. Nan, X. Wang, T. Kang, J. Zhang, L. Dong, J. Dong, P. Xia, and D. Wei, Micromachines, 13 (2022) 1395.
2. F. R. Fan, W. Tang, and Z. L. Wang, Adv. Mater., 28 (2016) 4283–4305.
3. S. S. Nardekar, K. Krishnamoorthy, P. Pazhamalai, S. Sahoo, and S. J. Kim, Nano Energy, 93 (2022) 106869.

BM-018

Charcoal (Carbon)- Cotton Networks for wearable and Sustainable Electronics

Abinash Bharadwaj[1], Prajwalita Hazarika[1], Hirakjyoti Choudhury[1]*, Rupam Goswami[1]

[1]*Tezpur University, Napaam, Tezpur, Assam, India 784028*

***Corresponding author e-mail:** hirakjyoti198@gmail.com

ABSTRACT

This work proposes cost effective solutions to integrate charcoal (carbon) with cotton fibers aimed for wearable and sustainable electronic applications. This work spans across four methods, namely, (a) Cotton Pellets, (b) Drop-Cast Test, (c) Unrolled and Coated Cotton, (d) 3D Printed Mechanism and (e) Smart Textile Prototype as shown in Figure 1. Although, Cotton was selected as the foundation material because of its flexibility, availability, and outstanding absorbent characteristics [1], whereas activated charcoal was considered as the conductive material because of its large surface area and superior electrical conductivity [2]. Polyvinyl alcohol (PVA) serves as a binder to improve coating uniformity and mechanical stability. The technology entails creating conductive cotton samples using drop-casting and an unrolled-coated-rolled procedure to optimize the conductive layer penetration and dispersion. Electrical characterization is carried out by measuring current-voltage (I-V) to determine resistance and linearity. Furthermore, a press-based packaging system and a pilot smart textile prototype are shown. The results reveal a significant improvement in conductivity, indicating that this method has the potential to be used for low-cost resistive elements and smart textile applications.

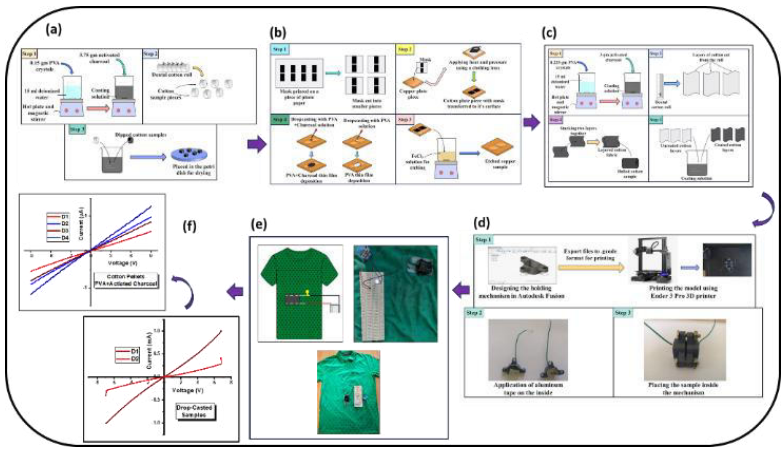


Fig. Charcoal-based cotton network (a) Cotton Pellets (b) Drop-Cast Test (c) Unrolled and Coated Cotton (d) 3D Printed Mechanism (e) Smart Textile Prototype (f) I-V Characteristics

Keywords: Activated Charcoal, Polyvinyl Alcohol, Cotton pellets, E-textiles

References:

1. M. Syduzzaman, S. U. Patwary, K. Farhana, and S. Ahmed, Text. Sci. Eng., 5 (2015) 1
2. K. L. Coates, C. P. Chien, Y. Y. R. Hsiao, D. J. Kovach, C. H. Tang, and M. H. Tanielian, Proc. Int. Conf. Multichip Modules High-Density Packag., (1998).

BM-019

Scalable Bio-Circular Radiative Cooling Coating: Simultaneous Extraction of Cellulose and Silica from Rice Husk

Hsin-Yu Fan[1], To-Yu Wang[1], Hsiu-Mei Yao[1] and Chao-Wei Huang[1]*

[1] *National Cheng Kung University - Department of Engineering Science*

***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

This study focuses on the application of scalable, high-efficiency, biomass-based radiative cooling (RC) coatings. Radiative cooling is a passive cooling technology, meaning it requires no external energy input to reduce system temperature, thereby mitigating global warming and the urban heat island effect.[1] When developing RC materials, we concentrate on two critical parameters. First one is "High Solar Reflectance (0.3-2.5um)", which is necessary to reflect solar radiation and block heat absorption. And second one call "High Mid-infrared Emissivity (8-13um)", which enables the transfer of excess heat to outer space.[2] However, conventional RC materials are typically derived from petrochemical products[3], which contradicts the original intention of environmental sustainability. Therefore, we propose a novel approach to synthesize RC materials using biomass to address this critical drawback.

We selected rice husk as the biomass raw material. Rice husk is a highly promising material because its cellulose component offers excellent potential for radiative cooling. Furthermore, rice husk is rich in silica[4], and the Si-O-Si bond can further enhance emissivity. In previous research, however, the common method of extracting silicon dioxide (calcination) utilized high temperatures that led to the pyrolysis of cellulose[5]. To overcome this technical challenge, we developed an improved extraction process. The highly effective RC material obtained from our optimized process was named BDRH. We then prepared a coating by incorporating BDRH with a binder, resulting in an exceptional RC material with a final reflectivity of 95.44% and an emissivity of 0.94. We employed Matlab for cooling power simulation and conducted further outdoor experiments. Compared to commercial white paint, our coating demonstrated a maximum temperature drop of 4.9˚C.

In summary, we successfully utilized biomass to fabricate a highly efficient cooling coating, simultaneously reducing carbon emissions and achieving circular bio-economy applications. Crucially, the improved extraction process we developed allows for the simultaneous recovery of both cellulose and silicon dioxide, a technology that can be expanded to various other application fields.

References:

1. Feng, K.; et al. Mater. Today Energy 43 (2024) 101575.
2. Gao, W.; Chen, Y. Small 19 (2023) 2206145.
3. Song, Y.; et al. Sol. Energy 256 (2023) 151–157.

BM-020

Electroencephalogram (EEG) Signals in the Diagnosis of Various Mental Disorders

Anshy Princella A. S[1], Harisudha Kuresan[1]*, M. Anand [2], G.Elavel Visuvanathan[1]

[1]*Department of Electronics and Communication Engineering, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603 203.*

[2]*Department of Networking and Communications, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India 603 203.*

***Corresponding author e-mail:** harisudk@srmist.edu.in

ABSTRACT

This research develops an advanced EEG electrode system that combines microneedles with microfluidic channels. The combination of these technologies creates a new electrode design that achieves excellent skin contact without causing discomfort, thereby helping to obtain high-quality signals with lower resistance values. The microneedle system achieves clear access to the epidermis, through which it reduces impedance problems from skin residues and hair, but the microfluidic channel system maintains consistent conductivity through steady contact surface hydration. The proposed electrode design combines positive features from both wet and dry electrodes to maximize EEG signal quality, thereby facilitating a more accurate neurological examination. The research applies EEG signal processing techniques to diagnostic applications within mental health diagnosis, including doubts about anxiety, depression, and post-traumatic stress disorder (PTSD). The symptoms produce modified brainwave patterns that neural signal analysis with machine learning platforms can identify through EEG recordings. The system combines signal processing procedures with deep learning models to evaluate EEG signal data, leading to improved detection of mental health conditions before regular diagnostic procedures.

A systematic evaluation of this electrode design uses performance metrics, which include impedance assessment and signal-to-noise ratio (SNR) measurements, in addition to comparing current electrode models. Testing by both simulation and experimentation verifies the reliability and efficiency elements of the proposed model design. The research objective leads to EEG signal clarity enhancement along with reduced impedance variation, which enables improved usability in clinical and portable EEG applications.

Keywords: Electroencephalogram electrodes, microneedles, microfluidic channels, signal acquisition, impedance measurement.

Reference:

1. Ren, Z.; Chen, et al. IEEE Trans. Instrum. Meas. 69 (2020) 8328–8334.
2. Jiang, Y.; et al. IEEE Sens. J. 21 (2021) 12255–12268.

BM-021

Competing Capillary and Magnetic Forces in Self-Assembled Magnetic Monolayers

Jagadishnaik[1], C Raghunatha[1], C Nishant[1,2], A R Usha Devi[1], Sarbari Bhattacharya[1]*

[1]*Department of Physics, Bangalore University, Bengaluru 560056, India*

[2]*Department of Physics, Mount Carmel PU College, Bengaluru 560052, India*

***Corresponding author e-mail**: sarbari.bhattacharya@bub.ernet.in

ABSTRACT

Pattern formation in floating magnetic dipoles emerges from the interplay between long-range magnetic dipole-dipole interactions and short-range attractive capillary forces at the air-water interface. By constraining dipoles to be perpendicular to the interface and parallel to each other, we ensure purely repulsive magnetic interactions. We investigate how capillary forces, induced by surface deformations, compete with this magnetic repulsion using macroscopic magnets mounted on floating boats. We find that capillary forces, while much weaker in range than magnetic interactions, can be surprisingly strong for certain boat geometries and are sufficient to suppress pattern formation entirely. Two-magnet dynamics on boats of differing shapes reveal that the magnitude and effect of capillary attraction depend strongly on boat geometry. When extended to multi-particle systems, these insights explain observed patterning behaviour: boat design can reverse the balance between competing interactions and restore pattern formation even when capillary forces would otherwise dominate. Our results highlight the critical role of experimental geometry and dipole orientation in controlling self-organization in magnetically interacting particle systems.

References:

1. C. Raghunatha et al., Macromol. Symp., 413 (2024) 2300030.
2. D. Vella and L. Mahadevan, Am. J. Phys., 73 (2005) 817–825.
3. I. Ho et al., Phys. Rev. Lett., 123 (2019) 254502.
4. A. Hooshanginejad et al., Nat. Commun., 15 (2024) 5466.

BM-022

Contribution Sustainable Manufacturing of a Component under Minimum Quantity Lubrication (MQL) Condition: A Comprehensive Review

Anbu Thamilarasan P, Sidhaart K, Madhan M, Haridass R*, Vinayak Arun Sankar Vijayasankar

Karpagam College of Engineering, Coimbatore, TN, India

***Corresponding author e-mail:** harimedesign@gmail.com

ABSTRACT

MQL may provide a feasible avenue to minimize fluid usage, emissions, and job exposure while maintaining or augmenting machining productivity. This review collates mechanistic associations of atomization, droplets deposited, base-oil chemistry, and tool–chip tribology to define the limits of applicability of nano-enhanced and cryogenic MQL. Comparative analysis compares the dry, flood, minimum quantity lubrication (MQL), nano-enhanced MQL, and cryogenic-assisted strategies in terms of tool life, surface integrity, energy per part, and lubricant footprints, considering combined experimental trends and typical case studies. Attention focused on delivery systems, nozzle geometry, atomizer type, and a flow control metering process including advanced atomizing methods such as ultrasonic excitation and electrostatic charging to increase deposition efficiency and minimize airborne fraction. The occupational and environmental consequences of nanoparticle inclusion are critically addressed, and smart design rules for a Safer-by-Design approach to nanoparticle choice, dispersion stability, and extraction location are presented. A practical pathway is articulated, identifying sensor-incorporated closed-loop control, pressure-driven injection and internal channel delivery, and artificial intelligence-facilitated parameter tuning to connect laboratory gains and the implementation at production scale. The identified gaps in knowledge are standardized aerosol characterization, long-term exposure evaluation, and techno- economic analysis of the hybrid systems. Prioritized recommendations include interoperable sensing standards, demonstrator implementations, and safer formulation protocols for fast adoption of sustainable MQCL-based manufacturing processes. Interdisciplinary work between the tribology, fluid dynamic, and digital manufacturing communities is required for successful implementation of the methodology.

Keywords: Sustainable manufacturing, minimum quantity lubrication, eco-friendly machining, surface integrity, energy efficiency, green manufacturing.

BM-023

Surfactant-Mediated Control of Pattern Formation in Magnetic Swimmers

Nishant R Chirania[1,2], C Raghunatha[1], Jagadishnaik[1], A R Usha Devi[1], Sarbari Bhattacharya[1]*

[1]*Department of Physics, Bangalore University, Bengaluru 560056, India*

[2]*Department of Physics, Mount Carmel PU College, Bengaluru 560052, India*

***Corresponding author e-mail:** sarbari.bhattacharya@bub.ernet.in

ABSTRACT

We investigate how surfactants modulate the dynamics and collective organization of magnetically repulsive swimmers at an air–water interface. Each swimmer consists of a floating boat embedded with a vertically aligned magnet, generating predominantly repulsive dipolar interactions. By varying surfactant concentration, we systematically tune surface tension and modify the hydrodynamic environment. Two-body repulsive dynamics are analyzed by fitting experimental trajectories to equations of motion incorporating magnetic repulsion, drag forces, and capillary interactions. The dependence of fit parameters on surfactant concentration reveals how surface tension mediates the effective interaction range between swimmers. We extend this analysis to many-body systems, using pattern statistics to quantify how surfactant-induced hydrodynamic modulation affects collective structure formation. Our results demonstrate that competing magnetic, hydrodynamic, and capillary interactions govern spatial order in interfacial soft-matter systems, offering new control strategies for engineering self-assembled structures.

References:

1. I. Varga, H. Yamada, F. Kun, H. G. Matuttis and N. Ito, Phys. Rev. E 2005 71, 051405 (1-7)
2. N. Yoshioka, I. Varga, F. Kun, S. Yukawa, N. Ito, Phys. Rev E 2005 72, 061403 (1-6)
3. C.Raghunatha, Nishant R. Chirania, M. Niranjan, A.R. Usha Devi, S.A. Rangwala, Sarbari Bhattacharya, Macromol. Symp. 2024 413, 2300030 (1-7)
4. D. Vella and L. Mahadevan, Am. J. Phys 2005 73(9) 817-825
5. A. Hooshanginejad, J-W Barotta, V. Spradlin, G. Pucci, R. Hunt, D.M. Harris, Nat. Commun. 2024 15 5466 (1-9)

BM-024

Effect of Co-Precipitation Assisted Hydrothermal Synthesis Time on Thermal and Magnetic Properties of $CoFe_2O_4$ for Magnetic Hyperthermia Applications

Devendra Kumar[1]*, B. K. Sahoo[1]

[1]*National Institute of Technology Raipur, Raipur, Chhattisgarh, India, 492010*

***Corresponding author e-mail:** dkumar.phd2023.phy@nitrr.ac.in

ABSTRACT

In recent years, the magnetic hyperthermia treatment (MHT) has been accepted worldwide as a cancer treatment strategy. Fe_3O_4 is utilized as the heating source in the presence of an alternating magnetic field (AMF). There is a necessity in exploring an alternating material for the heat source. This study concentrates on $CoFe_2O_4$, a promising magnetic nanoparticle (MNP) for MHT application. The MNPs were synthesized via a co-precipitation-assisted hydrothermal synthesis approach. The crystallite size of the MNPs varies between 14 to 16 nm. The Fourier Transform Infrared Spectroscopy (FTIR) gives the functional groups present, in addition octahedral and tetrahedral stretching near 450 and 550 cm-1 which confirms the spinel structure of the $CoFe_2O_4$ MNPs. To explore the usefulness of prepared MNPs for the MHT application, magnetic and thermal properties are investigated. The magnetization against the applied field verifies the soft ferrimagnetic characteristics, while the magnetization vs temperature plot validates the superparamagnetic nature near 320K, which is appropriate for MHT. Using FTIR data, the thermal conductivity (k) of the MNPs is determined by applying the Callaway-Klemen's formula and found to be 4.1(W/m·K) which closely aligns with the experimentally observed values. To study the heating nature of the sample, the thermal diffusion equation is studied using the obtained magnetic and thermal parameters. It is found that for appropriate heating, a higher value of k with larger saturation magnetization (Ms) is advantageous for the MHT application under the tolerable limit of the AMF.

References:

1. A. Zelenakova, Ľ. Nagy, P. Hrubovcak, M. Barutiak and M. Gerina, J. Alloys Compd., 2024, 989, 174415.
2. S. Fayazzadeh, M. Khodaei, M. Arani, S. R. Mahdavi, T. Nizamov and A. Majouga, J. Supercond. Nov. Magn., 2020, 33, 2227–2233.
3. J. Mucha, H. Misiorek and A. Jeżowski, Phys. Solid State, 2007, 49, 18–22.

BM-025

Heat Energy as Medicine Enabled by Fe_3O_4 Magnetic Nanoparticles for Cancer Treatment

Yashwant [1]*, B. K. Sahoo[1], Munna Dan[2]

[1]*National Institute of Technology Raipur, Chhattisgarh, India, 492010*

[2]*Amity University Raipur, Chhattisgarh, India, 493225*

***Corresponding author email:** yashwant.phd2025.phy@nitrr.ac.in

ABSTRACT

For cancer therapy, heat energy can be regarded as a form of medicine when it is appropriately generated and controlled at the nanoscale. Magnetic Hyperthermia is an oncologic treatment which uses the heating properties of magnetic nanoparticles (MNPs) under an alternating magnetic field (AMF). This work investigates the heating properties of magnetite (Fe_3O_4) MNPs for tumour heating. The MNPs were synthesised by the co-precipitation method and characterised by XRD, FTIR and SQUID measurements. XRD data gives particle size as 10.3nm and the unit cell as 0.833 nm. Using FTIR data, we get an average force constant of 201.67N/m, average phonon velocity 4321 m/s, Debye temperature 591K and phonon thermal conductivity 2.2 W/mK at 300 K. The obtained thermal conductivity and magnetic parameters are used in the thermal diffusion analysis to study heat transport behaviour of MNPs in the tumour region. The study finds that the localised thermal spread can be tuned by adjusting the MNPs concentration, magnitude and frequency of AMF and the thermal conductivity of the effective medium, which allows tailored Fe_3O_4-based magnetic hyperthermia to be a non-invasive, non-toxic thermal medicine instead of a bulk heating technique.

References:

1. Marta Vassalo, Daniele Martella, Gabriel Barrera, Federica Celegato, J. ACS Omega,8 (2023) 2143-2154.
2. Behnam Sabzi Dizajyekan, Arezou Jafari, Mohsen Vafaie-Sefti, Scientific report, 14 (2024) 1296.

BM-026

Magnetic and Dielectric Behaviour of Alkaline Doped $BiFeO_3$

Osheen Sharma[1], Jitendra Pal Singh[1]*, Pawan Kumar[2], Dinesh Kumar Shukla[3], Keun Hwa Chae[4] and Jaiparkash[1]*

[1]*Department of Sciences, Manav Rachna University, Faridabad, Haryana-121004, India*

[2]*Department of Physics, National Institute of Technology, Rourkela, Odisha 769008, India*

[3]*Advanced Analysis & Data Center, Korea Institute of Science and Technology, Seoul-02792, Republic of Korea*

[4]*UGC-DAE Consortium for Scientific Research, Indore 452017, India*

***Corresponding author e-mail:** jpsingh@mru.edu.in, jaiprakash@mru.edu.in

ABSTRACT

For this work, alkaline-doped (Ca^{2+}, Sr^{2+} and Ba^{2+}) bismuth ferrite (BFO) ceramic was synthesized via a conventional rapid two-stage reaction method to investigate the magnetic, and dielectric behaviour. X-ray diffraction patterns showed the presence of a pure crystalline phase of BFO in all synthesized materials. No impurity phase is observed with doping. Rietveld refinement validated the rhombohedral crystal structure with *R3c* space group in all materials. Fourier transform infrared spectroscopy exhibited the character of Fe-O stretching associated with FeO_6 octahedral in all materials. Raman spectroscopy analysis further evidenced lattice distortion and symmetric shift in Raman active phonon modes induced by doping. Field emission scanning electron microscopy (FESEM) showed the clear grains with distinct boundaries. The average particle size was 360±44, 297±9, and 219±7 nm for Ca^{2+}, Sr^{2+} and Ba^{2+} doped BFO. The Fe L-edge near-edge X-ray fine absorption spectroscopy (NEXFAS) spectra exhibited well-resolved L3 and L2 absorption features. These spectra also confirmed the Fe^{3+} oxidation state in synthesized materials. The O K-edge spectra displayed a prominent pre-edge feature highly influenced with doping. This may be due to the change in hybridization (O 2p and Fe 3d states) with doping ions. The magnetic measurement at room temperature showed that magnetic ordering is affected by the dopant ions. The dielectric constant and loss tangent were decreased for Ca^{2+} and Sr^{2+} substitution, followed by an increase for Ba^{2+} ions. Dielectric measurement revealed the decrease in dielectric constant accompanied by a significant reduction in the loss tangent as the frequency was increased. These findings demonstrated that alkaline metal ions may provide an effective route for tailoring the multifunctional properties of BFO.

Keywords: Rapid two-stage reaction Method, Ionic Radii, Rietveld Refinement, Dielectric Behavior, magnetic ordering

BM-027

Microstructural Dynamics of Stretching Nanofilm of Hydrogels: Effects of Film Thickness on Mechanical Properties

Chia-Yu Liao[1], Chih-Jung Lin[2], Yu-Jane Sheng[2]*, and Heng-Kwong Tsao[1]

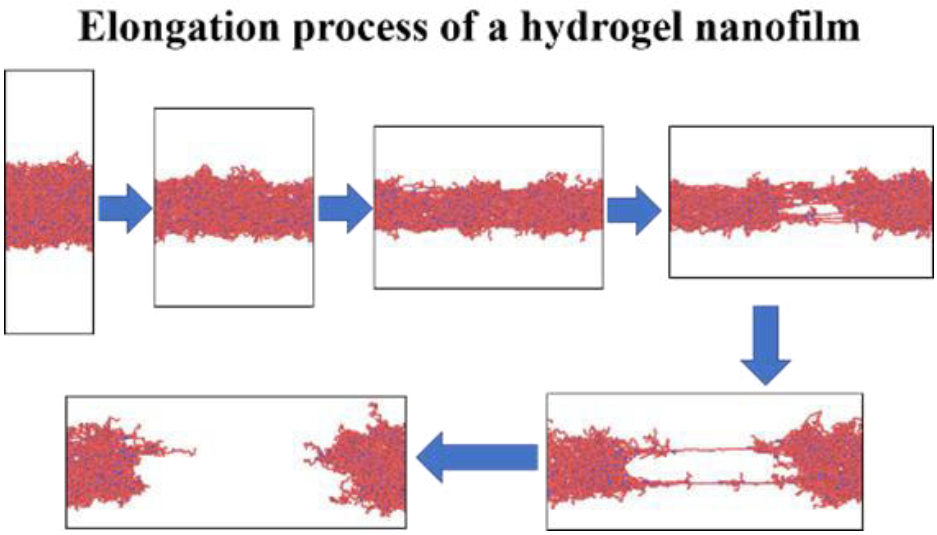
[1]*Department of Chemical and Materials Engineering, National Central University, Taoyuan 32001, Taiwan, ROC*

[2]*Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan, ROC*

***Corresponding author e-mail:** yjsheng@ntu.edu.tw

ABSTRACT

While stretching hydrogel nanofilms enables the acquisition of stress-strain curves, deciphering the internal structure and mechanisms through experiments remains challenging. In this work, dissipative particle dynamics simulations are employed to observe microstructural changes in elongated hydrogel nanofilms. The morphological changes of the film, up to the point of fracture, are observed, and the corresponding stress-strain curve is obtained. Microscopic characteristics, including polymer size, strand size, and bond length, are systematically analyzed to understand the network's deformation. Additionally, the breakages of polymers, strands, and bonds are closely monitored. In a thin film, the microstructure of the interfacial region differs from that of the bulk region, with the latter enduring more forces during extension. Consequently, as film thickness increases, the contribution from the bulk region becomes more pronounced, leading to a further enhancement of mechanical properties.



BM-028

Synergistic Tamra-Yasad Bhasma and Cinnamaldehyde Nano-shield Hydrogels for Diabetic Wound Repair

Suhela Tyeb [1]*, Nitesh Kumar [2], Vivek Verma [3], Ashok Kumar [4], Sanjana Kaul[1]

[1]*School of Biotechnology, University of Jammu, Jammu, J&K, India – 180006*

[2]*Department of Materials Engineering, Indian Institute of Technology Jammu, Jammu, J&K, India-181221*

[3]*Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, UP, India-208016*

[4]*Biosciences and Bioengineering Department, Indian Institute of Technology Kanpur, UP, India-208016*

ABSTRACT

Around 100 million people with diabetes in India are at risk of developing diabetic wounds in their lifetime. These wounds cause severe loss of quality of life to the patients due to increased economic burden and risk of limb amputations. Indigenous wound dressings are a cost-effective solution for the management and healing of such wounds. Loading bioactive formulations into passive dressing material led to successful intervention in the hampered wound-healing cascade. Role of traditional wound healing formulations such as aloe vera, turmeric, cinnamon oil extract loaded in hydrogels, hydrocolloids, sponges, and other dressing materials has been discussed earlier. Tamra and Yasada Bhasma are two types of ayurvedic formulations (bhamas) cited in Indian traditional medicinal text of "Rasa-shastra". These Bhasmas have been studied in isolation showing beneficial attributes such as free radical scavenging, hepatoprotective activity and anti-inflammatory effect. The present work aims to study the combinatorial effect of Tamra Bhasma and Yasad Bhasma in conjunction with the potent antimicrobial "Cinnamaldehyde Nano-emulsion (NE)" loaded into two different forms of a Polyvinyl alcohol (PVA) matrix: hydrogel and sponge. In-vitro studies on three cell lines, NIH3T3 and HaCaT and HuVECs showed sustained release of these Bhasmas and NE leading to enhanced cell proliferation, cell migration, free radical scavenging and collagen formation. The developed bioactive wound dressing show promise towards healing and management of infected diabetic wounds as compared to PVA hydrogel and sponge control.

Keywords: Tamra Bhasma, Yasad Bhasma, PVA hydrogel, Sponge, Cinnamaldehyde emulsion

BM-029

Trace Elemental Analysis of Benincasa hispida, an Anti-Jaundice Medicinal Plant from Telangana, India, Using ED-XRF Spectroscopy

D.Sammaiah[1], G. Manjula[2] and S. Jyothsna[3*]

[1]*Department of Botany, Kakatiya Govt. College (A), Hanamkonda -506001, Kakatiya University, Telangana, India*

[2]*Department of Physics, Kakatiya University, Warangal-506009, Telangana, India*

[3]*University College of Eng. & Tech. for Women, KU, Warangal-506009, Telangana, India*

***Corresponding author e-mail:** joshsriram123@gmail.com

ABSTRACT

Jaundice is a common liver disease that affects all age groups and continues to be a significant health burden in developing countries, including India. Traditional medicinal plants have long been used jaundice management due to their better therapeutic efficacy and minor side effects. In the present study, *Benincasa hispida* fruits, a potential anti jaundice medicinal plant from Telangana region, was selected for screening of its trace elemental concentration using EDXRF (Energy Dispersive X-ray Fluorescence) technique. Elemental analysis revealed that, the presence of thirteen (13) essential macro, micro and trace elements like K, P, Ca, Cl, Mn, S, Fe, Cu, Zn, Se, Br, Rb and Sr in varying concentrations. Quantitative comparison with the certified standard reference material NIST 1515 apple leaf showed higher levels of Mn, Cu, Fe, Zn, Cl, K, Se, Br, Sr and Rb, whereas P, S, and Ca were relatively present at lower levels. The improvement of these biologically important trace elements suggests a possible role of *Benincasa hispida* fruits in supporting for multiple processes such as liver metabolism, antioxidant defense, and hepatic homeostasis. These findings provide a scientific basis for the development of novel standardized dosage of herbal medications derived from this plant. Furthermore, future studies may explore its potential application as a natural, biocompatible antioxidant coating material for implantable medical devices to enhance tissue integration and reduce inflammation.

Keywords: Elemental screening, Trace elements, *Benincasa hispida*, Jaundice (Icterus) disease and EDXRF Technique.

BM-030

Advanced Bone Repair Solutions: A Mechanical-Assisted Post Bio-Printing Approach

Tharani Priya Ayyappan , Gobi Saravanan Kaliaraj*[3]

Centre of Excellence for Additive Manufacturing, Sathyabama institute of Science and Technology, Chennai, Tamil Nadu, India, 600119.

***Corresponding author e-mail:** gobisaravanan@sathyabama.ac.in

ABSTRACT

A bone fracture that is 1.5 times the diameter of the tubular bone is known as a critical-size bone defect, which takes a prolonged time to heal due to limited communication within the bone tissues. Herein, a piezoelectric scaffold (PZS) developed using Sodium alginate-metal (Ba, Sr, and Ba+Sr) composites (AMC) by applying mechanical stress. PZS has been proven to accelerate bone regeneration by triggering cellular communication. At 12, 24, and 36 hours of incubation with PZS, a 2-fold increase in 143B cell line confluence was observed, accompanied by significant cellular accumulation within scaffold-incubated cells. Additionally, the MTT assay confirmed that no cytotoxicity was generated. Antibacterial studies showed only noted amounts of E. coli and S. aureus colonies, while blood protein adsorption studies revealed substantial protein adsorption. Mechanical integrity was assessed using a universal tensile testing machine. FTIR, XRD, and SEM analysis shows proper metal incorporation and structural arrangements. Biodegradability and swelling characteristics indicate their suitability for bone scaffold applications. In summary, this study developed an electrically triggered alginate-based metallic scaffold that is promising as a conductive platform to expedite cellular induction and promote faster healing and complete regeneration of long bone fractures.

References:

1. L. Chastagnier, L. Essayan, C. Thomann, J. Niemann, E. Errazuriz-Cerda, M. Laithier, A. Baudouin, C. Marquette, and E. Petiot, Bioprinting, 50 (2025).
2. T. Tariverdian, A. Behnamghader, P. Brouki Milan, H. Barzegar-Bafrooei, and M. Mozafari, Ceram. Int., 45 (2019) 14029–14038.
3. D. Chawla, T. Kaur, A. Joshi, and N. Singh, Int. J. Biol. Macromol., 144 (2020) 560–567.

BM-031

Trace Element Profiling of Anti-Asthmatic Medicinal Plant Tephrosia purpurea Using EDXRF Technique

D. Sammaiah[1] and S. Jyothsna[2]*

[1]*Department of Botany, Kakatiya Govt. College (A), Hanamkonda -506001, Kakatiya University, Telangana, India*

[2]*Department of Physics, UCE&TW, Kakatiya University, WGL-506009, Telangana, India. (IISER) Tirupati, India*

***Corresponding author e-mail:** joshsriram123@gmail.com

ABSTRACT

Asthma is a chronic inflammatory disease of the airways, affecting millions of individuals worldwide. While synthetic corticosteroids remain the primary therapeutic option, their long term use can cause adverse effects, leading to growing interest in medicinal plant based therapies. Tephrosia purpurea is a traditionally used anti-asthmatic medicinal plant with promising therapeutic potential in respiratory disorders. The present study aims to evaluate the trace elemental consentration of T. purpurea fruit samples using Energy Dispersive X-Ray Fluorescence (EDXRF) spectroscopy, a rapid, non-destructive analytical technique. The analytical accuracy was compared with NIST 1515 apple leaf as a reference material. The results revealed that the presence of essential macro, micro and trace elements such as K, P, S, Ca, Mg, Fe, Zn, Cu, Mn, and Se. Notably, selenium (0.89±0.24ppm) and copper (7.99±1.01ppm) levels were found at high levels and are known to play key roles in reducing oxidative stress and airway inflammation associated with asthma. Simultaneously, potassium, calcium, zinc and manganese supports immune homeostasis, bronchial smooth muscle regulation and air way function. The findings highlight the significance of trace elemental profiling of fruit samples provides scientific evidence in understanding its ethno medicinal use in asthma treatment and management. However, further studies pharmacological efficiency and toxicological investigations are requires safety for pulmonary applications.

Keywords: Trace elements, Medicinal plant, Tephrosia purpurea, EDXRF technique, Asthma disease.

BM-032

Activatable Sulphur Dioxide (SO_2)-Releasing Probe Triggers Ferroptosis via Redox Imbalance in Cancer Cells

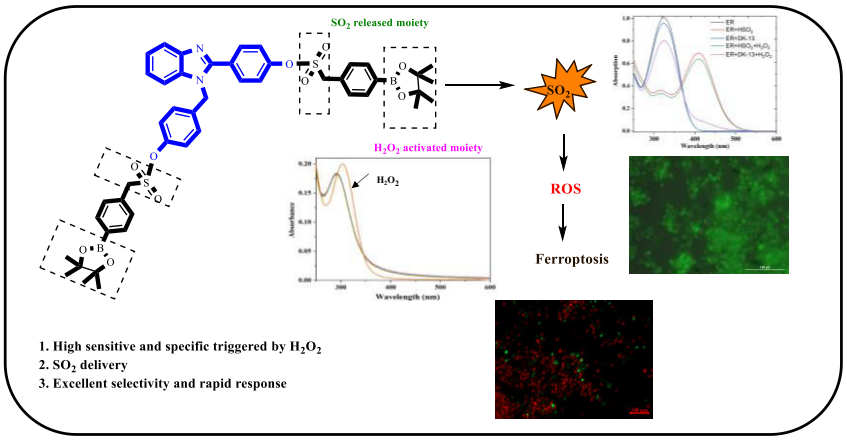
Deepak Bains and Asifkhan Shanavas*

Chemical Biology Unit, Institute of Nano Science and Technology (INST), Sector 81, Knowledge City, Mohali, Punjab 140306, India

***Corresponding author e-mail:** asifkhan@inst.ac.in

ABSTRACT

Ferroptosis is an iron-dependent, regulated cell death pathway driven by lipid peroxidation and represents a promising strategy to overcome apoptosis resistance in cancer therapy.[1] We designed and synthesized a dipodal benzimidazolium-based, ROS-responsive sulfur dioxide (SO_2) donor capable of controlled SO_2 release. The probe design incorporates a triggerable boronate linkages that undergoes selective activation in the presence of hydrogen peroxide (H_2O_2), as evidenced by pronounced spectral changes in UV–vis and fluorescence emission profiles after H_2O_2 treatment. Also, we monitored SO_2 release which is subsequently detected through its reaction with DEACA and Ellman's reagent using a convenient fluorescence and absorbance method. Further, to investigate whether the treatment influenced oxidative stress within the cells, intracellular reactive oxygen species levels were quantified using a fluorescence-based assay and visualized through microscopy analysis. *In vitro* studies demonstrate efficient cancer cell killing and a live/dead assay was performed on 4T1 cancer cells using the probe to evaluate its cytotoxic effects and ability to distinguish viable from non-viable cells. In addition, ferroptosis-associated lipid peroxidation is markedly elevated, as shown by strong red fluorescence staining in treated cells. Collectively, these results indicate that the designed donor not only enables ROS-triggered SO_2 release but also amplifies oxidative stress and promotes ferroptotic pathways, highlighting its potential as a chemical tool for studying redox-regulated cell death mechanisms.



References:

1. Jianfei Liu, Zipeng Li, Shuxin Peng, Jun Tang, Di Zhang, Yong Ye, Anal. Chemistry, 96 (2024), 2041–2051.

BM-033

Physiologically Based Pharmacokinetic Modelling of Liposomal Drug Delivery Regulated by Oleic Acid from Enteromorpha Intestinalis

Manega Ponmalai[1], Vijaykumar Sudarshana Deepa[2], Nazeer Abdul Azeez [1]

[1]*Department of Biotechnology, School of Bioengineering, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu - 603 203, India*

[2]*Department of Biotechnology, National Institute of Technology, Tadepalligudem, Andhra Pradesh – 534 101, India*

***Corresponding author e-mail:** abdulazn@srmist.edu.in

ABSTRACT

Increasing discoveries of new class drug delivery systems demands increasing animal studies, pressing an ethical concern. Hence the physiology of the animals are simulated using modelling tools to estimate the probable pharmacokinetic efficiency of the drug delivery systems. This study is an attempt to predict the pharmacokinetics of Aspirin delivered through Liposome using Physiologically Based Pharmacokinetics (PBPK) modelling. The liposome was stabilized using Oleic acid based bio-surfactant isolated from *Enteromorpha intestinalis*. The entrapment efficiency of the liposome was 93.33 ± 0.17% and HR-TEM revealed spherical liposomal micelles at 80-95 nm while the mean particle size was observed to be 77 nm from DLS. The release was observed 98-99% in simulated body fluid conditions (pH 1.2, 6.8 and 7.4). To Weibull dissolution factor was calculated from the release kinetics that helped define the release profile of aspirin from spherical liposome. East Asian male and female population, along with the physico-chemical properties of Aspirin were defined in PBPK modelling. The pharmacokinetics (PK) was estimated for 48 hours and PK parameters were mapped with their influencing physiological factors such as body weight, age, and chronic kidney disease. The results suggested the improved PK profile for Aspirin when stabilized using *E.intestinalis* extract.

Keywords: PBPK modelling; Oleic acid; Drug loading; Release Kinetics; Enteromorpha intestinalis

BM-034

Design of Electrospun Multi-Layered Nanofiber Platform for Improved Wound Healing in Diabetic Condition

Ashirbani Singh, Shazma Sarwat, Yash Srivastava, Koel Mukherjee*

Department of Bioengineering & Biotechnology, Birla Institute of Technology, Mesra, Ranchi, Jharkhand-835215

***Corresponding author e-mail:** koelmukherjee@bitmesra.ac.in

ABSTRACT

Diabetic wound management remains one of the major clinical concerns due to delayed healing, impaired cell proliferation, persistent inflammation, and susceptibility to infection. The present study aims to fabricate a multilayered electrospun nanofiber scaffold made according to the challenges faced in each stage of diabetic wound healing. Using serial electrospinning process three layers were fabricated, PVA added phytochemical as innermost layer, PCL-PVA associated antioxidant chemical as middle layer and cerium oxide nanoparticles composed outermost layer respectively. The fabricated scaffold then characterized using FESEM, FTIR and XRD for fiber morphology and chemical existence. To check antimicrobial efficacy, water retention and drug release, in vitro studies were performed. To evaluate in vivo wound healing efficacy, an STZ-induced diabetic mouse along with control was treated with fabricated nanofiber and was observed for 14 days. FESEM results provide insights for average diameters of 277.5, 242 nm, and 144.6 nm for respective layers. FTIR and XRD peaks shows the presence of phytochemicals and NPs in the layer. Holo zone indicates the antimicrobial activity where data represents good water retention capacity also. Healing was assessed through wound closure and histological analysis. Scaffold-treated mice exhibited faster wound closure, better inflammation control, and better collagen maturation compared to control groups.

Keywords: Nanoscafold, phytochemicals, in vivo study, diabetic wound

BM-035

Biofunctional Polydopamine/Gelatin Layer-by-Layer Self-Assembled Polycaprolactone Nanofibers for Wound Healing

Bharathraj Arumugam, Varsha Anand, Sahana Rajan Kalpana, Shivanee Kumar, Sushma Babu, Nagarajan Selvamurugan*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** selvamun@srmist.edu.in

ABSTRACT

Wound healing is a dynamic and tightly regulated biological phenomenon involving coordinated cellular and molecular events essential for tissue repair and regeneration. Despite this intrinsic capability, the rising incidence of non-healing wounds, often exacerbated by microbial infections, poses a major clinical challenge. However, conventional wound dressings often lack bioactivity, antibacterial properties, and structural features, necessitating advanced wound care strategies. Hence, the main objective of this study is to develop a novel nanofiber-based wound dressing by incorporating 4-methoxycinnamic acid (MCA), a natural bioactive compound, into polycaprolactone (PCL) nanofibers fabricated via electrospinning. To further enhance the biocompatibility and surface bioactivity, the MCA-loaded nanofibers were surface functionalized using polydopamine (PDA) and gelatin (GEL) containing MCA as coating layers. Comprehensive physicochemical and morphological analyses confirmed that MCA incorporation preserved the structural integrity without any significant alterations in the *in vitro* material characterization. Furthermore, biocompatibility was assessed using fibroblast cells, exhibiting favorable cell attachment, proliferation, and migration. Additionally, the dual-loaded LBL-nanofibers effectively enhanced the expression of wound healing-related genes. The fabricated nanofibers also exhibited potent antibacterial activity, with enhanced efficacy attributed to the presence of MCA within the nanofiber and the LBL coating. Overall, the incorporation of MCA in both the nanofiber matrix and surface coating exhibited enhanced potential as advanced wound dressings with dual regenerative and antimicrobial functionality.

References:

1. D. Cui et al., Polymers, 15 (2023) 3122.
2. A. Płowuszyńska and A. Gliszczyńska, Molecules, 26 (2021) 3827.

BM-036

Engineered Nanobiofertilizers Integrating Metal Oxides for Improved Growth Performance and Biochemical Response in Amaranthus Viridis

Prem Kumar Varadaraji[1], Geetha Sethuraj[2*], N. Angeline Little Flower[1*]

[1]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203*

[2]*Department of Basic Sciences, SRM College of Agricultural Sciences, SRM Institute of Science and Technology, Chengalpattu District, Tamil Nadu, India, 603203*

ABSTRACT

The accelerated increase in the global population has necessitated the requisite for sustainable agricultural practices that will guarantee long-term soil health and food security. Despite the fact that synthetic fertilizers enhance crop yield, their excessive application contributes to soil degradation and environmental pollution. Nanobiofertilizers—plant growth-promoting microorganisms with engineered nanomaterials are advanced techniques for improving nutrient availability and crop productivity. In this paper, the nanobiofertilizer formulations were developed using three plant growth-promoting bacteria, namely *Azospirillum brasilense*, *Pseudomonas fluorescens*, and *Bacillus subtilis*, in combination with metal oxide nanoparticles synthesized by sol–gel and co-precipitation techniques including mesoporous silica (SiO_2), zinc oxide (ZnO), titanium dioxide (TiO_2), and iron oxide (Fe_3O_4). Pot experiments were conducted on *Amaranthus viridis* to evaluate the growth response, nutritional enhancement, and phytochemical composition. Among the treatments, the ZnO–*B. subtilis* formulation produced the highest increase in the height of plants and nutrient content. Mineral profiling indicated enhanced uptake of essential macro- and micronutrients. GC–MS analysis identified some bioactive metabolites, including jasmonate derivatives, porphyrins, and anthraquinones associated with antioxidant activity, pigment biosynthesis, and growth promotion. Antioxidant activity tested in vitro using a DPPH assay showed a dose-dependent increase; *P. fluorescens* and *B. subtilis* exhibited 87.72% at 100 µg/mL, which was comparable to that of ascorbic acid. All these findings suggest that the nanobiofertilizer formulations significantly improved the physiological and biochemical attributes of *A. viridis*, thus underpinning its potential application as sustainable inputs for enhanced crop productivity.

Keywords: Metal oxide nanoparticles, Nano Bio fertilizers, *Amaranthus viridis,* Plant growth promoting bacteria, Sustainable agriculture.

BM-037

Curcumin-Loaded PCL/Chitosan Nanofibers: Comparative Evaluation of Antimicrobial Activity and Wound Healing Potential

Sunandita Vijayakumar, Varsha Krishnamoorthy, Shree Initha Mutharasan, S.Gnanavel*

Biomaterials Laboratory, Department of Biomedical Engineering, SRM Institute of Science and Technology, Kattarkulathur campus, Chengalpattu, Tamil Nadu, 603203, India

***Corresponding author e-mail:** gnanaves@srmist.edu.in

ABSTRACT

Chronic wounds affect 10.5 million beneficiaries of the U.S. Medicare, costing $22.5 billion annually in the U.S. alone and $148.65 billion globally. Traditional wound dressings only act as a passive barrier and do not possess antimicrobial or tissue regenerative capabilities which are necessary for dealing with persistent infections associated with such wounds. To address these limitations, this study develops a curcumin-loaded PCL/Chitosan nanofibrous patch which combines the mechanical stability of synthetic polymers with the biological activity of natural compounds. PCL was chosen for its structural stability, chitosan for its biocompatibility and antimicrobial properties and curcumin for its anti-inflammatory and wound healing effects. The patches were fabricated by blending PCL and chitosan in the ratio of 85:15 with and without curcumin integration. Curcumin (1% w/w) was dissolved in ethanol and incorporated into the polymer solution prior to electrospinning, resulting in the fabrication of two distinct electrospun nanofibrous meshes, namely curcumin-loaded and non-loaded PCL/Chitosan scaffolds. Characterization via SEM revealed a nanofibrous morphology mimicking the extracellular matrix. FTIR and XRD confirmed successful polymer blending and homogeneous curcumin dispersion. TGA validated thermal stability. Antibacterial testing demonstrated the superior antibacterial efficacy of curcumin-loaded PCL/Chitosan patch compared to the limited inhibition of non-loaded controls. These results demonstrate that the curcumin-loaded PCL/Chitosan patch serves as a promising platform for infection control and wound healing applications.

Keywords: Electrospinning, PCL, Chitosan, Curcumin, Chronic wounds, wound healing, Antimicrobial activity

References:

1. Yadav P.D. et al., Discover Materials, vol (2024) 4:99.
2. Nikfarjam S. et al., Polymers, vol (2023) 15, 2014.
3. Aranaz I. et al., Polymers, vol (2021) 13, 3256.
4. Kasprzak-Drozd K. et al., Int. J. Mol. Sci., vol (2024) 25, 3617.
5. Sen C.K., Adv. Wound Care, vol (2025) 14(9).

BM-038

Green synthesis of seaweed derived carbon dots via microwave assisted method for biomedical and environmental applications

Abinithi S[1], Sathishkumar K[2], Sabareesh K. P. V[1*]

[1]*Department of Physics, Rathinam College of Arts and Science, Coimbatore 641 021, Tamil Nadu, India*

[2] *Department of Biotechnology, Rathinam College of Arts and Science, Coimbatore 641 021, Tamil Nadu, India*

Corresponding author: dean.rd@rathinam.in

ABSTRACT

Sustainable nanomaterials derived from renewable resources have gained significant attention due to their eco-friendly synthesis, multifunctionality and potential applications in environmental and biomedical fields. In the present study, carbon dots (CDs) were synthesized from seaweed biomass using a facile and microwave-assisted method. The optical properties of the synthesized CDs were confirmed through UV–visible spectroscopy and photoluminescence (PL) analysis, demonstrating strong absorption and excitation-dependent emission behaviour. Functional group analysis using Fourier Transform Infrared Spectroscopy (FTIR) revealed the presence of oxygen- and nitrogen-containing surface functionalities, contributing to enhanced dispersibility and reactivity. The prepared CDs were further evaluated for multifunctional applications. Catalytic performance was assessed through the reduction of methylene blue, where the CDs exhibited efficient catalytic activity indicating their potential use in environmental remediation. In addition, *in vitro* wound scratch assay shown promising wound healing properties suggesting their applicability in biomedical applications. The intrinsic fluorescence characteristics of the CDs also enabled effective bioimaging, highlighting their suitability as biocompatible imaging probes. Overall, the study demonstrates a sustainable approach for converting marine biomass into value-added nanomaterials with significant catalytic, biomedical and imaging properties.

Keywords: Carbon dots, Catalytic activity, Wound healing, Bioimagi

BM-039

Phytofabrication of Zeolitic Imidazolate Frameworks as Potential Wound Healing Agents

Ayyanar R, S Sruthi, G R Rajarajeswari*

Department of Chemistry, College of Engineering, Anna University, Chennai, India, 600025

***Corresponding author *e-mail*:** rajiaravind@gmail.com

ABSTRACT

Evolving global burden of multi drug resistant microbes pose a serious challenge to health care in human population by causing an estimated amount of 4.7 million deaths in 2021. Especially in diabetic wounds, the multi drug resistance is known to cause sever effects that even led to the amputation of legs in patients. Addressing the challenges and limitations of the conventional therapeutics in drug delivery and an effective wound healing management is the need of the hour. Zeolitic Imidazolate Frameworks (ZIFs) are the next generation nano materials emerging as the advanced therapeutic and suitable drug carriers for various risky health conditions. The present study investigates the one pot syntheses of ZIF 8 and ZIF 67 by incorporating the extracts of traditional medicinal herbs that has potential wound healing activity, as sustainable drug delivery systems. For the encapsulation, the hydroethanolic extract of medicinal plants were made and utilised in one pot synthesis. The characterization for identifying functional groups using FT-IR confirmed the successful formation of the ZIF 8 and ZIF 67. The SEM images further confirmed the systems are in nano dimensions. Both the ZIF 8 and ZIF 67 is known to possess >90% cell viability at therapeutic concentrations, and having an excellent antimicrobial property against both gram negative *(Escherichia coli)* and gram positive bacteria *(Staphylococcus aureus, Streptococcus bacillus).* Thus, the incorporation of medicinal plants into versatile drug carriers such as ZIFs can be utilised as wound healing materials for treating diabetic foot ulcers, various chronic wounds and for a sustainable drug delivery for day-to-day health risks.

References:

1. L. Govindan, P. Raju, S. Kannaiah, N. Arunprakash, S. Alqahtani and K. Chidambaram, 3 Biotech, 2025, 15, 191
2. S. Puspitarini, M. Budiyanto and F. B. Ilhami, Plant Nanomater. J., 2025, 1, 1–10.
3. A. Arya, S. Kumar, H. Singh, D. Kain and A. M. Ahanger, Inorg. Chem. Commun., 2023, 157, 111394.
4. S. R. Rajpoot, H. M. Asif, K. Ahmad, M. W. Tasleem and K. Ahmad, J. Popul. Ther. Clin. Pharmacol., 2024, 31, 37–48.
5. P. Phatai, C. Pholtue, N. Sihanatang, N. Bantao, K. Prasitnok, P. Khemthong, S. Youngjan, T. Butburee, R. Khunphonoi, S. Kamonwannasit, S. Pinitsoontorn and O. Prasitnok, ChemistrySelect, 2025, 10, e05890.

BM-040

Tailoring the Gelation Kinetics and Visco-Elastic Properties of Pluronic Hybrid Hydrogels: Insights from Rheological Analysis

Aiswarya Gowri V. S[1], Anbumozhi Angayarkanni Somasundaram*[1]

[1]*Soft Matter Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur-603203.*

***Corresponding author e-mail:** anbumoza@srmist.edu.in

ABSTRACT

Structural integrity and mechanical strength are promising characteristics of hydrogels, making them suitable for various applications. Pluronic/chitosan hybrid hydrogel is a biocompatible, mechanically stable hydrogel matrix suitable for advanced biomedical applications. This study aimed to determine the impact of chitosan concentration (0-3% w/v) on physical properties and mechanical behavior of Pluronic/chitosan hybrid hydrogel. Rotational rheology measurements revealed that all formulations exhibited pronounced shear-thinning behaviour. Yield stress rose significantly from 0.16 kPa to 0.31 kPa, with increasing chitosan concentration confirming improved mechanical strength through hydrogen bonding and polymer entanglements. Amplitude sweeps tests identified a well-defined linear viscoelastic region (LVR), with a 21% increase in shear modulus at 0.1% strain, indicating strong hydrogen bonding and structural integrity of the hydrogel. Thixotropic recovery tests showed that with 3% w/v chitosan, accomplished highest structural recovery of 71.42% after complete distortion of the hydrogel at 100 s^{-1}, highlighting good self-healing capability. These finding highlights that the Pluronic/chitosan hybrid hydrogel system demonstrates excellent stability and injectability, making it suitable for various biomedical applications such as minimally invasive drug delivery, tissue engineering, and regenerative medicine.

References:

1. K. E. Enoch and A. A. S. Somasundaram, Surf. Interfaces, 50 (2024) 104475.
2. S. Chatterjee, P. C.-L. Hui, E. Wat, C.-W. Kan, P.-C. Leung, and W. Wang, Carbohydr. Polym., 236 (2020) 116074.

BM-041

Design and Development of Novel ZnZr Alloy Phases for Advanced Biomedical Applications

Smrithi Chandran[1], Hajeesh Kumar Vikraman[2], Sakshi Bajha[1], Anandhakumar Sundaramurthy[1], Kiran Mangalampalli SRN*[3], Ravikirana*[1]

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*Slovak University of Technology in Bratislava, 91724, Slovakia*

[3]*SRM University-AP, Amaravati, Andhra Pradesh, India, 522240*

***Corresponding author e-mail:** ravikirs@srmist.edu.in , kiran.k@srmap.edu.in

ABSTRACT

Alloys are combinations of metals or metals with other elements. Compared to pure metals, alloys offer better corrosion resistance, lower costs, higher strength, and improved workability. Among the various types of alloys, binary alloys have significant applications in mechanical, tribological, and biological fields, which can be beneficial for developing new ideas in the scientific community. Recent studies indicate that ZnZr alloy can be used in the development of vascular degradable stents; however, the single phase of the ZnZr alloy has not been extensively explored. In this work, ZnZr alloy was synthesized by Ball Milling followed by Vacuum Annealing. The backscattered SEM micrograph showed the presence of ZnZr, Zn_2Zr and $ZnZr_4$ multiphases. The finely crushed sample was subjected to Spark Plasma Sintering for high densification. The surface mechanical characteristics of the densified ZnZr pellet were studied with Nanoindentation and the multiphase demonstrated superior properties compared to bare Zn and Zr metal. Further investigations into the cytotoxicity and antibacterial properties of the ZnZr alloy demonstrated enhanced biological performance, thereby supporting its potential suitability for stent applications.

References:

1. N. Annonay et al., Bioact. Mater., 3 (2018) 385–388.
2. J.-J. Luo et al., TMS 2015 144th Annual Meeting & Exhibition: Supplemental Proceedings (2016) 115–121.

BM-042

Multifunctional ZnO/Y_2O_3–Nd_2O_3 Nanocomposite: A Novel Ternary Material for Enhanced Photocatalytic and Anticancer Behaviour

S. Pushpalatha[1*], T. Jose Antony[2, 3], J. Densiya [1], A. Rajendran [1]

[1] *Department of Physics, Nehru Memorial College, Affiliated to Bharathidasan University, Puthanampatti, Tiruchirappalli-621007, Tamil Nadu, India.*

[2]*Department of Physics, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Vadapalani Campus, No.1, Jawaharlal Nehru Road, Vadapalani, Chennai- 600026, Tamil Nadu, India.*

[3]*Sree Balaji Institute of Science and Technology (SBIST), Chromepet, Chennai-600044, Tamil Nadu, India.*

***Corresponding author e-mail:** *pushpithphy@gmail.com*

ABSTRACT

The rapid development of textile manufacturing results in a massive accumulation of dye pollutants in aquatic environments and ecosystems. The coprecipitation method was utilized in synthesizing the ZnO, Y_2O_3, Nd_2O_3, ZnO/Nd_2O_3, Y_2O_3/Nd_2O_3, and ZnO/Y_2O_3–Nd_2O_3 nanocomposites. The prepared materials were analyzed using X-ray diffraction (XRD), which demonstrated the hexagonal crystal structure of ZnO and Nd_2O_3, while Y_2O_3 exhibited a cubic phase. The field emission scanning electron microscopy (FESEM) revealed that the ZnO/Y_2O_3–Nd_2O_3 nanocomposites possess a spherical morphology with smaller particle size and reduced agglomeration. Fourier transform infrared (FTIR) spectroscopy revealed the presence of functional groups in the ZnO/Y_2O_3–Nd_2O_3 samples. Further, UV–visible diffuse reflectance spectroscopy (UV–DRS) was employed to determine the optical bandgap of the nanocomposites, demonstrating that successful tuning of the optical bandgap was achieved. Photoluminescence (PL) analysis confirmed the reduced recombination of photogenerated electron–hole (e^-/h^+) pairs in the ZnO/Y_2O_3–Nd_2O_3 nanocomposite. The antibacterial and antifungal activities of the samples were evaluated against one Gram-positive and three Gram-negative bacterial strains. Cytotoxicity against MCF-7 cells was determined using the MTT assay. The synthesized samples exhibited highly efficient photocatalytic degradation of Methylene blue under UV irradiation, following a pseudo-first-order kinetic model. Notably, the ZnO/Y_2O_3–Nd_2O_3 nanocomposite demonstrated the highest photocatalytic efficiency of 93.6% within 150 min, with a rate constant of 0.01781 min^{-1} and a correlation coefficient (R^2) of 0.98686. Enhanced light absorption across the solar and visible regions confirms the superior photocatalytic performance of the ZnO/Y_2O_3–Nd_2O_3 nanocomposite under UV–Vis light.

Keywords: Coprecipitation method; ZnO/Y_2O_3–Nd_2O_3; Photocatalysis; Anticancer behaviour.

BM-043

Design and Evaluation of a Bioactive Nanocomposite-Coated 3D-Printed PLA Cranial Implant for Enhanced Osseointegration and Antibacterial Performance

R. Sai Sharan, R. Venket Ramanan, V. Nithish Kumar, Fabiola Jemmie Shilparani F, S. Gnanavel*

Department of Biomedical Engineering, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** gnanaves@srmist.edu.in

ABSTRACT

Cranial reconstruction is performed on millions annually, yet conventional materials such as titanium and Polymethyl methacrylate (PMMA) present high complication rates due to infection and poor biological integration. This study proposes a customizable, 3D-printable cranial implant integrating Polylactic Acid (PLA), Hydroxyapatite (HA), Chitosan and Titanium dioxide (TiO_2) to combine bone-mimicking bioactivity with antimicrobial protection. The design aims to promote natural bone regeneration while safely resorbing, reducing long-term infection risks associated with permanent metal or plastic implants. The implant was modelled in AutoCAD using open-source CT datasets and its mechanical behavior was analyzed through ANSYS Finite Element Analysis (FEA). Simulations demonstrated reduced stress shielding by mimicking the elastic modulus of bone, alongside optimized load distribution and minimized peak deformation. PLA was 3D printed using Fused Deposition Modelling (FDM) technique, followed by surface modification to overcome PLA's inherent bio-inertness. 3D printed PLA substrate was surface modified using two different nanocomposite coatings—HA/TiO_2 (NC-1) and HA/Chitosan (NC-2) through controlled spray deposition method to achieve uniform coverage. FTIR, XRD, and SEM confirmed phase integration and homogeneous morphology, while thermogravimetric analysis showed enhanced thermal stability in coated samples. In vitro studies revealed increased cell proliferation and cell viability compared to uncoated PLA and conventional cranial implant materials. Both composites exhibited strong antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*, significantly inhibiting bacterial growth and biofilm formation. Overall, NC-1 and NC-2 transform 3D-printed PLA into a multifunctional, bioactive implant that enhances osteointegration, biocompatibility and mitigates infection risk, offering a cost-effective strategy for patient-specific cranial reconstruction.

Keywords: Fused Deposition Modelling, Bioactive implant, Spray deposition, Finite Element Analysis.

References:

1. J. R. Barcena et al., Bioengineering (Basel), 11 (2024) 705.
2. M. Stevanović et al., J. Mater. Res. Technol., 15 (2021).

BM-044

Biomechanical Analysis of Biodegradable PLA-PCL Screws in Hammer Toe Surgery Using 3D Finite Element Modelling

Yazhini D, Gnanavel S*

[1]SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** gnanaves@srmist.edu.in

ABSTRACT

The foot is one of the most anatomically complex structures in the human body and is highly susceptible to biomechanical disorders due to its dynamic weight-bearing loading conditions. Hammer toe deformity, characterized by plantar flexion at the proximal interphalangeal joint, is one of the most common foot deformities that may require surgical correction in symptomatic or severe cases. Internal fixation screws are widely used to correct the deformity and provide postoperative joint stability, and are commonly made from titanium alloys and stainless steel. However, the high stiffness of metallic implants may contribute to stress shielding at the bone–implant interface. In this study, a bioabsorbable poly (lactic acid)-poly(caprolactone) (PLA-PCL) blend was investigated for its biodegradability and tunable mechanical properties relative to conventional implants. A three-dimensional finite element model was constructed in SolidWorks and implemented in ANSYS to simulate physiological loading conditions and study the stress distribution and load transfer characteristics of the PLA-PCL screw in comparison with titanium and polyetheretherketone (PEEK) fixation screws. The PLA-PCL demonstrated reduced peak von Mises stress and more uniform stress distribution relative to the other evaluated implants.

Keywords: Hammer toe deformity, finite element analysis, internal fixation screws, PEEK, PLA-PCL.

References:

1. Moayedi M, Arshi AR, Salehi M, Akrami M, Naemi R, *Comput. Biol. Med.*, **vol. 135 (2021) 104598*.
2. Basile A, Albo F, Via AG, *J. Foot Ankle Surg.*, vol. 54 (2015) 910–916.
3. Wei RX, Ling SK, Lui TH, Yung PS, *J Orthop Surg (Hong Kong)*, vol. 28 (2020) 2309499020911168
4. Franciosa P, Gerbino S, *Proc. COMSOL Conf. Paris*, (2010).
5. Antunes PJ, Dias GR, Coelho AT, Rebelo F, Pereira T, *Non-linear finite element modelling of anatomically detailed 3D foot model*, Report paper, vol. 1 (2008) 1–11.

BM-045

Tunable Magnetic Hyperthermia Performance of Superparamagnetic Iron Oxide Nanoparticles Through Zinc Doping: A Structural, Magnetic and Relaxation Mechanisms Analysis.

Rahulgorky Sahayaraj, Anbumozhi Angayarkanni Somasundaram*

Soft Matter Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India – 603203

***Corresponding author e-mail:** *anbumoza@srmist.edu.in*

ABSTRACT

Zinc-doped superparamagnetic iron oxide nanoparticles with zinc concentrations of 0, 2, 5, and 10 wt% were synthesized via a co-precipitation method and systematically investigated for their structural, magnetic, and magnetic hyperthermia performance. X-ray diffraction confirmed the formation of single-phase cubic spinel structures with increasing lattice parameters upon Zn incorporation, indicating successful substitution of Zn^{2+} ions into the Fe_3O_4 lattice. FTIR analysis further corroborated the preservation of the spinel framework with progressive shifts in Fe-O vibrational modes due to zinc substitution. Magnetic measurements revealed superparamagnetic behaviour at room temperature for all samples, accompanied by a monotonic decrease in saturation magnetization and coercivity with increasing Zn content, attributable to the replacement of magnetic Fe^{3+} ions by non-magnetic Zn^{2+} ions and reduced magneto crystalline anisotropy. Electron spin resonance spectroscopy demonstrated a systematic reduction in effective anisotropy constant and variations in interparticle interactions as a function of zinc concentration. Magnetic hyperthermia studies conducted under clinically safe alternating magnetic field conditions (500 kHz, 8 kA/m) exhibited a non-monotonic dependence of heating efficiency on Zn doping, with the highest specific absorption rate (18.6 W/g) and effective specific absorption rate (0.58 $nH \cdot m^2 \cdot kg^{-1}$) observed for the 10 wt% Zn-doped sample. The observed enhancement in hyperthermia efficiency at higher Zn concentrations is attributed to the combined effects of optimized particle size, reduced anisotropy, and relaxation dynamics. These findings demonstrate that controlled zinc doping provides an effective route to tuning the magnetic and hyperthermic performance of SPIONs, highlighting their potential for magnetic hyperthermia applications.

References:

1. X. Liu et al., J. Phys. Chem. C, 120 (2016) 1328–1341.
2. G. Kasparis et al., J. Mater. Chem. B (2022). (Volume and pages not provided)
3. Q. Li et al., Sci. Rep., 7 (2017). (Article number not provided)
4. P. Franciosa and S. Gerbino, Proc. COMSOL Conf. Paris (2010).

BM-046

Development of Manganese-Impregnated Nanohydroxyapatite Functionalised with Alendronate as a Synergistic Metalloimmunotherapeutic Adjuvant.

Ashitha K.C and Rajashree Padmanaban*

Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy campus, Chennai – 600025.

***Corresponding author email:** drprajashree@gmail.com

ABSTRACT

Current immunotherapeutic strategy against cancer usually requires accompanying adjuvants to increase the immune response to tumor antigens. Hydroxyapatite (HAP) has emerged as adjuvant for vaccines as it has immunomodulatory potency based on its physiochemical properties. However, a major challenge is to develop immune adjuvants that has stronger immunogenicity, at lower dose and also has no or minimal adverse effect. The incorporation of metallo-immunology principles into cancer vaccine adjuvant development has the potential to enhance their clinical efficacy. Accordingly, manganese (Mn^{2+}), a powerful activator of the cGAS-STING pathway and alendronate (ALN), an activator of mevalonate pathway, a druggable targets for vaccine adjuvant were chosen, yet they show rapid systemic clearance and potential toxicity. The HAP has high affinity for ALN, we designed ALN-functionalized Mn-HAP nanoparticles as an organic-inorganic hybrid adjuvant. In this study, synthesized manganese-impregnated hydroxyapatite (Mn-HAP) followed by the surface functionalisation of ALN. The developed Mn-HAP-ALN nano adjuvant were characterised by XRD, FTIR, SEM. Alendronate release assay in in vitro condition in both physiological and pathological pH depicted a controlled release of ALN. Cytotoxicity of Mn-HAP-ALN nanoadjuvant was tested using dose dependent MTT method, hemocompatibility assay. A protein adsorption was also assessed. Finally, immunomodulation assays with PBMC showed optimal immunostimulation required for the ideal vaccine, thus Mn-HAP-ALN nanoadjuvant system effectively bridges metallo-immunotherapy, this platform represents a promising strategy for next-generation vaccine adjuvant formulation.

Keywords: Hydroxyapatite, Manganese, Alendronate, Vaccine Adjuvant, cGAS-STING pathway.

References:

1. Zhang, X., Wei, M., Zhang, Z., Zeng, Y., Zou, F., Zhang, S., ... & Xia, N. (2024). Risedronate-functionalized manganese-hydroxyapatite amorphous particles: A potent adjuvant for subunit vaccines and cancer immunotherapy. *Journal of Controlled Release*, *367*, 13-26.
2. Bulut, O., Kilic, G., Debisarun, P. A., Röring, R. J., Sun, S., Kolkman, M., ... & Netea, M. G. (2024). Alendronate modulates cytokine responses in healthy young individuals after BCG vaccination. *Immunology letters*, *267*, 106851.
3. Russell, R. G. G., Xia, Z., Dunford, J. E., Oppermann, U. D. O., Kwaasi, A., Hulley, P. A.& Ebetino, F. H. (2007). Bisphosphonates: an update on mechanisms of action and how these relate to clinical efficacy. *Annals of the New York Academy of Sciences*, *1117*(1), 209-257.

BM-047

Design and Development of Biomimetic Ti_6Al_4V Scaffolds Via Metal Additive Manufacturing: Bio-Functionalization, *In-Vitro* and *In-Vivo* Studies

K. Venkatesan[1, 2,3], Deepak K. Pattanayak[1, 2*]

[1]*Electrochemical Process Engineering Division, CSIR- Central Electrochemical Research Institute, Karaikudi- 630003, Tamil Nadu, India.*

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.*

[3]*Institute for Frontier Materials, Deakin University, Australia*

ABSTRACT

Additive manufacturing (AM) of metallic implants is an upcoming technology where any customized and complex structured implants or scaffolds could be developed. However, osseointegration and infection resistance of AM Ti_6Al_4V(Ti_{64}) scaffolds are poor and thus lead to implant loosening and failure. Hence, the present study aimed to develop biomimetic strategies to overcome these drawbacks. Initially, process parameters of Selective Laser Melting (SLM) and post-treatment techniques of Ti_{64} alloy were optimized to manufacture a biomimetic scaffold. Further, it was biofunctionalized through chemical/electrochemical technique by forming a nano-network and an array of titania nanotubes (TNTs) with the incorporation of Ca/Ag. The functionalization triggered antibacterial activity against *S. aureus* and *E. coli* bacterial strains. The *in-vitro* cytotoxicity test using cell lines revealed more than 90 % cell viability and excellent cell adhesion characteristics. It also induced bioactivity and increased corrosion resistance behavior in the SBF medium. The *in-vivo* evaluation of the surface-modified 3D-Ti_{64} scaffolds in the rabbit model demonstrated excellent osteointegration ability. These findings suggest that the chemically/electrochemically modified scaffolds possess the necessary bioactivity, osseointegration ability, antimicrobial properties, and corrosion resistance for effective use in hard tissue replacement applications.

Keywords: Additive Manufacturing, Ti_{64} scaffolds, anti-bacterial, biocompatibility, osseointegration and corrosion resistance.

BM-048

Sustainable Co-Doping Strategy in TiO_2 Nanoparticles Using Kalanchoe pinnata: A Green Route to Enhanced Functional Nanomaterials

Arun Kumar D[1], Anushiya S[1], Satish Kumar R.C.[1], Kesavan M[1]*

[1]*Interdisciplinary Institute of Indian System of Medicine, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203.*

***Corresponding author e-mail:** kesavanm@srmist.edu.in

ABSTRACT

Titanium dioxide (TiO_2) nanoparticles are widely recognized for their photocatalytic, antibacterial, and antioxidant properties, but concerns over chemical methods have driven interest in green synthesis alternatives. This study presents the eco-friendly synthesis of Strontium (Sr) and Magnesium (Mg) co-doped TiO_2 nanoparticles using *Kalanchoe pinnata* leaf extract as a reducing and stabilizing agent. The synthesis involved preparing aqueous leaf extract from fresh *Kalanchoe pinnata* leaves, mixing it with titanium precursor (Titanium Tetra Isopropoxide) and dopants Strontium and Magnesium Nitrates. The nanoparticles were characterized using Fourier Transform Infrared (FTIR) spectroscopy, X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), UV-Visible spectroscopy and Cyclic Voltammetry (CV) to confirm phase formation, morphology, composition, and electrochemical behaviour. The doped TiO_2 nanoparticles demonstrated enhanced antibacterial activity against *Escherichia coli* and *Staphylococcus aureus* via well diffusion method compared to undoped TiO_2. They also exhibited improved antioxidant potential in DPPH assays, superior photocatalytic dye degradation, and promising electrochemical performance relative to undoped counterparts. These multifunctional Sr/Mg-doped TiO_2 nanoparticles, synthesized sustainably using *Kalanchoe pinnata* extract, shows promising biomedical, environmental and energy storage applications.

References:

1. Tasisa, Y.E., Gunasekaran, M. & Krishnaraj, R. Green synthesis of Ca/Sr co-doped TiO_2 nanoparticles: impact on morphology, band gap reduction, supercapacitor, and visible-light photocatalytic efficiency. *Discov Appl Sci* 7, 979 (2025). https://doi.org/10.1007/s42452-025-06976-5.
2. Shanavas, S., Priyadharsan, A., Karthikeyan, S., Dharmaboopathi, K., Ragavan, I., Vidya, C., ... & Anbarasana, P. M. (2020). Green synthesis of titanium dioxide nanoparticles using Phyllanthus niruri leaf extract and study on its structural, optical and morphological properties. *Materials Today: Proceedings*, *26*, 3531-3534.
3. Tasisa, Y.E., Gunasekaran, M., Sarma, T.K. *et al.* Enhanced photocatalytic and electrochemical properties of green synthesized strontium doped titanium dioxide nanoparticles for dye removal and supercapacitor applications. *Sci Rep* **15**, 10452 (2025). https://doi.org/10.1038/s41598-025-95111-w.

BM-049

Evaluating the Influence of Material Composition on Dental Restoration Systems Using Finite Element Analysis

Fabiola Jemmie Shilparani F[1], Gnanavel S[1*] and Vamsi Krishna Dommeti[2]

[1]*Biomaterials Laboratory, Department of Biomedical Engineering, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Tamilnadu, 603203, India*

[2]*Department of Mechanical Engineering, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, TamilNadu, 603203, India*

***Corresponding author e-mail:** gnanaves@srmist.edu.in

ABSTRACT

Implant-supported dental restoration systems are a well-recognised method for permanent tooth replacement. The long-term performance and fatigue life of these systems are significantly affected by the materials utilised in the production of their components, including the crown and implant fixture (abutment and screw). Contemporary commercial systems often utilise zirconia for the crown and 316L stainless steel for the other components. Emerging materials, such silica-based ceramics for crowns and low-modulus titanium alloys such as Ti-$_6$Al-4V and Ti-13Nb-13Zr for structural components, have opportunities for improved biomechanical performance and biocompatibility. This work utilised finite element analysis (FEA) to assess the distribution of von Mises stress and Mohr-Coulomb Stress ratio, safety factor, and anticipated fatigue life of the dental restoration system under masticatory forces at 100 N. Four distinct materials, comprising two notional nanocomposites, were investigated for the crown, while three materials—316L stainless steel, Ti-6Al-4V, and Ti-13Nb-13Zr—were analysed for the implant fixture. Results demonstrated that both nanocomposites surpassed conventional zirconia in diminishing stress and stress ratio, exhibiting a favourable safety factor and prolonging fatigue life in the crown. Ti-13Nb-13Zr demonstrated the most advantageous stress response, safety factor, and fatigue resistance among load-bearing components, exceeding the performance of both 316L stainless steel and Ti-6Al-4V. These findings highlight the significance of material selection in enhancing the durability and mechanical integrity of dental implant systems. The research offers a computational framework for the preclinical evaluation of innovative biomaterials, including nanocomposites, intended for next-generation dental prosthesis

References:

1. Tiu J, Al-Amleh B, Waddell J N and Duncan W J *J Prosthet Dent* **113** (2015) 175-84
2. Koc D, Dogan A and Bek B *European Journal of Dentistry* **04** (2019)223-32
3. Abu Kasim N H, Madfa A A, Hamdi M and Rahbari G R *Dent Mater J* **30 (**2011**)** 869-80
4. Huang J, Yao M, Lin J and Yao X *Materials Letters* (2022)**307**

BM-050

Bioactive Thiolated Mesoporous Silica @ L-Arginine modified Sodium Alginate/ Guar Gum Thin films for Blood compatible Wound Healing

Anishia Ambrose[1], Kalaivizhi Rajappan[1*], Ganesh Munuswami Ramanujam[2], Aswathy Karanath Anilkumar[3]

[1] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu-603203, Tamilnadu, India*

[2] *Molecular Biology and Immunobiology Division, Interdisciplinary Institute of Indian System of Medicine,*

SRM Institute of Science and Technology, Kattankulathur, Chengalpattu-603203, Tamilnadu, India.

[3] *Department of Biotechnology, Faculty of Engineering and Technology,*

SRM Institute of Science and Technology, Kattankulathur-603203, Tamilnadu, India

***Corresponding author e-mail:** kalaivir@srmist.edu.in

ABSTRACT

Wound healing is a significant worldwide health issue that may complicate the regular activities of human life. Notwithstanding the widespread availability of several wound healing materials, the quest for an optimum blood compatible wound healing substance persists. This study aims to develop an optimal wound healing material that is blood compatible, exhibiting enhanced biocompatibility and wound healing efficacy. Sodium alginate (SA) is utilized for its efficacious healing properties and its capacity to sustain a moist microenvironment. It is additionally functionalized with L-arginine to augment the production of collagen, epithelialization and wound healing. L-arginine-modified SA is subsequently mixed with guar gum (GG) to improve its characteristics. Thiol-functionalized mesoporous silica nanoparticles were utilized for their enhanced antioxidant capacity and hemocompatibility. The solvent casting method is adopted for the preparation of films. The prepared films and the nanocomposites underwent physicochemical and biomedical characterizations to confirm their suitability for wound healing applications. The hemocompatibility studies shows 92 % compatibility with blood and the resultant material exhibits 86 % wound closure over 24 hours. The evaluations explain that the prepared Thiolated mesoporous silica @ l-arginine modified SA/ GG thin films are ideal for wound healing applications. In the future, advancing *in-vivo* investigations will be crucial for clinical applications.

Keywords: L-arginine, Thiolated, Mesoporous silica nanoparticles, hemocompatibility, in-vitro scratch assay, cytocompatibility, guar gum

References:

1. Dam, P., Celik, M., Ustun, M., Saha, S., Saha, C., Kacar, E. A., ... & Mandal, A. K. (2023). Wound healing strategies based on nanoparticles incorporated in hydrogel wound patches. *RSC advances*, *13*(31), 21345-21364.
2. Lin, X.; Yang, X.; Li, P.; Xu, Z.; Zhao, L.; Mu, C.; Li, D.; Ge, L. Antibacterial Conductive Collagen-Based Hydrogels for Accelerated Full-Thickness Wound Healing. *ACS Appl Mater Interfaces* **2023**, *15* (19), 22817–22829. https://doi.org/10.1021/acsami.2c22932.

BM-051

Nanostructured Hydroxyapatite Derived from Cowrie Shells Incorporated into PCL for Enhanced Osteogenic Differentiation

Stephen S, Kalaivizhi R*

Department of Chemistry, Faculty of Engineering and Technology,

SRM Institute of Science and Technology, Kattankulathur, Chengalpattu-603203, Tamilnadu, India

***Corresponding author e-mail:** kalaivir@srmist.edu.in

ABSTRACT

Bone tissue regeneration remains a critical challenge in orthopedics particularly in the treatment of osteoporosis and larger bone defects. Conventional techniques have several drawbacks, such as poor bioactivity and infection. Polymer based scaffolds attracted increasing interest in bone tissue regeneration due to their tunable properties and biocompatibility. Polycaprolactone (PCL) is a synthetic polyester with a hydrophobic nature and inadequate bioactivity. PCL has been widely used in the fabrication of polymeric scaffolds in bone tissue regeneration, providing adequate mechanical strength and biocompatibility. Cowrie shell is a natural biomimetic source that can be synthesized into hydroxyapatite (HA), which adds bioactivity and osteoconductivity when added with PCL matrices. Combining PCL/HA enhance the scaffolds porosity and mimics the natural mineral composition of human bone. This scaffold enhances cell proliferation and mineralization which accelerates bone healing. This study aims to develop a biomimetic scaffold derived from natural shell sources. The hypothesis is to combine modern polymer science with biomineral sources to yield hybrid scaffolds for effective bone tissue regeneration.

Keywords: Polycaprolactone, Hydroxyapatite, Bone Tissue Regeneration

Reference:

1. Mejía Suaza, M. L., Leos Rivera, J. C., Moncada Acevedo, M. E., Ossa-Orozco, C. P., Uribe Yunda, D., & Zarate Triviño, D. G. Polycaprolactone, silk fibroin and silver nanoparticles scaffolds as a substrate for bone tissue engineering. *Materials Technology*, 40(1), 2529502.
2. Danagody, B., Bose, N., & Rajappan, K. Bioinspired hydroxyapatite-incorporated polyacrylonitrile nanofiber and amoxicillin-loaded cellulose acetate bilayer membrane with tunable osteoconductivity for bone regeneration. *ChemNanoMat*, 00, e202400576.

BM-052

Liposomes Containing Zinc-Based Chemotherapuetic Drug Block Proliferation and Trigger Apoptosis in Breast Cancer Cells

Radhakrishnan Sarankumar[1], Mallayasamy Siva[1], Priyadip Das*[1]

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** priyadip@srmist.edu.in

ABSTRACT

Platinum-based chemotherapeutic drugs are effective in killing malignant cells but often trigger drug resistance or off-target side effects. Unlike platinum, zinc is used as an endogenous cofactor for several cellular enzymes and may, thus, display increased biocompatibility. In this study, it focuses on designation and development of two substituted phenanthro[9,10-d]imidazole-based ligands, L1 and L2, bearing pyridine and quinoline substitution at the 2-position, along with their corresponding Zn(II) complexes, $(L1)_2Zn$ and $(L2)_2Zn$. These complexes were characterized using standard analytical and spectroscopic methods. Notably, $(L2)_2Zn$, but not $(L1)_2Zn$, exhibited intrinsic fluorescence, indicating its potential utility in imaging applications. To facilitate cellular uptake, liposomal formulations were generated using the phospholipid DMPC (1,2-dimyristoyl-sn-glycero-3-phosphocholine) through molecular self-assembly. The resulting liposomal complexes, Lip-$(L1)_2Zn$ and Lip-$(L2)_2Zn$, successfully entered breast cancer cells, induced DNA fragmentation, arrested the cell cycle at the G0/G1 phase, decreased cellular proliferation, and promoted apoptosis via activation of the DNA damage response.Importantly, both Lip-$(L1)_2Zn$ and Lip-$(L2)_2Zn$ reduced the size of breast cancer cell-based spheroids, suggesting their potential to suppress tumor growth. Overall, this work represents an important proof-of-concept demonstrating that liposomal formulations of phenanthro[9,10-d]imidazole-based Zn(II) complexes with inherent optical properties hold significant promise for the development of imaging probes and efficient anticancer therapeutics.

References:

1. M. Siva, K. Das, S. Guha, S. Sivagnanam, G. Das, A. Saha, A. Stewart, B. Maity, P. Das, ACS Appl. Bio Mater., 6 (2023) 5310–5323.

BM-053

Boerhavia Diffusa-Assisted Green Synthesis of Gold Nanoparticles with Enhanced Heavy Metal Sensing, Catalytic, and Antimicrobial Properties

Divya Arulraj[1], John Dennis[1], Kesavan. M[3], Jegadheeshwari. S[2,3], Tapan Kumar Mistri[1,*]

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur - 603 203, Tamil Nadu, India.*

[2]*Department of Biotechnology, School of Bioengineering, SRM Institute of Science and Technology, Kattankulathur – 603 203, Tamil Nadu, India.*

[3]*Interdisciplinary Institute of Indian System of Medicine, SRM Institute of Science and Technology, Kattankulathur – 603 203, Tamil Nadu, India.*

***Corresponding author e-mail: tapankum@srmist.edu.in**

ABSTRACT

The green synthesis of gold nanoparticles using *Boerhavia diffus*a (*B. diffusa*-AuNPs) leaves extract provides an eco-friendly alternative to chemical methods. The present study reports the rapid, one-pot synthesis of stable AuNPs, characterized by UV-Vis, FTIR, HR-TEM, XRD, and DLS, revealing spherical particles of 37 ± 4 nm stabilised by plant polyphenols. B. diffusa-AuNPs selectively detected Fe^{3+} and Hg^{2+} ions through a red shift in their LSPR band, indicating colorimetric sensing capability. SEM analysis confirmed that ion-induced nanoparticle aggregation was responsible for the sensing response. *B. diffusa*-AuNPs scavenged 75% of stable and toxic 1,1-diphenyl-2-picryl-hydrazil (DPPH) radicals. Moreover, the antibacterial study revealed that B. diffusa-AuNPs exhibited strong activity against both Gram-positive and Gram-negative bacterial strains. Remarkably, *B. diffusa*-AuNPs achieved photocatalytic degradation efficiencies of 98.99% for methylene blue and 99.74% for congo red dyes within 10 minutes. These versatile AuNPs show significant potential for applications in environmental remediation and biomedical fields.

Keywords: Gold nanoparticles, antibacterial activity, antioxidant activity, catalytic degradation, colourimetric sensor.

References:

1. M.S. Kirans et al. Green synthesis and characterization of gold nanoparticles from Moringa oleifera leaves and assessment of antioxidant, antidiabetic and anticancer properties, *Chemical Data Collections* 33 (2021) 100714.
2. M. Hosny et al. Comparative study between Phragmites australis root and rhizome extracts for mediating gold nanoparticles synthesis and their medical and environmental applications, *Advanced Powder Technology* 32 (2021) 2268–2279.
3. N. Alikhani, et al. Green synthesis of gold nanoparticles (Au NPs) using Rosa canina fruit extractand evaluation of its catalytic activity in the degradation of organic dye pollutants of water, Inorg. Chem. Commun. 139 (2022) 109351.
4. T. Do Dat et al. Green synthesis of gold nanoparticles using Andrographis paniculata leave extract for lead ion detection, degradation of dyes, and bioactivities, Biochem. Eng. J. 200 (2023) 109103.

BM-054

Investigating the Antibacterial Activity of Homoleptic Bipyridine-Based Polypyridyl Iron(II) Complexes: Probing the Role of Ligand Design in Antibacterial Function

Porshia R[1], Naveen Malik*[1]

[1] *SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** naveenm1@srmist.edu.in

ABSTRACT

Novel Fe(II) complexes featuring (I) 4,4'-dimethyl-2,2'-bipyridine and (II) (E)-4-methyl-4'-(2-(pyridin-4-yl)vinyl)-2,2'-bipyridine ligands, coordinated in an octahedral geometry, were successfully synthesized and characterized using UV-visible, Infrared, NMR (nuclear magnetic resonance), and Mass spectroscopies, along with electrochemical techniques. Their antibacterial activity was evaluated against both Gram-positive and Gram-negative bacteria. In agar well diffusion assays, complex (II) demonstrated susceptibility against Escherichia coli, a Gram-negative bacterium and moderate activity against Salmonella enterica, also a Gram-negative bacterium. Additionally, both complexes (I) and (II) exhibited significant antimicrobial activity against Gram-positive strains, including Staphylococcus epidermidis, Staphylococcus aureus, and Bacillus subtilis. The presence of a free ligand, specifically the addition of a pyridine arm in complex (II), appears to contribute to the enhanced antibacterial activity observed; however, the underlying mechanism remains under investigation.

References:

1. Julia A. Eremina, Ekaterina A. Ermakova, Ksenia S. Smirnova, Polyhedron, 206 (2021) 115352.
2. Oladipo Mary Adelaide, Olaoye Oluwabiyi James, Elixir Applied Chemistry, 67 (2014) 21413-21420.
3. Carol, D., C. Barry, M. McCann, Chemico-biological interactions, 164 (2006) 115-125.

BM-055

A Strategy to Inhibit Protein Corona Formation and Bacterial Infection Using Fluorinated Silver Nanoparticles for Infection-Resistant Wound Dressings

Shyam Ganesh, Hemanathan Elango, Suman Nayak, Priyadip Das*, Abhijit Saha*

Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu-603203, India

*** Corresponding author. Email ID:** saha.abhijit.g3@gmail.com; abhijits@srmist.edu.in, priyadipcsmcri@gmail.com; priyadip@srmist.edu.in

ABSTRACT

Protein corona formation, followed by biofilm formation at the wound site, promotes infection spread and delays wound healing. Therefore, we need a material that can simultaneously prevent protein and bacterial adhesion on the surface. In this manuscript, we showed a fluorinated silver nanoparticle-based strategy to inhibit protein corona formation and bacterial adhesion for infection-resistant wound dressing applications. We coated silver nanoparticles (Ag NPs) with 2,2,2-trifluoroethyl amine and 4-fluorobenzyl amine and prepared fluorinated silver nanoparticles, C_1 and C_2, respectively. The C_1 and C_2 were characterized by UV, FT-IR, XPS, DLS, Zeta potential, SEM, and TEM analysis. We observed that C_1 and C_2 absorbed a very small amount of protein compared to bare Ag NPs, as well as preventing bacterial adhesion on the surface. For application, a common bandage was coated with C_1 and C_2, and we observed no bacterial growth on the bandage, and the C_1 and C_2 also reduced the bacterial growth in the surrounding medium, i.e., providing a solution to reduce bacterial infection at the wound site.

BM-056

Structural and Functional Evaluation of a Protein-Derived Nanofibrillar Hydrogel for Skeletal Muscle Engineering

Ankit Srivastava[1]*

[1]*Department of Biotechnology & Chemical Engineering, Manipal University Jaipur, Jaipur 303007, Rajasthan, India*

***Corresponding author e-mail:** ankitsreevastava@gmail.com, ankit.srivastava@jaipur.manipal.edu

ABSTRACT

Nanofibrillar protein hydrogels provide biomimetic architectures suitable for skeletal muscle tissue engineering. A nanofibrillar lysozyme hydrogel was fabricated and comprehensively characterized to assess its structural, mechanical, and biological performance as a three-dimensional scaffold. CD spectroscopy showed an α-helix to β-sheet transition (~218 nm), while FTIR revealed a dominant amide I band at 1624 cm^{-1}, confirming cross-β assembly. Oscillatory rheology and AFM nanoindentation demonstrated stable viscoelastic behavior ($G' = 1.8 \pm 0.2$ kPa) and a homogeneous Young's modulus of 2.1 ± 0.3 kPa. The hydrogel showed an equilibrium swelling ratio of $420 \pm 35\%$ and limited mass loss (~18%) under physiological conditions. Electron microscopy revealed an interconnected porous network (20-80 µm pores) and confirmed nanofibrillar scaffold (8-12 nm diameter). Rabit skeletal muscle cells exhibited >92% viability, enhanced metabolic activity, and expression of MyoD and myosin heavy chain with aligned multinucleated myotube formation. These results validate nanofibrillar lysozyme hydrogel as a mechanically appropriate and biocompatible scaffold for muscle regeneration.

Keywords: Nanofibrils; Hydrogel scaffold; Myoblast viability; Regenerative biomaterials; Tissue scaffold; Biocompatibility

BM-057

Bagasse-Derived Graphene Quantum Dots Eco - Friendly Synthesis, Characterization and its Anti-oxidant Activity

S. Vignesh [1], J. Judith Vijaya [2], A. John Bosco [1*]

[1] *Department of chemistry, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu District, Tamil Nadu – 603 203, India.*

[2] *Department of chemistry, Loyola College (Autonomous), Nungambakkam, Chennai,Tamil Nadu – 600034*

Corresponding authors e-mail: johnbosa@srmist.edu.in, judithvijaya@loyolacollege.edu.in

ABSTRACT

Green synthesis of Graphene Quantum Dots (GQD's) is a promising strategy in maintaining sustainable environment. Main motivation of this work is to convert carbon based agricultural waste sugarcane bagasse into value added product (GQD's). Selective degradation of the raw material were carried out using hot water pretreatment method. Here, we report the synthesis of (GQD's) by hydrothermal method. Surface morphology, electronic structure, band gap energy and functional group of the prepared material were analyzed using characterization techniques. Antioxidant activity of the green synthesized (GQD's) were examined in comparison with the standard ascorbic acid. 50 µg/mL concentration of material showing optimum antioxidant activity of 86% confirming the excellent antioxidant activity of GQD.

Keywords: Green synthesis, hot water pretreatment, hydrothermal method, antioxidant activit.

References

1. Abbas, Aumber, Lim Tuti Mariana, and Anh N. Phan. "Biomass-waste derived graphene quantum dots and their applications." Carbon 140 (2018): 77-99.
2. Kharangarh, Poonam R., et al. "Synthesis of luminescent graphene quantum dots from biomass waste materials for energy-related applications—an Overview." Energy Storage 5.3 (2023): e390.
3. Chai, Xinyu, et al. "A hydrothermal-carbonization process for simultaneously production of sugars, graphene quantum dots, and porous carbon from sugarcane bagasse." Bioresource technology 282 (2019): 142-147.

BM-058

Hybridizing Coumarins with IMiDs: A Platform for Structure-Guided Design of Bioactive Small Molecules

Nikila C[1] and R Mohan Kumar[1, 2*]

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur – 603203.*

[2]*Interdisciplinary Institute of Indian System of Medicine, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur – 603203.*

***Corresponding author e-mail:** mohankur@srmist.edu.in

ABSTRACT

Immunomodulatory drugs (IMiDs) such as lenalidomide are clinically vital molecular glues that recruit neo-substrates to cereblon (CRBN) for ubiquitination and degradation. Herein, we describe a versatile hybrid platform in which the glutarimide nitrogen of lenalidomide is directly functionalised with diversely substituted coumarin-3-carboxylic acids.[1-4] Amide coupling under mild conditions afforded all hybrids in good to excellent yields. Molecular docking into the CRBN-lenalidomide co-crystal structure revealed that the coumarin appendage is well accommodated in solvent-exposed regions, with 7-hydroxy and 7-methoxy derivatives displaying the most favourable predicted binding poses. Antiproliferative screening against cervical (SiHa) and colorectal (HCT116) cancer cell lines identified several hybrids exhibiting low- to sub-micromolar potency, with the 7-hydroxycoumarin–lenalidomide conjugate emerging as the lead compound. This work establishes a robust scaffold for further development of cereblon-modulating agents and theranostic probes.

Keywords: cereblon; lenalidomide; amide coupling reaction; benzotriazole-mediated coupling; bioactive scaffold

References:

1. Y.R. Prasad, A.L. Rao, and L. Prasoona, Bioorganic & Medicinal Chemistry Letters, 2005, 15, 5030-5034.
2. N. Gökhan-Kelekçi, S. Yabanoglu, and E. Küpeli, Bioorganic & Medicinal Chemistry, 2007, 15, 5775-5786.
3. J. Venkatesan, B.N. Sinha, and G. Ucar, Bioorganic & Medicinal Chemistry Letters, 2008, 18, 6362-6368.
4. M.J. Matos, D. Viña, and E. Quezada, Bioorganic & Medicinal Chemistry Letters, 2009, 19, 3268-3270.

BM-059

Rational Design of Enzyme-Responsive Fluorescent Organoruthenium Prodrug for Real-Time Tracking of Cargo Release and Cytotoxicity

Karnan Sugantharam,[1] Chezhiyan Sumithaa[1], Vadde Ramu,[2] and Nils Metzler-Nolte,[2] and Mani Ganeshpandian[1]*

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603203, India.*

[2]*Faculty of Chemistry and Biochemistry, Chair of Inorganic Chemistry I – Bioinorganic Chemistry, Ruhr University Bochum, Universitätsstraße 150, 44801 Bochum, Germany.*

***Corresponding author e-mail:** ganeshpm@srmist.edu.in

ABSTRACT

Stimuli-responsive controlled delivery and real-time release monitoring are crucial for metallo-chemotherapeutics to overcome the obstacles they face during (pre)clinical development. In this study, we structurally modified a conventional half-sandwich Ru(arene) complex into a single-component fluorogenic as well as esterase-responsive nanosystem via functionalizing the NN-bidentate ligand with 10,12-pentacosadiynoic acid (PCDA) derivative, thereby designing amphiphilic complex and further adopting the co-assembly strategy. Prior to obtain the nanoassembly, in an attempt to infer the benefits of functionalizing the ligand, a series of four organoruthenium complexes including the amphiphilic complex were prepared and characterized well. This nano-assembly is found to release the Ru complex in the presence of porcine liver esterase in concomitant with the four-fold increase in its fluorescence intensity. Such a stimuli-responsive behaviour is exploited for real-time release monitoring of Ru complex and understanding its functionality to induce cell death in THP-1 cancer cells. Compared to free Ru complex, this nanosystem exhibited higher cytotoxicity towards HeLa cells and lower toxicity in non-cancerous GM-5756 cells. Zebrafish embryo toxicity analysis confirmed its biocompatibility and uptake for further possible *in vivo* studies. GSH-binding could be a possible mechanism of cytotoxic action of the released Ru complex.

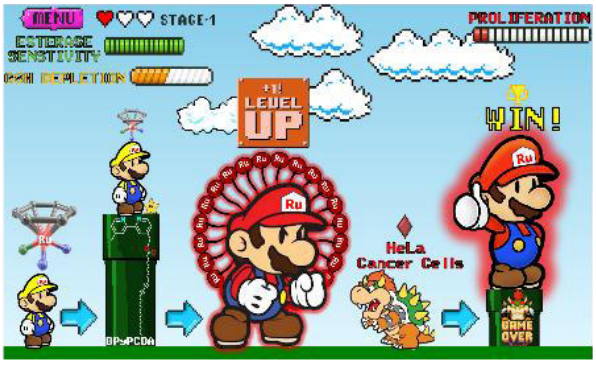


Fig. 1. Graphical abstract

Keywords: Real-time release monitoring; metallo-chemotherapeutics; amphiphilic complex

References:

1. F. Zheng, W. Xiong, S. Sun, P. Zhang and J. J. Zhu, *Nanophotonics*, **8**(2019), 391–413.

2. Sumithaa, C., Sugantharam, K., Karanath-Anilkumar, A., Munuswamy-Ramanujam, G. and Ganeshpandian, *Chem. Comm.*, **60**(2024), 9566-9569.

BM-060

Mechanical Flexibility, Photosalience, and Acidochromism of Benzylidene Indanone-Based Molecular Crystals

Riyaaz Ahamed, Soumyajit Ghosh*

Crystal Engineering and Supramolecular Chemistry Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603 203, Tamil Nadu, India.

***Corresponding author mail:** soumyajitghosh89@gmail.com, soumyajs@srmist.edu.in

ABSTRACT

Molecular crystals that respond to multiple external stimuli are of great interest in smart, responsive materials in various fields.[1] However, the integration of multiple responsive properties within the same crystal remains a significant challenge for materials scientists due to the complex structural and electronic interactions. This work pushes that frontier further by showcasing how benzylidene indanone derivatives can integrate mechanical flexibility, photosalience, and acidochromism[2] in crystalline system. Here crystal 1 is mechanically brittle but exhibits light-induced photosalient splitting and jumping when exposed to UV light. This dynamic response is attributed to a [2+2] cycloaddition reaction, where strain energy accumulates and is subsequently released, causing fragmentation and jumping. Interestingly, crystal 1 retains its photosalient behavior even after acid treatment. In contrast, crystal 2 demonstrates anisotropic mechanical flexibility, showing elasticity on one face and plasticity on others. This distinct mechanical behavior is linked to the weak noncovalent interactions within its layered crystal structure. Both crystals 1 and 2 also exhibit reversible acidochromism. They undergo a reversible color change from pale-yellow to orange-red (crystal 1) or orange-yellow (crystal 2) when exposed to acid vapor and revert to their original color upon exposure to base vapor. This phenomenon results from the protonation and deprotonation of the carbonyl group, which significantly influences the electronic conjugation and intramolecular charge transfer within the molecules. With this successful integration of these multistimuli-responsive features, these materials are highly promising and leap towards significant potential applications, including flexible acid sensors, multifunctional responsive smart devices, and actuators, paving the way for advanced smart or intelligent molecular materials with tunable mechanical and optical properties.[3]

Keywords: Mechanical flexibility, Photosalient and Reversible acidochromism.

References

1. L. Li et al., *Chem. Sci.*, 2019, **10**, 7327–7332.
2. T. Parthasarathy et al., *Cryst. Growth Des.*, 2024, **25**, 309–318.
3. C. Wei et al., *Chem. Soc. Rev.*, 2024, **53**, 3687–3713.

BM-061

IoT-Enabled Paper-Based Colorimetric Sensor Using Nanomaterials for Detection of Urinary Biomarkers

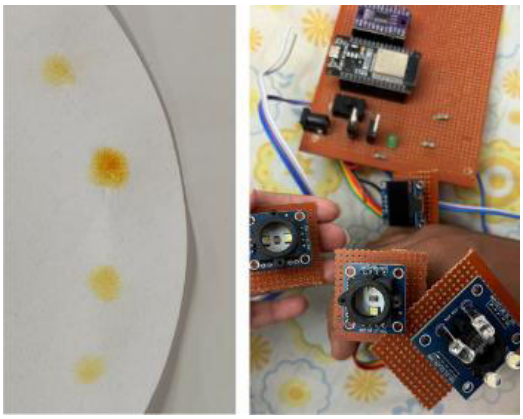
Hiruthic Roshan.M[1], Ravinna P S[1], Dr. Sruthi Ann Alex[1]*

[1] *Department of Biomedical Engineering, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, India – 603203*

***Corresponding author e-mail:** sruthia@srmist.edu.in

ABSTRACT

Urinary biomarkers such as glucose, urea, and creatinine are important indicators for monitoring metabolic activity and kidney function. The detection of these biomarkers plays a key role in the early diagnosis of diseases such as diabetes and renal disorders. However, conventional urinalysis techniques generally require laboratory instruments and trained personnel, which limits their use for rapid and routine monitoring outside clinical settings. In this study, a paper-based colorimetric sensor was developed for the simultaneous detection of glucose, urea, and creatinine in urine samples. Silicon dioxide (SiO_2) and reduced graphene oxide (rGO) were incorporated to enhance sensing performance. The sensor was designed with separate reaction zones containing specific reagents for each biomarker. Visible color changes were analyzed using an RGB sensor and transmitted to a mobile device through an IoT system.



Keywords: Paper-based sensor, Colorimetric detection, Glucose detection, Urea detection, Creatinine detection, Silicon dioxide (SiO_2), Reduced graphene oxide (rGO), RGB sensing.

References

1. A. K. Yetisen, M. S. Akram, C. R. Lowe, *Lab Chip*, 13 (2013) 2210–2251.
2. C. Parolo, A. Merkoçi, *Chem. Soc. Rev.*, 42 (2013) 450–457.
3. A. K. Geim, K. S. Novoselov, *Nat. Mater.*, 6 (2007) 183–191.
4. K. S. Novoselov, A. K. Geim, S. V. Morozov, *Science*, 306 (2004) 666–669.
5. J. Li, Y. Kuang, Y. Shi, *ACS Appl. Mater. Interfaces*, 4 (2012) 645–650.

BM-062

Mechanically Flexible Pentadienenitrile Derivative Based Molecular Crystals Exhibiting Distinct Photoresponsive Behavior

Vishnukumar Thanasekar, Soumyajit Ghosh*

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** soumyajitghosh89@gmail.com, soumyajs@srmist.edu.in

ABSTRACT

Photoresponsive molecular crystals constitute an emerging class of functional crystalline smart materials that have garnered considerable attention due to their capacity to convert light energy into mechanical motion.[1] These light-induced responses, known as photomechanical effects, render these crystals promising candidates for advanced photoactuators, photonic devices, and intelligent materials. In this study, we synthesized two novel diphenylpenta-2,4-dienenitrile derivative crystals (Crystals **1** and **2**), which demonstrate mechanical flexibility[2] and distinct photomechanical responses[3] to 420 nm LED irradiation. Notably, Crystal **1** exhibited sequential bending, initially away from the light source and subsequently towards it upon prolonged exposure, whereas Crystal **2** exhibited photosalient breaking. These divergent responses are attributed to [2+2] photocycloaddition reactions occurring within the crystal lattice.[4,5] The variations in kinematic behavior are ascribed to differences in the accumulation and subsequent release of strain energy during photocycloaddition. The synergistic integration of photomechanical activity and mechanical flexibility underscores the multifunctional nature of these materials, offering critical insights for the design of crystals with potential applications in optoelectronics, photonics, and molecular switches, thereby expanding the scope of future photoresponsive organic materials.

Keywords: Mechanical flexibility; Photomechanical responses; [2+2] Photocycloaddition; Structure-property correlation.

References:

1. Q. Yu, B. Aguila, J. Gao, P. Xu, Q. Chen, J. Yan, D. Xing, Y. Chen, P. Cheng, Z. Zhang, and S. Ma, *Chem. Eur. J.* **25** (2019) 5611–5622.
2. S. Saha, M. K. Mishra, C. M. Reddy, and G. R. Desiraju, *Acc. Chem. Res.* **51** (2018) 2957–2967.
3. S. Tang, J. Lin, J. Zhou, C. Zhao, Y. Liu, K. Li, S. Wu, and J. Gong, *Cryst. Growth Des.* **25** (2025) 2206–2214.
4. S. Nag, F. Emmerling, S. Tothadi, B. Bhattacharya, and S. Ghosh, *CrystEngComm* **26** (2024) 2871–2882.
5. T. Parthasarathy, B. Bhattacharya, F. Emmerling, and S. Ghosh, *CrystEngComm* **26** (2024) 4634–4642.

BM-063

Tuning Mechanical Flexibility and Photomechanical Bending in Cyanostilbene Cocrystals

Sanjay Gopal[1], Soumyajit Ghosh[1]*,

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603 203, Tamil Nadu, India.*

***Corresponding author E-mail**: soumyajs@srmist.edu.in

ABSTRACT

Intermolecular interactions and crystal packing significantly influence the mechanical adaptability of organic molecular crystals; however, the majority of π-conjugated molecular crystals are inherently brittle. In this study, we present a cocrystallization-driven approach to systematically modify the mechanical and photomechanical properties of the BPPA crystal. The unmodified BPPA crystal demonstrates brittle mechanical behavior due to its rigid packing structure. To address this limitation, we cocrystallized BPPA with two aromatic carboxylic acid coformers, namely 3,4-dichlorobenzoic acid (DCBA) and terephthalic acid (TPA), resulting in the formation of structurally distinct cocrystals, DCBA–BPPA and TPA-2(BPPA). Notably, the DCBA–BPPA cocrystal exhibits flexibility and photomechanical bending under UV irradiation, attributed to photoinduced strain within an anisotropically packed lattice. Conversely, the TPA-2(BPPA) cocrystal, formed in a 2:1 stoichiometric ratio, displays shearing and plastic bending, indicative of a layered packing arrangement. Structural analysis reveals that the differing mechanical responses are governed by variations in supramolecular interactions, hydrogen-bonding motifs, and packing anisotropy imposed by the selected coformers. Overall, cocrystallization is demonstrated to be an effective crystal engineering strategy for transforming brittle molecular crystals into mechanically adaptive and multifunctional materials, while providing valuable insights into structure–property relationships for the rational design of mechanically and photomechanically responsive organic crystals.

Keywords: Cocrystallization, Flexibility, Photomechanical bending, Shearing, Plastic bending, and Crystal engineering

References:

1. S. Ghosh, M. K. Mishra, S. Ganguly, and G. R. Desiraju, *J. Am. Chem. Soc.* **137**, 9912–9921 (2015).
2. S. Li and D. Yan, *ACS Appl. Mater. Interfaces* **10**, 22703–22710 (2018).
3. Y. Wei, K. Chen, S. Zhu, W. Wu, H. Zhao, X. Huang, N. Wang, L. Zhou, T. Wang, J. Wang, and H. Hao, *Small* **20**, 2307756 (2024).
4. T. Parthasarathy, M. K. Mishra, B. Bhattacharya, F. Emmerling, and S. Ghosh, *Cryst. Growth Des.* **25**, 309–318 (2024).
5. A. Bhowmik, S. Bamane, A. K. Saxena, and M. K. Mishra, *Cryst. Growth Des.* **25**, 5007–5021 (2025).

BM-064

Design of Flexible Chiral Organic Molecular Crystals using Crystal Engineering Approach for Optical Waveguiding and Self-Powered Piezoelectric–Triboelectric Devices.

Jothiprakasam Alaguvel[1], Soumyajit Ghosh[1]*

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603203, Tamilnadu, India.*

***Corresponding author e-mail:** soumyajs@srmist.edu.in

ABSTRACT

Flexible chiral organic molecular crystals have emerged as promising multifunctional materials for advanced photonic and energy-harvesting applications. In this study, we present the design of flexible chiral organic molecular crystals through a rational crystal engineering approach for optical waveguiding and self-powered piezoelectric–triboelectric devices. π-Conjugated chiral molecules are systematically designed to modulate intermolecular interactions, including hydrogen bonding, π–π stacking, and van der Waals forces, facilitating non-centrosymmetric crystal packing and mechanical flexibility. The resulting single crystals exhibit strong solid-state fluorescence and efficient optical waveguiding with low propagation loss, rendering them suitable for miniaturized photonic components. Furthermore, the chiral non-centrosymmetric crystal arrangement induces intrinsic piezoelectric properties, enabling the conversion of mechanical stimuli into electrical signals. To further exploit their energy-harvesting potential, the crystals are incorporated into triboelectric nanogenerator (TENG) architectures, where contact electrification generates electrical output under mechanical motion. The integration of optical functionality, mechanical flexibility, piezoelectricity, and triboelectric performance demonstrates the multifunctional capability of these materials. This study underscores the potential of crystal-engineered chiral organic crystals as promising candidates for flexible photonic devices, self-powered sensors, and next-generation wearable optoelectronic systems.

Keywords: Flexible molecular crystal; Chiral organic molecular crystal; Optical waveguides; Piezoelectric crystal.

Reference:

1. S. Ghosh and C. M. Reddy, *Angew. Chem*., **124**, (2012), 10465–10469.
2. K. Arora, D. Saini, S. Naskar, S. C. Sahoo, D. Mandal, and P. P. Neelakandan, *J. Am. Chem. Soc*. **147**, (2025), 25498–25507.
3. J. Lin, J. Zhou, Z. Wang, L. Li, M. Li, J. Xu, S. Wu, P. Naumov, and J. Gong, *Angew. Chem. Int. Ed*. **64**, (2025), e202416856.
4. P. Marandi, D. Saini, K. Arora, R. Garg, U. Sarkar, K. Parida, D. Mandal, and P. P. Neelakandan, *J. Am. Chem. Soc.* **146**, (2024), 26178–26186
5. V. Gupta, A. Kumar, B. Mondal, A. Babu, S. Ranpariya, D. K. Sinha, and D. Mandal, *ACS Sustainable Chem. Eng*. **11**, (2023), 6173–6182.

BM-065

Audible Sound Controlled Spatiotemporal Patterning of Supramolecular Aggregates

K. Arjun[1] and Rahul Dev Mukhopadhyay[1*]

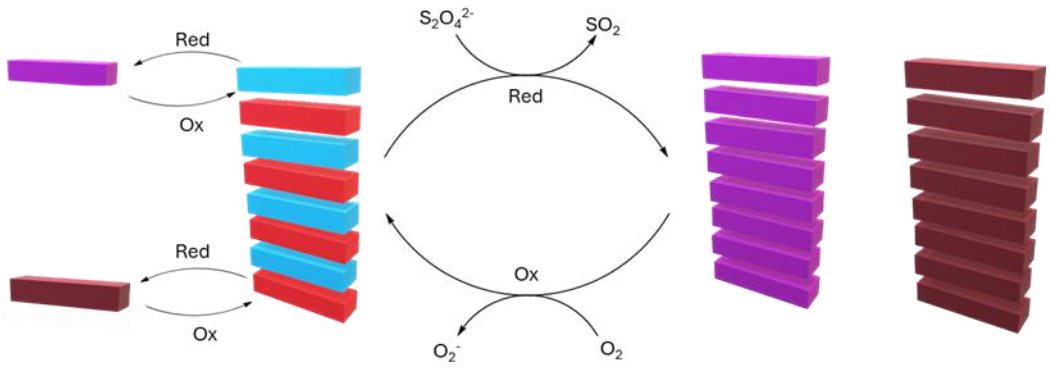
[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603203, India.*

***Corresponding author e-mail:** rahuldem@srmist.edu.in

ABSTRACT

Designing stimuli-responsive systems, which form different supramolecular structures in response to external stimuli, remains a key challenge. Among other external stimuli that have been utilised so far, redox-responsive molecules have gained special attention due to their redox state-dependent self-assembling behaviour. This has led to the development of controlled spatiotemporal patterning of supramolecular aggregates and monomers,[1] as well as segregation of oppositely chiral supramolecular aggregates,[2] in a single solution. One of the well-studied redox-responsive systems is perylenediimide (PDI) and NDI-based dyes. They exhibit reversible redox-responsive response between their neutral, radical anion and dianion states. Herein, we report the synthesis and characterisation of PDI and NDI dyes, and the redox-responsive supramolecular self-assembly of the PDI and NDI systems, as well as their co-assembly, will be studied. We therefore investigated the aggregation behaviour of these molecules under normal (oxidised) conditions and under reduced conditions by using UV-vis spectroscopy. The morphological investigations were also carried out for the PDI, NDI assemblies and PDI-NDI co-assembly under normal (oxidised) and reduced conditions by using scanning electron microscopy (SEM). Finally, we generate the spatiotemporal pattern of the redox-responsive PDI, NDI assemblies and PDI-NDI co-assembly in the presence and absence of audible sound.

Scheme:



Reference

1. Hwang et al., *Nat. Chem.*, **2020**, *12*, 808.
2. Sen et al., *Chem.* **2023** 9, 1–1.

BM-066

Bioinspired Hierarchical Hydroxyapatite Nanorod-Reinforced Composite Coatings for Durable and Corrosion-Resistant Implant Surfaces

Abimanyu. R[1], Saibabu. A[1], Ballamurgan.A.M[1]*

[1] *Department of Nanoscience and Technology, Bharathiar University, Coimbatore, Tamilnadu, India, 641046*

***Corresponding author e-mail:** balamurugan@buc.edu.in

ABSTRACT

Bioinspired structural materials found in nature provide valuable design strategies for developing advanced protective coatings for biomedical implants. Among these, the radular tooth architecture of marine gastropods exhibits a highly organized mineral–organic composite structure with exceptional mechanical durability. Inspired by this hierarchical natural design, this study explores the development of a multifunctional bioinspired composite coating reinforced with hydroxyapatite (HAp) nanorods to enhance the surface stability and corrosion resistance of metallic implant substrates in physiological environments. The coating was fabricated through a solution-based deposition method to produce a nanostructured organic–inorganic composite layer on medical-grade stainless steel substrates. Hydroxyapatite nanorods were incorporated as the reinforcing inorganic phase within a biopolymeric matrix to mimic the mineralized fibrous arrangement found in natural radular teeth. Structural and morphological properties were analyzed using X-ray diffraction, Fourier transform infrared spectroscopy, and scanning electron microscopy. Electrochemical performance was evaluated in simulated physiological media at 37 °C using open circuit potential monitoring, potentiodynamic polarization, and electrochemical impedance spectroscopy. The bioinspired hierarchical composite coating significantly improved surface stability and corrosion resistance compared with uncoated substrates.

Keywords: Bioinspired Coatings, Nanomaterials, Biopolymers, Hierarchical composite structures, Corrosion resistance

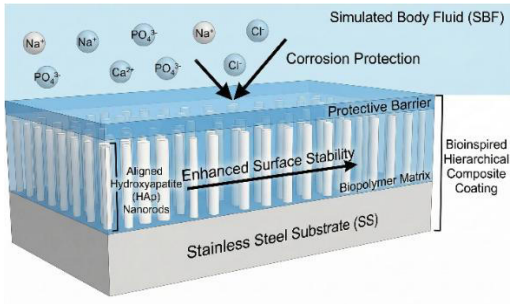


Fig.1. Bioinspired HAp nanorod-reinforced coating for improved corrosion resistance of implants.

References:

1. Gupta, A., & Hiremath, S. S. (2023). Morphological Evolution and Electrochemical Corrosion Behaviour of Bio-Inspired Hierarchical Micro-/Nano- Structured Ti-6Al-4V ELI Surface Targeting Potential Biomedical Applications.
2. Makhlouf, A. S. H., & Rodriguez, R. (2020). Bioinspired smart coatings and engineering materials for industrial and biomedical applications (pp. 407–427). Elsevier.

BM-067

Electrospun PVA/Kapok Gum (Ceiba pentandra) Nanofibrous Mats for Bioactive Wound Healing Applications

Abimanyu. R[1], Anwar Javeed. H[1], Ballamurgan.A.M[1]*

[1] *Department of Nanoscience and Technology, Bharathiar University, Coimbatore, Tamilnadu, India, 641046*

***Corresponding author e-mail:** balamurugan@buc.edu.in

ABSTRACT

Advanced wound dressing materials that mimic the structural and functional characteristics of the extracellular matrix are increasingly explored for improved wound management and tissue regeneration. Electrospun nanofibers are particularly attractive due to their high surface area, interconnected porosity, and ability to support cell attachment and proliferation. In this study, polyvinyl alcohol (PVA) blended with natural kapok gum was used to fabricate nanofibrous mats via electrospinning for potential wound healing applications. Kapok gum derived from Ceiba pentandra, a plant-derived polysaccharide, was incorporated into the PVA matrix to enhance hydrophilicity, bioactivity, and biological interactions within the fibrous scaffold.The structural and morphological characteristics of the fabricated nanofibers were analyzed using Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The resulting nanofibrous mats exhibited uniform fiber morphology and a porous architecture that can facilitate oxygen permeability and maintain a moist microenvironment favorable for wound healing. In addition, the incorporation of kapok gum may contribute to antibacterial protection and improved biological performance of the dressing material. Overall, the developed PVA–kapok gum nanofibrous scaffold demonstrates promising potential as a bioactive wound dressing for advanced wound care applications.

Keywords: Nanofibers, Kapok Gum, Biopolymers, Wound Dressing, Tissue Regeneration

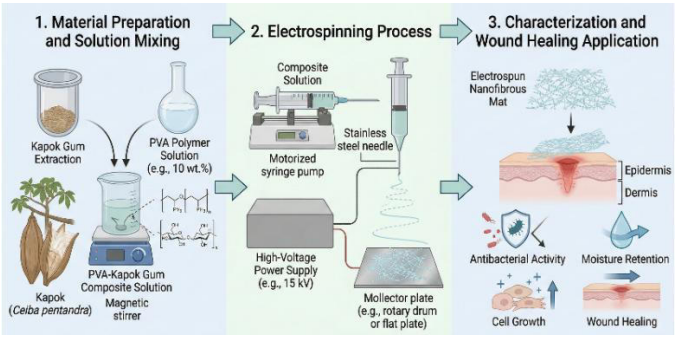


Fig.1. Electrospun PVA–kapok gum nanofibers for wound healing applications.

References:

1. Liu, Q., Luo, S., Peng, J., & Chang, R. (2024). Electrospun Nanofibers from Plant Natural Products: A New Approach Toward Efficient Wound Healing. International Journal of Nanomedicine, 19, 13973–13990.
2. Kumar, K. P. A., Ramakrishnan, R. K., Černík, M., & Padil, V. V. T. (2022). *Tree gum-based nanostructures and their biomedical applications* (pp. 383–407).

BM-068

Biogenic Mg-HAp from Salmacis Virgulata for Advanced Bone Tissue Engineering and Osteogenic Enhancement

Abimanyu. R[1],Nivetha .R[1], Ballamurgan.A.M[1]*

[1] *Department of Nanoscience and Technology, Bharathiar University, Coimbatore, Tamilnadu, India, 641046*

***Corresponding author e-mail:** balamurugan@buc.edu.in

ABSTRACT

Biogenic materials provide sustainable and highly functional alternatives for biomedical applications, and in this study, magnesium-doped hydroxyapatite (Mg–HAp) was synthesized using sea urchin shells derived from Salmacis virgulata, a naturally calcium-rich marine source. The shells were purified, thermally converted from $CaCO_3$ to CaO, hydrated to form $Ca(OH)_2$, and reacted with di-ammonium hydrogen phosphate through a wet chemical co-precipitation process to obtain Mg–HAp, followed by drying and calcination. Comprehensive structural and functional characterization using XRD, FTIR, Raman spectroscopy, SEM, and EDX confirmed the formation of phase-pure, nanocrystalline hydroxyapatite with naturally incorporated magnesium and a porous morphology favorable for cellular interaction. Biocompatibility studies using MG-63 osteoblast-like cells demonstrated excellent cytocompatibility and a marked increase in cell proliferation, indicating strong osteogenic potential. Developmental toxicity evaluation using zebrafish (Danio rerio) embryos showed no mortality, deformities, or behavioral abnormalities at all tested concentrations, confirming the material's high biosafety. Overall, these findings establish Salmacis virgulata–derived Mg–HAp as a bioactive, cytocompatible, and developmentally safe biomaterial with significant promise for bone regeneration and tissue engineering applications.

Keywords: Magnesium-doped Hydroxyapatite (Mg–HAp), Biogenic Calcium Source, Wet Chemical Co-precipitation, Osteogenic Potential, Zebrafish Toxicity Assessment.

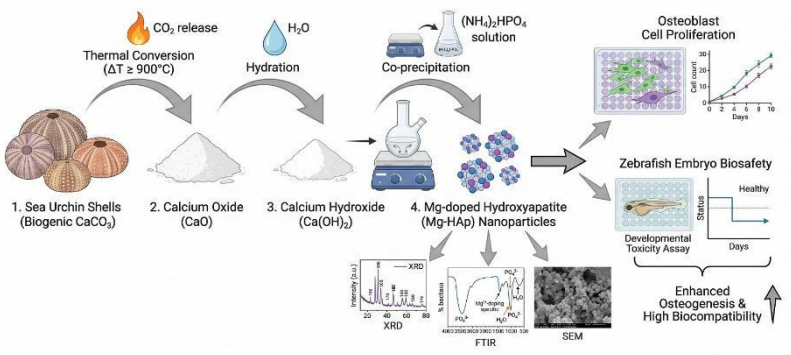


Fig.1. Schematic illustration of biogenic Mg–HAp synthesis and its potential for bone tissue engineering.

References:

1. Gómez Vázquez, N. S., Luque Morales, P. A., Gomez Gutierrez, C. M., Nava Olivas, O. de J., Villarreal Sánchez, R. C., Vilchis Nestor, A. R., & Chinchillas Chinchillas, M. de J. (n.d.). Hydroxyapatite Biosynthesis Obtained from Sea Urchin Spines (Strongylocentrotus purpuratus): Effect of Synthesis Temperature. *Multidisciplinary Digital Publishing Institute*.

BM-069

Preclinical Evaluation of Vitamin-C Boosted Nano-Liposome Curcumin for Targeted Breast Cancer Therapy

Manikandan. S[1], Abimanyu.R[1], Pavithra .V[1] , Ballamurgan.A.M[1]*

[1] *Department of Nanoscience and Technology, Bharathiar University, Coimbatore, Tamilnadu, India, 641046*

***Corresponding author e-mail:** balamurugan@buc.edu.in

ABSTRACT

Curcumin's therapeutic potential for breast cancer treatment is well recognized, but its clinical application is hindered by challenges such as poor bioavailability, rapid degradation, and limited solubility. To overcome these limitations, this study focuses on the encapsulation of curcumin and a curcumin/vitamin C combination into liposomal carriers, aimed at enhancing their stability and therapeutic efficacy in breast cancer applications. The research involved encapsulating curcumin and curcumin/vitamin C within liposomes, followed by extensive characterizations of the formulations. In vitro cytotoxicity tests, conducted using MTT assays on breast cancer cells, revealed that the encapsulated formulations significantly increased cancer cell death. Additionally, the study performed antioxidant assays, which demonstrated the potential of the curcumin/vitamin C combination to reduce oxidative stress, a critical factor in cancer development. Moreover, studies on drug release kinetics showed a controlled and sustained release of the encapsulated agents, suggesting a prolonged therapeutic effect. These results highlight the promise of liposome-encapsulated curcumin and curcumin/vitamin C combinations as effective treatments for breast cancer, paving the way for further preclinical investigations and potential clinical applications.

Keywords: Curcumin, Vitamin C, Liposomes, Breast Cancer Therapy, Controlled Drug Release

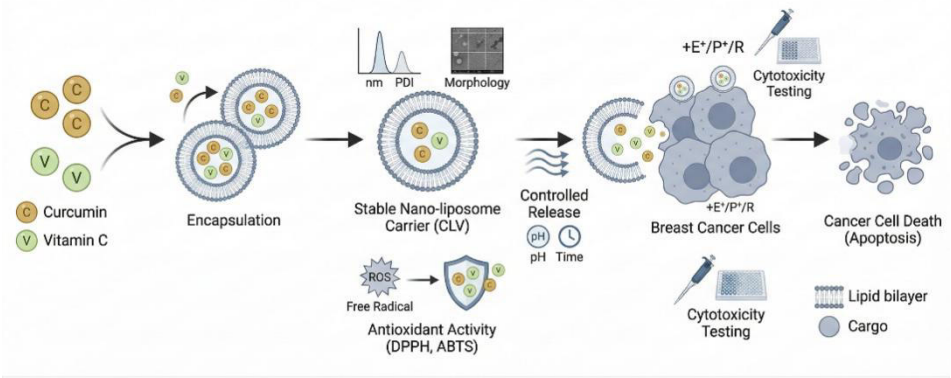


Fig.1. Schematic illustration of liposome-encapsulated curcumin and vitamin C for targeted breast cancer therapy.

References:

1. Fulton, M. D., & Najahi-Missaoui, W. (2023). Liposomes in cancer therapy: how did we start and where are we now. *International Journal of Molecular Sciences*, *24*(7), 6615.
2. Jain, A., Tiwari, A., Verma, A., Saraf, S., & Jain, S. K. (2020). Combination cancer therapy using multifunctional liposomes. *Critical Reviews™ in Therapeutic Drug Carrier Systems*, *37*(2).

BM-070

Electrophoretic Deposition of Hybrid Nanostructured β-TCP/HAp/MWCNT Coatings for Enhanced Corrosion Resistance and Mechanical Stability of 316L Stainless Steel

Mahendran Logesh[1], Abimanyu. R[1], Ballamurugan.A.M[1]*

[1] *Department of Nanoscience and Technology, Bharathiar University, Coimbatore, Tamilnadu, India, 641046*

***Corresponding author e-mail:** balamurugan@buc.edu.in

ABSTRACT

Surface modification of metallic implants is an effective strategy to enhance their corrosion resistance, mechanical stability, and biological performance in physiological environments. In this study, a composite coating composed of β-tricalcium phosphate (β-TCP), hydroxyapatite (HAp), and multi-walled carbon nanotubes (MWCNTs) was successfully deposited onto 316L stainless steel substrates using the electrophoretic deposition (EPD) technique. The incorporation of bioactive calcium phosphate phases with MWCNT reinforcement aims to improve both the structural integrity and surface functionality of the coating. The structural and morphological characteristics of the deposited coatings were investigated using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and transmission electron microscopy (TEM), confirming the formation of a homogeneous composite coating with well-dispersed components. Electrochemical corrosion behavior was evaluated in simulated body fluid (SBF) to assess the protective performance of the coatings under physiological conditions. Additionally, micro hardness measurements were performed to examine the mechanical strengthening effect provided by the MWCNT reinforcement. The coated samples exhibited enhanced corrosion resistance and improved surface hardness compared with uncoated substrates. Furthermore, immersion studies in SBF indicated the formation of apatite-like layers on the coating surface, suggesting good in vitro bioactivity. These results demonstrate that β-TCP/HAp/MWCNT composite coatings prepared via EPD hold significant promise for improving the durability and biological performance of stainless steel implants

Keywords: Electrophoretic Deposition (EPD), Bioactive Coatings, MWCNTs, 316L Stainless Steel, Corrosion Resistance

References:

1. Nguyen, T. T., Pham, T. N., Nguyen, T. P., Cao, T. H., Nguyen, V. T., Nguyen, T. X., & Dinh, T. M. T. (2017). Electrodeposition of Hydroxyapatite/Functionalized Carbon Nanotubes (Hap/Fcnts) Coatings on The Surface Of 316l Stainless Steel. *Vietnam Journal of Science And Technology*, *55*(6).
2. Abudalazez, A. M. A., Kasim, S. R., Ariffin, A., & Ahmad, Z. A. (2012). Preparation and Characterization of Biphasic Calcium Phosphate Coatings on 316L Stainless Steel Fabricated by Electrophoretic Deposition. *Advanced Materials Research*, *620*, 373–377.

BM-071

Characterization and Mechanical Evaluation of Biodentine with Nano Zirconia, Nano Graphene and Calcium Phosphate

Rumesa Batul[1], Saleem D. Makandar [1], Nik Rozainah Nik Abdul Ghani [1], Huwaina Abd Ghani [1], Mohamad Arif Awang Nawi [1]

[1] *School of Dental Sciences, Health Campus, Universiti Sains Malaysia 16150, Kubang Kerian, Kelantan, Malaysia*

***Corresponding author e-mail:** saleemdm@usm.my

ABSTRACT

Biodentine is a notable representative of calcium silicate-based materials. [1]. It holds few drawbacks [2]. We enhanced the properties of Biodentine by incorporating nano materials like nano zirconia and nano graphene along with calcium phosphate. Nanotechnology is an emerging field where nanoparticles improve the physio-mechanical properties of dental materials. Four groups were formed, and twenty samples were prepared, consisting of five samples from every group. FTIR and SEM EDX analysis was performed. The "Vickers microhardness tester" was used to record microhardness, and a universal Instron testing machine was used to check the compressive strength. Nano zirconia calcium silico phosphate group in this study showed favorable results.

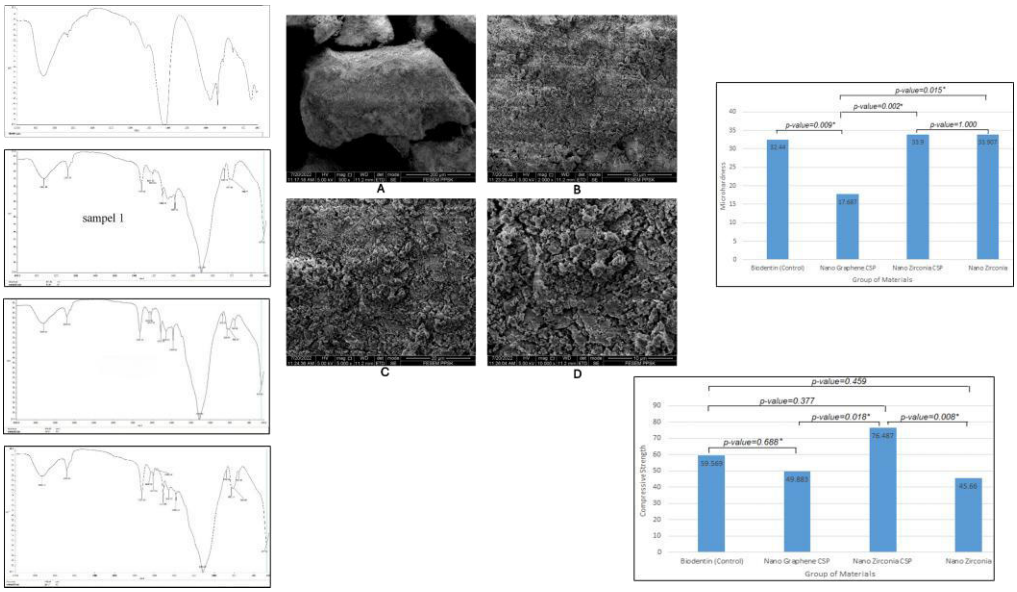


Fig. 1 FTIR, SEM, Microhardness and Compressive strength of modified Biodentine

Keywords: Dental Materials; Silicates; Hardness; Material Testing; Compressive strength; Calcium Phosphate; Nanoparticles, Zirconium; Graphite; Microscopy; Electron Scanning; Fourier Transform Infrared.

References:

1. Batul, R., et al., Comparative evaluation of microhardness, water sorption and solubility of biodentin and nano-zirconia-modified biodentin and FTIR analysis. Applied Sciences, 2023. 13(3): p. 1758.
2. Kaur, M., et al., MTA versus Biodentine: review of literature with a comparative analysis. Journal of clinical and diagnostic research: JCDR, 2017. 11(8): p. ZG01.

BM-072

Multiscale Structural and Functional Analysis of Radular Teeth from Patella vulgata: Evaluating Natural Biomineral Architecture for Biomaterial Design

Abimanyu. R[1], Nishad.S[1], Ballamurgan.A.M[1]*

[1] *Department of Nanoscience and Technology, Bharathiar University, Coimbatore, Tamilnadu, India, 641046*

***Corresponding author e-mail:** balamurugan@buc.edu.in

ABSTRACT

Biological mineralized structures exhibit exceptional durability arising from hierarchical organization and optimized mineral–organic interfaces. In this study, the radular teeth of Patella vulgata were systematically investigated to understand structural and functional features that may inform the design of advanced biomaterials. Detailed morphological and compositional analyses were performed using scanning electron microscopy (SEM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR) to identify mineral phases and hierarchical architecture within the radular tooth. Mechanical behavior was examined through localized hardness measurements to determine functional property gradients along the tooth structure. In addition, environmental stability studies were conducted in aqueous physiological conditions to examine structural evolution and mineral stability. Preliminary cytocompatibility evaluation using osteoblast-like cells was performed to assess potential biological interactions with the mineralized surface. The results reveal a complex hierarchical composite system with functionally graded mechanical properties and stable mineral reinforcement. These findings provide fundamental insights into the structural principles governing the remarkable durability of radular teeth and highlight their relevance as a natural model for the development of next-generation biomaterial surfaces.

Keywords: Radular Teeth, Biomineralization, Hierarchical architecture, Bioinspired biomaterials.

References:

1. Chellapandian, H., Jeyachandran, S., Park, K.-C., & Kwak, I.-S. (2025). Marine-Derived Functional Biomaterials: Advancements in Biomedicine and Drug Delivery Applications. *Natrual Product Communication.*
2. Krings, W., Gorb, S. N., Neumann, C., & Wägele, H. (2024). *Radular tooth coating in members of Dendronotidae and Flabellinidae (Nudibranchia, Gastropoda, Mollusca)*.
3. Gorb, S. N., & Krings, W. (2021). Gradients of Mechanical Properties in Taenioglossan Radular Teeth is Linked with Specific Function and Ecological Niche. *Social Science Research Network*.

BM-073

Development of Magnesium sample using wire arc additive manufacturing for automobile and biomedical applications

Basireddy Pranitosh Reddy[1], Gangeyula Jyothiradithya[2], Akash Vincent, N. Harshavardhana*

SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail**: harshavn@srmist.edu.in

ABSTRACT

Magnesium (Mg) and its alloys have emerged as promising lightweight structural and biodegradable materials for automotive and biomedical applications due to their low density and favourable mechanical-to-weight ratio respectively. However, fabrication of Mg alloys remains challenging because of inherent material limitations, including poor room-temperature formability due to limited plasticity, high chemical reactivity, low melting and boiling points, and electrochemical instability that leads to rapid corrosion. Robot-assisted wire arc additive manufacturing (WAAM) is an emerging technology for the fabrication and repair of Mg alloy components, offering improved process control and geometric flexibility. In the present study, Mg deposition was achieved through process parameter optimization using bead-on-weld experiments. Based on the optimized parameters, bulk samples of 50 X 100 X 10 mm^3 (height X length X thickness) were successfully fabricated. The fabricated samples were characterized to evaluate their mechanical and microstructural properties. Mechanical performance was assessed through tensile and hardness testing, while microstructural analysis was conducted using optical microscopy, high-resolution scanning electron microscopy (HR-SEM), X-ray diffraction (XRD), and electron backscatter diffraction (EBSD). The study demonstrates the feasibility of WAAM for Mg fabrication and provides insights into the structure–property relationship, the mechanical performance, and the processing challenges encountered during fabrication.

Keywords: Wire Arc additive manufacturing, Magnesium alloys, Mechanical properties, microstructure, structure property relationship

BM-074

Eu^{3+}-Doped Fe_3O_4 Mesocrystals for Magneto–Optic Synergistic Cancer Therapy and Bioimaging

Akash Marsalin[1], Anandhakumar Sundaramurthy[2], Vishwajeet M. Khot[3] & Rajaboopathi Mani[1]*

[1] *Key Laboratory of Emergent Materials (KLEM), Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203, Chengalpattu, Tamil Nadu, India.*

[2] *Biomaterials Research Laboratory (BMRL), Department of Chemical Engineering, SRM Institute of Science and Technology, Kattankulathur 603203, Chengalpattu, Tamil Nadu, India.*

[3] *Department of Medical Physics, Centre for Interdisciplinary Research, D. Y. Patil Education Society (Deemed to be University), Kolhapur, 416006, Maharashtra, India.*

***Corresponding author e-mail:** rajaboom@srmist.edu.in

ABSTRACT

Magnetic hyperthermia (MHT) is a minimal, non-invasive therapeutic methods utilize alternative magnetic field to generate localized heat. However, its clinical application remains restricted in patients with metallic and magnetic implants, due to the risk of eddy currents induced off target heating[1]. To address this, we developed a multifunctional therapeutic agent based on Eu doped Fe_3O_4 mesocrystals design to integrate magnetic hyperthermia, near-infrared photothermal therapy (PTT) and imaging within a single nanoarchitecture. The crystallographically aligned mesocrystals were synthesized via modified solvothermal method[2]. Where, XRD confirms the phase purity without the formation of secondary phase upon Eu doping. Raman spectroscopy indicates a minor surface transformation from magnetite to maghemite. This surface oxidation is further supported by XPS analysis through the change in the Fe^{2+}/Fe^{3+} ratio and proximity of oxygen vacancy. Morphological analysis indicates that higher Eu^{3+} concentrations can suppress mesocrystal self-assembly by increasing local electron density, which promotes the formation of additional nucleation sites thus reducing its particle size. Among the dopant concentration, Eu 3% doped achieved an optimal balance by retaining high magnetization of 73 emu/g, while exhibiting distinct photoluminescence at 614 nm and nIR absorption for PTT. MHT studies confirm that pristine and low-doped samples reach therapeutic temperatures ~42°C. Furthermore, the pristine and 3% sample demonstrates better PTT heating under 808 nm laser irradiation. *In vitro* studies demonstrate the 3% Eu-doped sample exhibits ~80% viability with L-929 normal cells and ~20% cell viability against A-549 cancer cells upon laser irradiation. In brief, these Eu-doped mesocrystals are robust therapeutic agents, possessing magnetic, photothermal, and luminescent functionalities for synergistic hyperthermia and image-guided cancer therapy.

Keywords: Magnetic Hyperthermia; Photothermal Therapy; Cancer Apoptosis; Mesocrystal.

References:

1. Fu et al., “Photothermal Effect of Superparamagnetic Fe3O4 Nanoparticles Irradiated by Near-Infrared Laser” J. Nanomater., 2020, 1, 1687-4110.
2. Marsalin et al., “Multifunctional Fe3O4 mesocrystals for cancer therapy: integrating hyperthermia and targeted drug delivery”, J. Mater. Chem. B, 2025,13, 10635-10647.

BM-075

Fabrication of Mothership Capsules using Polymers for Lipase Enzymes Delivery to Treat Pancreatic Insufficiency

Johnson Thinakaran[1], Anandhakumar Sundaramurthy[2*]

[1] *Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2] *Department of Chemical Engineering, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** anandhas@srmist.edu.in

ABSTRACT

Pancreatic lipase deficiency leads to impaired lipid digestion and malabsorption, resulting in significant gastrointestinal and nutritional complications. Although oral lipase supplementation is a promising therapeutic strategy, its efficacy is limited by degradation in the acidic gastric environment. To overcome this challenge, stimuli-responsive mothership capsules (MCs) have been developed as an advanced platform for the encapsulation and controlled release of enzymes. In this study, we fabricated MCs using a simple extrusion method using an anionic polymer, gellan gum (GG), and a cationic polymer, poly (allylamine hydrochloride) (PAH), through electrotactic charge interactions, as result forming the MCs. The pH-responsive MCs exhibited enhanced stability in a 1% PAH solution at pH 5. The formed capsules exhibited smooth, spherical structures with a diameter ranging from 2 to 3 mm. The MCs served as compartments for carrying and releasing the lipase in the small intestine. To assess lipase release, the MCs were exposed to simulated gastric fluid (SGF) for 2 hours. While the MCs remained stable, only a small amount of lipase was released. The MCs were then incubated in simulated intestinal fluid (SIF) at pH 6.8 for 8 hours, which triggered the breakdown of the polymeric capsules and facilitated the release of lipase. The release of lipase was quantified spectrophotometrically, revealing minimal leakage under acidic conditions and enhanced release in SIF due to pH-induced destabilisation of the polyelectrolyte network. The preserved enzymatic functionality of the released lipase highlights the protective capability of the mothership capsule system. Overall, this study demonstrates that pH-responsive GG/PAH mothership capsules represent a promising strategy for targeted intestinal enzyme delivery and offer significant potential for improving oral enzyme replacement therapy in pancreatic lipase deficiency.

References:

1. Sharma, Varsha, Maarten Vergaelen, Sangamithra Nehru, Richard Hoogenboom, and Anandhakumar Sundaramurthy. "Poly (2-n-propyl-2-oxazoline)/tannic acid nanocapsules with in-situ synthesized gold nanorods for cancer theranostics." European Polymer Journal 198 (2023): 112409.
2. Sharma, Varsha, Gokul Paramasivam, Maarten Vergaelen, Richard Hoogenboom, and Anandhakumar Sundaramurthy. "Tannic acid-stabilized self-degrading temperature-sensitive poly (2-n-propyl-2-oxazoline)/gellan gum capsules for lipase delivery." ACS Applied Bio Materials 4, no. 9 (2021): 7134-7146.

BM-076

Investigation of Implant Corrosion-Induced Toxicity in Zebrafish (Danio rerio): A Systemic Evaluation of Cellular and Metabolic Stability

Bharath Sankaralingam, Gobi Saravanan Kaliaraj*, Sankar Jamuna, Rathinavel Ashokkumar

Centre of Excellence for Additive Manufacturing, Sathyabama Institute of Science and Technology, Chennai 600119, Tamil Nadu, India

***Corresponding author e-mail:** gobisaravanan@sathyabama.ac.in

ABSTRACT

The long-term performance of metallic implants is governed by coupled electrochemical, transport, and biological processes, in which corrosion-mediated ion release acts as a time-dependent forcing function that drives systemic toxicity. In this study, the corrosion behaviour of SS304L, SS316L, titanium, and Ti6Al4V alloy was quantitatively evaluated, and the resulting biological impact was analysed using Danio rerio as an integrative in vivo model. Electrochemical characterisation in simulated body fluid (SBF) was conducted using potentiodynamic polarisation, yielding the corrosion potential (Ecorr) and corrosion current density (icorr), which directly represent the rate of anodic dissolution. Stainless steels exhibited significantly higher icorr values of -0.4 to -0.8 mA/cm2 compared to titanium-based materials, indicating enhanced metal flux across the implant-electrolyte interface. Inductively coupled plasma analysis revealed concentration- and time-dependent accumulation of Fe >1mg/mL, Cr >1mg/mL, and Ni <1mg/mL ions, with SS304L and SS316L showing the steepest concentration gradients, confirming inferior corrosion resistance. Histopathological analysis showed lamellar fusion and hypertrophy in gill filaments, hepatocellular vacuolization and necrosis in liver tissue, disrupted metabolic homeostasis, and villus degeneration in the intestine, resulting in reduced absorptive surface area. Metallo-toxicological stress was investigated by estimating metabolic end products linked to various organ which met pronounced oxidative and inflammatory stress confirmed by increased LPO in brain (30.4% in SS316; 55.9% in SS304L), elevated MPO in gills (45% in SS316L; 57% in SS304L) and significant up regulation of oxidative enzymes catalases and SOD (37% in SS316L; 56.8% in SS304L). Overall, the results establish a direct functional relationship among corrosion kinetics, metal ion transport, and systemic biological response, for the integrative analysis and points of care to be taken to improve fabrication methods.

References:

1. Hsiao, V.K.S.; Lin, Y.-C.; Wu, H.-C.; Wu, T.-I. Surface Morphology and Human MG-63 Osteoblastic Cell Line Response of 316L Stainless Steel after Various Surface Treatments. Metals 2023, 13, 1739.

BM-077

Dissolution of Calcium Oxalate Kidney Stones Using Nutraceutical Phosphates

Bhavani Iyer Suriyanarayanan, Palash Sanphui

Department of Chemistry, SRM Institute of Science and Technology (SRM IST),

Kattankulathur,

***Corresponding Author e-mail:** bs7126@srmist.edu.in

ABSTRACT

Calcium oxalate (CaOx) accounts for nearly 70–80% of human kidney stones, with calcium oxalate monohydrate (COM) being the most thermodynamically stable and clinically difficult form to dissolve. Current treatments primarily involve surgical removal or citrate supplementation; however, the high recurrence rate of kidney stones highlights the need for alternative, non-invasive dissolution strategies. In this study, we systematically investigated the in-vitro dissolution ability of three nutraceutical agents—sodium tripolyphosphate (STPP), sodium hexametaphosphate (HMP), and potassium citrate (KCIT)—toward calcium oxalate crystals. Solid-state characterization using powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FT-IR), and scanning electron microscopy (SEM) revealed that STPP and HMP can partially convert COM into metastable phases such as calcium oxalate dihydrate (COD) and trihydrate (COT). Among the tested agents, STPP exhibited the strongest lattice-disrupting and calcium-chelating ability. Dissolution experiments demonstrated that STPP achieved nearly complete dissolution of CaOx crystals (>90% in water) and significant dissolution of human kidney stones (63% in artificial urine without CaCl2), outperforming both HMP and KCIT. Zeta potential measurements (–53.4 mV) indicated the formation of highly stable CaOx dispersions in the presence of STPP, while SEM images showed pronounced morphological disintegration of COM crystals. Additionally, STPP displayed superior moisture stability compared with HMP and KCIT, suggesting improved practical applicability. Overall, the results identify STPP as a safe, food-grade phosphate capable of effectively destabilizing calcium oxalate crystals and promoting dissolution. This work highlights the potential of nutraceutical phosphates as promising candidates for non-invasive management of calcium oxalate kidney stones.

Keywords : Calcium Oxalate, Kidney Stones, Sodium Tripolyphosphate, Crystal Dissolution, Nutraceutical Phosphates

BM-078

3D Printing of Biocompatible Cobalt–Chromium Metals with Functional Hydroxyapatite Surface Layers

Nirmal Raj V[1], Pranav Ramanan N[1], Niranjankumar S[1], Arun Kumar K[2]

[1] *Department of Mechanical Engineering, Karpagam College of Engineering, Coimbatore, India*

[2] *Assistant Professor, Department of Mechanical Engineering, Karpagam College of Engineering, Coimbatore, India*

ABSTRACT

This paper investigates the fabrication and surface modification of cobalt–chromium (Co–Cr) alloys using additive manufacturing (AM) to produce biocompatible metallic implants with functional hydroxyapatite (HA) coatings. Cobalt–chromium alloys are known for their excellent mechanical strength, corrosion resistance, and load-bearing capacity, yet their inert surfaces limit bone bonding. In this study, Co–Cr samples were fabricated by Selective Laser Melting (SLM) and coated with hydroxyapatite using electrophoretic deposition (EPD) to improve biocompatibility and corrosion resistance. The surface morphology, phase composition, and adhesion strength of the coatings were analyzed using Scanning Electron Microscopy (SEM), Energy Dispersive X-ray (EDX) spectroscopy, and X-ray Diffraction (XRD). Electrochemical tests in simulated body fluid (SBF) demonstrated a significant reduction in corrosion rate and enhanced bioactivity in coated samples. The combination of additive manufacturing and surface modification provides a promising pathway to produce customized and durable implants with improved biological performance.

Keywords 3D Printing; Additive Manufacturing; Cobalt–Chromium Alloy; Hydroxyapatite Coating; Electrophoretic Deposition; Biocompatibility; Corrosion Resistance; Biomedical Implants; Surface Modification; Selective Laser Melting

AFM - 001

Material Innovation in FinFETs: Reviewing the role of Gate Metal, Gate Oxide, Channel Engineering

Suganyadevi M[1], ShirlyEdward A[2]*

[1]*SRM institute of Science and Technology, Vadapalani, Tamilnadu, India, 600026*

[2]*SRM institute of Science and Technology Vadapalani, Tamilnadu, India, 600026*

***Corresponding author e-mail:** sm1184@srmist.edu.in

ABSTRACT

With a focus on material evolution in channel layers, gate oxides, and gate metals, this paper provides an extensive review of recent developments in Multigate FET (FinFET) technologies. FinFET development was initially by silicon, but new materials like germanium, gallium nitride, III-V compounds (InGaN, GaAs, InP, and InGaAs), and 2D materials like molybdenum disulphide have shown a lot of promise. Gate materials such as titanium nitride, platinum, aluminium, and tungsten are discussed along with high-k dielectrics such as hafnium oxide, aluminium oxide, zirconium oxide, titanium nitride, and hafnium zirconium oxide. The study uses TCAD simulation to guide next-generation CMOS innovation by assessing the effects of material selection on short-channel effects, carrier mobility, leakage current, electrostatic control, and fabrication challenges. The results illustrate both the pros and cons of employing new materials. This can help with the next step in CMOS innovation. Ultimately, the integration of material science, device physics, and simulation-driven design will likely dictate the trajectory of multigate transistor technologies as we progress in scaling and integrating various device types.

References:

1. S. K. Mah, P. J. Ker, I. Ahmad, N. F. Z. Abidin, and M. M. A. Gmel, Materials, 14 (2021) 5721.
2. Z. Rethlei, R. S. Dhar, and S. Nanda, J. Phys. Conf. Ser., 1921 (2021) 012001.
3. Y.-J. Yao et al., Nanomaterials, 13 (2023) 1310.
4. M. N. Reddy and D. K. Panda, Multiscale Multidiscip. Model. Exp. Des., 7 (2024) 2179–2188.

AFM - 002

A Review on Self-healing Characteristics of Laminated Polymer Composites

Ragavendra S[1], Nishkinth M[2], Vishwa R[3]*

[1,2,3]*Department of Mechanical Engineering, Karpagam college of engineering, Coimbatore, Tamilnadu, India,641032*

***Corresponding author e-mail:** ragavsudha2@gmail.com

ABSTRACT

Self-healing laminated polymer composites (LPCs) are advanced material systems functioning to heal autonomously regain its structural integrity upon damage. This review provides an overview on self-healing systems like Extrinsic, intrinsic and hybrid self-healing strategies, with an emphasis on their mechanical, thermal and interfacial bonds. Extinsic procedures system such as Microcapsule and vascular systems facilitate in rapid, localized repair reaching as much as 90% healing efficiency, in contrast intrinsic mechanisms derived on covalent, supramolecular, and shape-memory chemistries provides multi-cycle healing with lees degradation of mechanical properties. Hybrid systems unify both healing mechanisms to attain enhanced functionality and extended service life. Elucidation via fracture, impact, fatigue, and microscopic (SEM, μCT) or Spectroscopic (FTIR, DSC, DMA) inquiries reveals healing kinetics and Efficiency (η) with respect to mechanical and multifunctional behaviors. Self-healing behavior or performance significantly depends on the laminate architecture, fiber orientation, and interfacial adhesion. Aerospace, Automotive, marine, and wind energy sectors applications indicates extended operational lifespan and improved sustainability. Subsequent Research should accentuate standardized characterization, scalable production techniques and predictive modeling to enable industrial deployment.

References:

1. Bodiuzzaman et al (2018), Repeatable self-healing of thermosetting fiber reinforced polymer composites with thermoplastic healant, Smart Materials and Structures 28-025037
2. Stefano Paolillo et al (2021), Intrinsic Self-Healing Epoxies in Polymer Matrix Composites (PMCs) for Aerospace Applications, Polymers 13(2), 201
3. Sepanta et al (2025). Shape Memory Alloy assisted healing of thermoplastic composite laminates under repeated impact loading, Composite Structures, 358:118977
4. Iee et al., (2016), Self-Healing Polymer Composites: Prospects, Challenges, and Applications, Polymer Reviews, (56) 225-261
5. Norris et al (2012), Autonomous stimulus triggered self-healing in smart structural composites, Smart Materials and Structures, 21-094027

AFM - 003

Evaluation of Self-healing Characteristics of FRP Composite Honeycomb

Akash R, Balaji S, Ganesh S*

Department of Mechanical Engineering, Karpagam College of Engineering, Coimbatore, India

ABSTRACT

Fiber-reinforced polymer (FRP) honeycomb composites represent a new type of clever building material designed to increase the service life by working autonomously through self-healing. Although the traditional FRP honeycombs provide a superb stiffness to weight balance, they are susceptible to core crushing, delamination, face-skin debonding and impact induced microcracking. New developments have incorporated micro capsule-driven healing systems of local crack repair in a single use, vascular systems of repeatable continuous healing of wounds, intrinsically self healing polymers of reversible covalent chemistry, supramolecular interaction, thermal re-bonding, and shape-memory effects. These processes significantly enhance damage recovery, impact resistance fatigue life, and environmental life without loss of consumption of light weight performance. Some issues have been the fine balance between the incorporation of healing agents and mechanical strength, long-term reliability of healing, and size ability to manufacture the large parts. Self-healing FRP honeycomb constructions with incorporated sensing technologies can support the real-time sensing and on-commit repair, they are thus an attractive addition to future aerospace, marine, and high-performance engineering utilizations.

References:

1. White, S. R., Sottos, N. R., Geubelle, P. H., Moore, J. S., Kessler, M. R., Sriram, S. R., Brown, E.N., & Viswanathan, S. (2001). Autonomic healing of polymer composites. Nature, 409(6822), 794–797. https://doi.org/10.1038/35057232.
2. Gupta, N., & Shukla, S. (2018). Advanced FRP composites for structural applications. Composite Structures, 195, 537–555.
3. Mohan, T. P., & Kanny, K. (2012). FRP honeycomb structures under fatigue loading. Composite Structures, 94, 174–182.
4. Bond, I. P., et al. (2008). Self-healing FRP composites. MRS Bulletin, 33, 770 774.
5. Hager, M. D., et al. (2014). Self-healing: Systems and applications. Advanced Materials Interfaces, 1, 1400004.

AFM-004

Development and Testing of 3d Printable Natural Fiber Reinforced PLA Material

Subramani N[1]*, Dr. S. Marimuthu[1], Barani Selvan S[1], Durai Vadivel V[1], Pradeep S[1]

[1]*Karpagam College of Engineering, Coimbatore, Tamilnadu,641032*

***Corresponding author e-mail**: subramani.n@kce.ac.in

ABSTRACT

Additive manufacturing via fused deposition modelling (FDM) is increasingly recognized as a pathway for sustainable materials development, particularly when combined with bio-based composites. Hemp fibre-reinforced polylactic acid (PLA) filaments are essential feedstock in a promising class. They deliver biodegradability, higher stiffness, renewable material content by incorporating these characteristics into the printed components. This review comprises of sustainable development of hemp/PLA filaments, particular focus on inter-relationships of process, structure and properties interact. This begins by summarization of key physiochemical and mechanical traits of hemp fibres and PLA with their shortcomings and strengths. Then, it reviews the main steps of fabrication sequence, compounding extrusion, and diameter control, important factors like moisture management, compatibilization and quality testing. The discussion on printability includes factors such as rheology, selection of nozzle and bed temperatures, infill design, and layer height optimization. This is supported by reported parameter ranges from the literature. Performance results show that low to moderate fibre loadings can enhance stiffness and improve crystallinity through nucleation. However, the issues such as porosity, interlayer cohesion, brittleness and moisture sensitivity remain causing constrained performance. Applications of hemp/PLA extends up to prototyping, tissue engineering scaffolds, lightweight automotive parts and sustainable packaging. Further research promises integration of nano-cellulosic fillers, hybrid bio-polyester systems, improved recyclability and life cycle assessments. Overall, this review offers design guidelines and a plan for scalable hemp/PLA filaments. It provides both technical insights and sustainability views for future FDM applications.

References:

1. M. N. Ahmad, M. Ishak, M. M. Taha, F. Mustapha, and Z. Leman, Materials 16 (2023) 4052.
2. W. K. Ahmed, F. Alnajjar, E. Zaneldin, A. H. Al-Marzouqi, M. Gochoo, and S. Khalid, Materials 13 (2020) 4065.
3. V. H. M. Almeida, R. M. Jesus, G. M. Santana, and T. B. Pereira, J. Compos. Sci. 8 (2024) 67.
4. V. H. M. Almeida, R. M. Jesus, G. M. Santana, et al., Polymers 16 (2024) 1757.
5. U. Arumaiselvan, M. Kalimuthu, R. Nagarajan, M. Mohan, S. O. Ismail, H. A. Al-Lohedan, and K. Krishnan, Bioresources 19 (2023) 3740–3754.

AFM-005

Performance Evaluation of Cutting Tools with Multi-Layered Nano Coating of Al_2O_3, Tin and Ti

Sathish R[1]*, Adithya V K[1], Barath Kalyan D[1], Charan Kumaar S[1]
[1]*Department of Mechanical Engineering, Karpagam College of Engineering, Coimbatore, Tamil Nadu, India, 641032*
***Corresponding author e-mail**: sathish.r@kce.ac.in

ABSTRACT

Cutting tools experience severe wear, friction, and thermal degradation during machining and surface finish. Multi-layer nano-coatings based on aluminium oxide (Al_2O_3), titanium nitride (TiN) and titanium (Ti) have emerged as high-performance surface treatments to enhance tool life, hardness, and oxidation resistance. titanium nitride (TiN) interlayer between Al_2O_3 and Ti. Comparative evaluations show that these layers improve crack arresting and thermal barrier efficiency over single-layer coatings. Moreover, hybrid and multilayer systems demonstrate superior wear reduction and cutting-edge retention under dry and high-speed machining. The article also identifies critical research gaps, including the need for heat resistance at elevated temperatures, and real-time monitoring of coating degradation. By integrating materials science with manufacturing performance, this review plays a critical role in advancing manufacturing productivity, operational efficiency, and long-term industrial competitiveness.

References:

1. M. Alhaddad and A. Shawky, Ceramics International 47 (2021) 9763–9770.
2. H. Boyle, et al., Wear 523 (2023) 204786.
3. H. Chen, et al., Tribology International (2024).
4. J. Fu, D. Chen, C. Xie, and C. Li, Materials Today 34 (2020) 92–113.
5. J. Liu, et al., Journal of Materials Research and Technology (2020).

AFM-006

Effect of tandem-type stabilization of two-dimensional (2D) Nb_2CT_x MXene on their colloidal and cytotoxic properties

M. Jakubczak[1] and A. M. Jastrzębska[1]
[1]*Faculty of Mechatronics, Warsaw University of Technology, św. Andrzeja Boboli 8, 02-525 Warsaw, Poland*

ABSTRACT

Two-dimensional (2D) Nb2CTx MXene holds great promise for biomedical applications due to its tunable surface chemistry and biocompatibility. However, their practical use requires long-term colloidal and oxidative stability. Here, we propose a tandem-type stabilization strategy that combines antioxidant protection with macromolecular surface functionalization. Nb2CTx was first treated with L-ascorbic acid (LA) to suppress oxidation by binding to reactive edges, followed by modification with polyethylene glycol (PEG), poly-L-lysine (PLL), or polydopamine (PDA). This dual approach enhanced stability in biological media — phosphate-buffered saline (PBS) and Dulbecco's Modified Eagle's Medium (DMEM) — while maintaining non-cytotoxicity toward A375 and HaCaT skin cell lines across a concentration range of 0–100 mg·L−1. Among the tested systems, LA/PEG and LA/PDA-modified MXenes maintained stable zeta potentials (−15 to −12 mV) and particle sizes for 72 h, whereas LA/PLL samples showed aggregation and charge loss. This tandem stabilization effectively prevents oxidation and aggregation without compromising biocompatibility, offering a versatile route for developing oxidation-resistant MXenes for biomedical and nanomedicine applications.

AFM-007

A Comprehensive Review on Mechanical Properties of Metal Hybrid Nanoparticle–Modified Glass Fiber Polymer Composites

Subramani N[1]*, S. Marimuthu[1], Ciril Roshan M[1], Dijo V[1], Mohamad Hisam G S[1]

[1]*Karpagam College of Engineering, Coimbatore, Tamilnadu,641032*

***Corresponding author e-mail**: subramani.n@kce.ac.in

ABSTRACT

This article summarises the progress of recent developments of metal/metal-oxide hybrid nanoparticle-modified glass-fibre polymer composites (GFRPs). It's about how those things work, mechanically, and how they're designed. Here, we detail the ideal ingredients to choose and how to make the material. We will also show how hybrids such as TiO_2, SiO_2, Al_2O_3, ZnO, Ag, or magnetic oxides (often engineered with CNTs/graphene or thermoplastics) alter the matrix geometry and fibre/matrix interface to improve tensile/flexural/impact/fatigue/wear performance. There are mechanisms such as interphase thickening, crack deflection and bridging, and interfacial friction to enhance multifunctionality (for example, EMI shielding and sensing as well as thermal pathways) in addition to particle-induced shear banding percolating networks. Some quantitative examples include that multipart epoxy cures become much tougher, and transportation polymers retain their modulus while weight decreases. Vat-photopolymerization resins, however, demonstrate that it can be feasible to grow their strength at low loads. Such modelling encompasses analytical micromechanics with interphase and percolation determination, traction laws derived from molecular dynamics, and process-informed finite-element models that illustrate how strength varies with nanoparticle fraction as the limit of dispersion is approached. There are still some persisting challenges due to handling agglomeration, viscosity, and cure control, as well as ensuring the material remains stable over time when temperature and moisture change. It is the authors' opinion that researchers should focus on standardised dispersion metrics, operando characterisation of network topology, coupled ageing under environmental and multiaxial loads, additive manufacturing interphases, embedded health monitoring networks, and circularity. These paths collaborate in converting laboratory findings into durable, certified, and application-oriented (GFRP structure) results

References

1. Abbasi, et al., Prog. Mater. Sci. 101 (2019) 1–45.
2. Abhishek, et al., Inorg. Chem. Commun. 145 (2023) 111–334.
3. Akhtar, et al., RSC Adv. 15 (2025) 1821–1850.
4. Ali, et al., Compos. Part C: Open Access 100 (2024) 434–450.

AFM-008

Dual-Ceramic Reinforcement-Enabled Functional Tribological Behavior in Zinc Metal Matrix Composites

Sanjay Savithendhiraa P[1]*, Sanjay Priyan1, Santosh. S[1]

[1]*Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, INDIA.*

***Corresponding author e-mail:** psanjay2410926@ssn.edu.in

ABSTRACT

Zinc-based metal matrix composites reinforced with ceramic particulates are increasingly explored for applications requiring improved wear resistance and surface durability. In the present study, a dual-reinforced Zn–SiC–Al_2O_3 composite was developed by stir casting of pure zinc metal with 1% SiC and 1% Al_2O_3 under the inert condition with constant stirring at 400 rpm. Nine samples of diameter 10 mm and length 30 mm were prepared using wire EDM and evaluated to understand the influence of hybrid ceramic reinforcements on tribological behavior under dry sliding conditions. The combined addition of SiC and Al_2O_3 altered the wear response of the zinc matrix by enhancing load-bearing capacity, limiting micro-ploughing, and improving surface stability during sliding.

Tribological performance was examined using pin-on-disc testing under the ASTM-G99. the experiments were conducted by varying the load (10, 30 and 50 N) and sliding velocity (1, 2 and 3m/s) keeping the sliding distance and temperature constant. The worn surfaces were systematically characterized using scanning electron microscopy (SEM), energy dispersion spectroscopy (EDS), and non-contact 3D surface analysis along with roughness measurement. SEM examination revealed distinct variations in wear-track morphology, with the dual-reinforced composite exhibiting smoother worn surfaces and reduced material removal compared with pure zinc. EDS analysis indicated the presence of oxide-rich regions within the wear tracks, suggesting the formation of mechanically mixed and tribo-oxidative layers during sliding. Non-contact 3D surface analysis provided quantitative information on wear-track topography, demonstrating reduced wear-track depth and the roughness. SiC particulates contributed in hard load-supporting that restricted severe abrasive wear, while Al_2O_3 contributed to the development and stabilization of compacted oxide layers. The synergistic interaction between these reinforcements promoted a transition from abrasion dominated wear toward oxidation and tribofilm controlled wear mechanisms.

Overall, the results demonstrate that dual ceramic reinforcement significantly enhances the tribological performance of zinc matrices, highlighting the potential of Zn–SiC–Al_2O_3 composites for wear-critical engineering applications.

References:

1. O.P. Modi, S. Rathod, B.K. Prasad, A.K. Jha, G. Dixit, Tribology International, 40 (2007) 1137–1146
2. N. Radhika, R. Raghu, Tribology in Industry, 37 (2015) 20–28.

AFM-009

Influence of Laser Remelting Parameters on Surface Integrity and Near-Surface Hardness of SS316 Deposits Fabricated by Directed Energy Deposition

Teja Swarup Kakumanu[1], Dilli Babu Guruswamy[2]*

[1]*Research Scholar, Department of Mechanical Engineering, Siddhartha Academy of Higher Education, Deemed to be University, Vijayawada 520 007, Andhra Pradesh, India*

[2]*Associate Professor, Department of Mechanical Engineering, Siddhartha Academy of Higher Education, Deemed to be University, Vijayawada 520 007, Andhra Pradesh, India*

***Corresponding author e-mail:** gdillibabu@gmail.com

ABSTRACT

Directed Energy Deposition (DED) of SS316 stainless steel is widely utilized for additive manufacturing and repair of functional components; however, the as-deposited surfaces are often characterized by high roughness, geometric non-uniformity, and near-surface defects arising from complex thermal histories. Laser remelting (LRM) provides a localized and material-efficient post-processing approach to modify surface morphology and microstructural characteristics without additional powder consumption. In the present study, the influence of laser remelting parameters on surface integrity, bead geometry, and near-surface hardness of single-layer SS316 DED deposits was systematically investigated. A Taguchi L9 orthogonal experimental design was employed to evaluate the effects of remelt laser power, remelt scan speed, and track overlap, with three replicates conducted for each experimental condition. Surface roughness (Ra) measurements were performed at multiple locations across each coupon, bead width and height were quantified using a coordinate measuring machine, and microhardness (HV0.1) was measured at the remelted surface and at a subsurface depth of 0.1 mm. Microstructural characterization was carried out to assess porosity evolution and grain refinement induced by laser remelting. The results indicate that laser remelting significantly enhances surface integrity, achieving up to a 70% reduction in surface roughness and approximately a 20% increase in near-surface hardness compared to the as-deposited condition. An optimized parameter combination of 900 W laser power, 300 mm/min scan speed, and approximately 40% track overlap produced a flatter bead profile with reduced porosity and refined surface microstructure. Analysis of variance (ANOVA) identified remelt scan speed as the most influential factor affecting surface roughness, followed by remelt laser power. The findings demonstrate that laser remelting is an effective post-deposition strategy for tailoring the surface and near-surface properties of DED-fabricated SS316 components for functional applications.

References:

1. T. DebRoy, H. L. Wei, J. S. Zuback, et al., Prog. Mater. Sci. 92 (2018) 112–224.
2. D. Herzog, V. Seyda, E. Wycisk, and C. Emmelmann, Acta Mater. 117 (2016) 371–392.
3. K. Zhang, S. Wang, W. Liu, and X. Shang, Mater. Des. 55 (2014) 104–119

AFM-010

Hierarchical Nanostructure and Optical Response of Ag-Modified reduced Graphene Oxide/La_2O_3 Electrospun Fibers

Bibhu Prasad Swain[1]*

[1]*Department of Physics, National Institute of Technology Manipur, Langol, Imphal, Manipur-795004*

***Corresponding author e-mail:** bibhuprasad.swain@gmail.com, bpswain@nitmanipur.ac.in

ABSTRACT

Ag-doped rGO/La_2O_3 nanocomposites were synthesized via a facile chemical method by varying rGO content, and Ag/rGO/La_2O_3-PVP nanofibers were subsequently fabricated through electrospinning. The morphology, structure, chemical bonding, and optical properties were characterized using SEM, XRD, FTIR, Raman, UV–Vis, PL spectroscopy, and SAXS. SEM revealed uniform nanofibers with diameters ranging from 154–330 nm. XRD confirmed the presence of PVP (22°), rGO (002) at 24°, Ag (111) at 38°, and La_2O_3 phases at 15.7°, 27.2°, 28.1°, 39.4°, and 48.6°, with crystallite sizes between 13.1–56.7 nm. FTIR spectra exhibited distinct bands at 3322.6, 2950, 1649.6, 1390.1, 1284.3, 667, and 584 cm^{-1}, corresponding to O–H, N–H, C=O, C–H, C–O, La–O, and Ag vibrations. Raman analysis showed D and G bands at 1352.2 and 1573.2 cm^{-1}, with an I_D/I_G ratio of 0.76–0.92, indicating oxidation and rGO nanocluster formation. UV–Vis absorption peaks appeared at 247–253 nm with a broad band at 413 nm, while PL exhibited a dominant emission at 394 nm. SAXS revealed insights into correlation length, scaling behavior, micro-void density, grain boundaries, and radius of gyration in the nanofibers.

Keywords: Ag/rGO/La_2O_3-PVP nanofibers; chemical bonding; optical properties; SAXS

References:

1. Suveksha Tamang; Sadhna Rai; Rabina Bhujel; Nayan Kamal Bhattacharyya; Bibhu Prasad Swain; Joydeep Biswas. J. Alloys Compd. 2023, 947, 169588.
2. Sayantan Sinha; Naorem Aruna Devi; Sumitra Nongthombam; Rabina Bhujel; Sadhna Rai; Goutam Sarkar; Bibhu P. Swain. Diamond Relat. Mater. 2020, 107, 107885.
3. Sagolsem Nonganbi Chanu; Pukhrambam Sushma Devi; Bibhu Prasad Swain. J. Mater. Sci.: Mater. Electron. 2024, 35, 646.
4. Sagolsem Nonganbi Chanu; Pukhrambam Sushma Devi; Bibhu Prasad Swain. Inorg. Chem. Commun. 2023, 155, 110978.
5. Pukhrambam Sushma Devi; Sagolsem Nonganbi Chanu; Soumyadeep Laha; Bibhu Prasad Swain. Appl. Phys. A 2023, 129, 446.

AFM-011

Designing Functional Graded Ceramics with High dc-Tunability Using Core-Shell Approach

Lavinia-Petronela Curecheriu[1]*, Larisa Mazilu[1,2], George Stoian[1,2], Maria Teresa Buscaglia[3]

[1]*Dielectrics, Ferroelectrics & Multiferroics Group, Faculty of Physics, "Al. I. Cuza" University of Iasi, 11 Carol I Bv., 700506, Iasi, Romania*

[2]*National Institute of Research and Development for Technical Physics, Iasi 700050, Romania*

[3]*Institute of Condensed Matter Chemistry and Technologies for Energy, National Research Council, Via de Marini 6, 16149, Genoa, Italy*

***Corresponding author e-mail:** lavinia.curecheriu@uaic.ro

ABSTRACT

The capability to understand and manipulate materials has been fundamental to the technical evolution of humanity. Among the innovative materials, a special class is that of functionally graded materials (FGMs) due to their unique characteristics: the two or more materials are present, and the microstructure/composition/porosity varies in a discrete or continuous way over a definable geometry [1]. FGMs have gained interest because their properties can be easily tailored due to the absence of well-defined boundaries or interfaces between different regions which are common in conventional composite materials [2]. Considering the advantages of FGMs, we proposed to design tunable materials that fulfil technological requirements by exploiting microstructure particularities of FGCs obtained from core-shell structures.

In this talk we will discuss the role of local composition gradients generated by core-shell structure in $BaTiO_3$@$SrTiO_3$ ceramics on the low and high field properties of these functionally graded ceramics. The samples were prepared by different sintering strategies (traditional two step sintering and spark plasma sintering (SPS)) and the graded composition was checked by SEM technique. The low field properties were investigated in a large temperature and frequence range of (25 to 150)°C and 1Hz – 1MHz and a composition-induced ferroelectric-to-relaxor crossover with compositional-dependent shifts of the structural transition temperatures by comparison with the pure $BaTiO_3$ was obtained. The dc-tunability for all ceramics show a non-histeretic behaviour and a strong variation of tunability with applied fields manly in case of graded ceramics.

Keywords: FGC- functional graded ceramics, core-shell, dc-tunability

References:

1. Bharti, N. Gupta, K.M. Gupta, Int.J.Mater.Mech.Manuf. (2013) 1, 221-224
2. R.S. Parihar, S.G. Setti, R.K. Sahu, Sci Eng Compos Mater, (2018) 25 (2), 309-336.
3.

AFM-012

High Durability Poly(styrene-b-isoprene-b-styrene) Nanocomposites for Corrosion-Resistant and Antifouling Coatings

Sangeetha Vijayagopal[1], Sanjeevi Prasath Sridhar[1]*, Nagaraj Alangi[2], Velraj Parthiban[1], Sudha Uthaman[1]

[1]*Centre for Nanoscience and Nanotechnology, Sathyabama Institute of Science and Technology, Chennai 600 119, Tamil Nadu, India.*

[2]*Beam Technology Development Group Advanced Tunable Laser Applications Division, Bhabha Atomic Research Centre, Mumbai-400085.*

***Corresponding author e-mail:** sanjeeviprasath.irc@sathyabama.ac.in

ABSTRACT

In this study, graphene oxide (GO), magnetite (Fe_3O_4), and nickel oxide (NiO) nanoparticles were synthesized, and both binary (Fe_3O_4-NiO) and ternary (GO-Fe_3O_4-NiO) nanocomposites were prepared through a ball-milling process using graphene oxide (60 wt%), magnetite (20 wt%), and nickel oxide (20 wt%). These nanocomposites were incorporated into a poly(styrene-b-isoprene-b-styrene) (pSIS) matrix, selected for its inherent softness, flexibility, stretchability, and excellent ability to uniformly disperse functional fillers. The inclusion of these fillers significantly improves the thermal and corrosion-resistant performance of the pSIS matrix. Graphene oxide acts as an efficient physical barrier, reducing heat transfer and slowing the diffusion of chloride ions toward the metal surface. Magnetite limits the transport of corrosive species and supports the formation of a protective oxide layer, while nickel oxide enhances the overall thermal stability of the composite system. Thermogravimetric analysis demonstrated that the prepared nanocomposite sheets remain thermally stable up to approximately 300-400 °C. Beyond mechanical and thermal enhancements, the ternary GO-Fe_3O_4-NiO fillers significantly improve the corrosion resistance of SIS films by creating a dense and robust barrier against corrosive ion diffusion. The composites also exhibit effective antifouling behavior, primarily due to the hydrophobic nature of the pSIS matrix, which minimizes bio-adhesion on the surface. Structural and phase identification were confirmed by XRD and Raman spectroscopy. Surface area and porosity were evaluated using BET analysis, while FESEM was employed to examine surface morphology and filler dispersion. Overall, these pSIS based nanocomposites demonstrate strong potential as highly durable, corrosion-resistant, and antifouling protective materials for marine and aerospace applications.

References:

1. Chandran, S., Sridhar, S. P., Soman, A. K., Joseph, B., Mater. Lett., 349 (2023) 134813.
2. Dam, D. T., Wang, X., Lee, J.-M., ACS Appl. Mater. Interfaces, 6 (2014) 8246–8256.
3. Maan, A. M. C., et al., ACS Appl. Mater. Interfaces, 15 (2023) 19682–19694.

AFM-013

Lanthanide Fluoroborates: Synthesis, Structure–Property Correlations and Eu^{3+} Photoluminescence for Efficient Red Emission

Arunima Prasannan[1], Durga Lalitha Bai Kshatri[1], U.V. Varadaraju[1] and Pardha Saradhi Maram[1]*

[1]*Department of Chemistry, School of Engineering and Sciences, SRM University – AP, Andhra Pradesh 522240, India*

*** Corresponding author e-mail:** pardha.m@srmap.edu.in

ABSTRACT

A new series of fluoroborates, BaLnBF (Ln = La, Pr, Nd, Sm, Eu, Gd, and Dy), were successfully synthesized via a solid-state reaction method. Rietveld refinement confirmed that these phases crystallize in the monoclinic crystal system with $P2_1/c$ space group. The photoluminescence properties were investigated by doping Eu3+ ions into the Gd-site in the BaGdBF host. Upon excitation at 394 nm (NUV) and 465 nm (blue), the phosphors exhibited characteristic Eu3+ emissions with intense red luminescence at 595 nm and 614 nm, corresponding to the $^5D_0 \rightarrow {}^7F_1$ and $^5D_0 \rightarrow {}^7F_2$ transitions, respectively. The optimum luminescence intensity was achieved at a doping concentration of x = 0.7 in BaGdEuBF. The presence of a strong electric dipole transition ($^5D_0 \rightarrow {}^7F_2$) indicates that the Eu^{3+} ions occupy a non-centrosymmetric site within the host lattice. The combination of efficient excitation by near-UV/blue light makes this phosphor a promising candidate for making red emitting diodes for applications.

Keywords: Photoluminescence

References:

1. P. R. Rani, M. Venkateswarlu, Sk. Mahamuda, K. Swapna, N. Deopa, A. S. Rao, and G. V. Prakash,Mater. Res. Bull. 110, 159–168 (2019).
2. D. L. Dexter,J. Chem. Phys. 21, 836–850 (1953).

AFM-014

Exploration of structure-property evolution in non-equimolar high entropy rare-earth doped $(Na_{0.5}Bi_{0.5})TiO_3$ ferroelectric ceramics

D. Shunmugasundarapandian, R. Thillaimari, Sondhar Longvah, and N.V. Giridharan*

Advanced Functional Materials Lab, Department of Physics, National Institute of Technology, Tiruchirappalli 620015, India

***Corresponding author e-mail:** giri@nitt.edu

ABSTRACT:

With the growing demand for efficient energy storage materials, lead-free dielectrics like $(Na_{0.5}Bi_{0.5})TiO_3$, $(K_{0.5}Bi_{0.5})TiO_3$ are receiving significant attention due to their inherent relaxor nature. Among different techniques and strategies to improve relaxor behaviour, high-entropy strategy stands out as a potential candidate due to its role in increasing energy storage density (Wrec), energy storage efficiency (η) and enhancing dielectric breakdown strength (Eb). In this study, we have prepared rare-earth doped high entropy NBT-based ceramics using solid state reaction method. The effect of high-entropy on structural and electrical properties of NBT ceramics is studied.

Reference:

1. L. Wang et al., Ceram. Int., 2025, 51, 52227–52237.
2. Y. Ning et al., Appl. Phys. Lett., 2025, 127, 203901.

AFM-015

Process–Geometry Relationships and Dimensional Fidelity in SS316 Deposits Fabricated by Directed Energy Deposition

Teja Amareswar Jagu, Dilli Babu Guruswamy*, Adnan Mohammad, Fayaz Mohammad,

Mani Muramurlla, Abdul Malik Mohammad

Department of Mechanical Engineering, Siddhartha Academy of Higher Education, Deemed to be University, Vijayawada 520 007, Andhra Pradesh, India

***Corresponding author e-mail:** gdillibabu@gmail.com

ABSTRACT

Directed Energy Deposition (DED) is increasingly utilized for near-net-shape fabrication and repair of metallic components; however, achieving consistent dimensional fidelity remains a significant challenge due to thermally driven melt pool instabilities and layer-wise heat accumulation. These effects strongly influence bead geometry and surface flatness, which are critical for functional performance and post-processing requirements. In the present study, the influence of key DED process parameters—laser power, travel speed, and powder feed rate—on the dimensional accuracy of SS316 stainless steel deposits was systematically investigated.

A Box–Behnken response surface methodology was employed to design fifteen multi-layer single-track experiments, each comprising ten deposited layers with a nominal track length of 50 mm. Dimensional responses, including bead height, bead thickness, and surface flatness, were measured to quantify geometric deviation. Quadratic regression models developed for bead height and thickness exhibited strong predictive capability, with coefficients of determination exceeding 0.98, while surface flatness demonstrated a moderate but meaningful correlation with process parameters. Analysis of variance revealed laser power and travel speed as the dominant factors governing melt pool behaviour and geometric stability, whereas powder feed rate primarily influenced dimensional outcomes through interaction effects. Multi-response optimization identified a stable process window that minimizes geometric deviation while maintaining uniform layer buildup and reduced flatness distortion. The results provide quantitative insights into process–geometry relationships in DED of SS316 and establish practical guidelines for achieving improved dimensional fidelity, supporting the application of DED in precision-critical functional components.

Keywords: Directed Energy Deposition; SS316; Dimensional Fidelity; Melt Pool Stability; Response Surface Methodology.

References:

1. D. Shao, X. Bi, M. Hong, and R. Li, Materials, 18 (2025) 883.
2. J. R. Qiu, Y. X. Chen, Y. K. Hwang, W. L. Chang, and S. J. Hwang, Int. J. Adv. Manuf. Technol., 132 (2024) 5329–5350.
3. E. Amar, V. Popov, V. M. Sharma, S. A. Batat, D. Halperin, and N. Eliaz, Materials, 16 (2023) 7253.

AFM-016

Microstructural and Mechanical Characterization of Si-Modified Cu-Ni-Al Shape Memory Alloys Processed via Powdered Metallurgy

Priyasruthi Srinivasan[1], Sanchitha Shankar[1], Santhosh Sampath[1]*

[1]*Programmable Responsive Intelligent Structures and Materials (PRISM) Group, Department of Mechanical Engineering, Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, INDIA.*

***Corresponding author e-mail:** santoshs@ssn.edu.in

ABSTRACT

This study examines the microwave-sintered Cu–Ni–Al shape memory alloys (SMAs) with incremental silicon additions of 0, 0.5, 1.0 and 1.5 wt.%, which were fabricated using optimized powder metallurgy techniques. Processing parameters including traverse distance, rotational speed, sintering duration and applied load were optimized to achieve uniform densification and refined microstructures suitable for mechanical and tribological evaluation. SEM analysis revealed that 0.5–1.0 wt.% Si addition promoted the formation of fine intermetallic precipitates and a refined, martensite-dominated matrix. These hard silicide phases enhanced matrix stiffness and phase stability. Mechanical testing showed that the alloy containing 0.5 wt.% Si exhibited the highest Vickers hardness and compressive strength compared to the Si-free alloy, while further Si additions led to a slight decline, indicating an optimum Si content. Tribological testing demonstrated a steady reduction in wear rate and coefficient of friction with increasing Si content. The Si-free alloy showed the highest wear and friction, whereas Si-modified alloys formed a stable protective tribo-layer that resisted abrasion. Overall, microwave-processed Si-modified Cu–Ni–Al SMAs demonstrate significant potential for wear-critical smart material applications.

References:

1. S. N. Saud, E. Hamzah, T. A. A. Bakar, and R. Hosseinian, Jurnal Teknologi, — (2013) 51–56.
2. M. K. Ibrahim, E. Hamzah, S. N. Saud, E. N. E. A. Bakar, and A. Bahador, Jurnal Teknologi, — (2018) 80.
3. D. Casellas, A. Beltran, J. M. Prado, A. Larson, and A. Romero, Wear, — (2004) 730–739.
4. A. M. Sankhla, K. M. Patel, M. A. Makhesana, K. Giasin, D. Y. Pimenov, S. Wojciechowski, and N. Khanna, J. Mater. Res. Technol., — (2022) 282–292.
5. O. P. Modi, S. Rathod, B. K. Prasad, A. K. Jha, and G. Dixit, Tribol. Int., 40 (2007) 1137–1141.

AFM-017

Effective Photocatalytic behavior of Gallium oxide-based nanocomposites for degradation of methylene blue and ciprofloxacin

Samreen Fathima, Surya Sathiyamoorthy, Pragathi Murugan, Balaji Manavaimaran *

Chemical vapour deposition Lab, Department of Materials Science, University of Madras, Guindy, Tamil Nadu, India, 600025

***Corresponding author e-mail:** drbalajimaran@gmail.com

ABSTRACT

A wide range of harmful substances such as dyes, industrial waste, pharmaceutical waste, pesticides and heavy metals get mixed into the water bodies [1]. Methylene blue (MB) is a cationic dye commonly used for dying textiles, printing and food colouring. It is highly toxic and carcinogenic and causes adverse side effects such as bladder irritation, anaemia, etc [2]. On the other hand, antibiotics are found in various water bodies but are only partially eliminated by standard water-treatment methods. Ciprofloxacin (CIP) is a second-generation fluoroquinolone, widely used to treat infectious diseases [3].

Recently gallium oxide (β-Ga_2O_3) has gained attention of researchers as it is non -toxic and has excellent thermal and chemical stability [4]. It is emerging as superior candidate compared to commercial TiO_2 due to its strong redox ability [5]. Heterojunction with 2D transition metal dichalcogenide (TMDCs) is an effective strategy employed in improving photocatalytic performance. 2D Tungsten disulphide (WS_2) is corrosion-resistant, has high surface area and biocompatible [6].

In this work Ga_2O_3 was synthesized by co-precipitation method followed by calcination at 800°C. X-ray diffraction pattern indicates the formation of monoclinic phase of Ga_2O_3. Prepared samples were characterized using UV-Vis, RAMAN and FE-SEM techniques. The photocatalytic degradation of MB using pristine β-Ga_2O_3 was found to be 90% in 150 minutes. Further, β-Ga_2O_3/WS_2 nanocomposites have been synthesized and its photocatalytic application will be discussed in detail.

Keywords: Gallium oxide; Methylene blue; Ciprofloxacin; Hydrothermal

References:

1. Ś. K., M. A. and M. J., Pollut. 273 (2021).
2. R. B., P. S., and S. N. K., New J. Chem. 42 (2018).

AFM-018

Exploring MBene: 2D Materials Pathways in Synthesis and Characterization for Optoelectronics devices

Madhurya Chandel [1]*

[1]*Faculty of Mechatronics, Warsaw University of Technology, Warsaw, Poland*

***Corresponding author e-mail:** madhurya.chandel@pw.edu.pl

ABSTRACT

Following the breakthroughs of graphene and MXenes, MBenes, early transition metal borides, have emerged as a compelling new class of two-dimensional (2D) materials. While they share nominal similarities with MXenes, the incorporation of boron introduces complex crystallographic arrangements and distinct transition metal–boron chemistry, resulting in alternative reaction pathways and structural transformations. These unique features position MBenes as a promising frontier in materials science, particularly for optoelectronic applications.

A major challenge in MBene synthesis lies in their pronounced susceptibility to oxidation, which limits the effectiveness of conventional wet-chemical etching and often leads to the formation of oxy-borides rather than pure MBenes. To overcome this, we employed microwave-assisted hydrothermal etching, combined with acid (HCl) and base (NaOH) pretreatments, to successfully remove aluminum from MoAlB and yield multilayered 2D MBene structures. This approach provides a controlled pathway for scalable synthesis, enhancing the structural integrity of the resulting materials.

Comprehensive characterization using X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), electron microscopy, and spectroscopic methods revealed fundamental insights into MBene chemistry and behavior. Optical absorption studies and time-resolved photoluminescence (TRPL) further demonstrated tunable optical properties, underscoring their potential in optoelectronic and energy-related technologies. Together, these findings establish a foundation for advancing MBene synthesis strategies and integrating these materials into next-generation device architectures.

Keywords: 2D materials, MBene; Characterization; Optical properties; optoelectronic devices

References:

1. M. Chandel et al., Mater. Horiz., 12 (2025) 3473–3484.

AFM-019

Microstructural and Mechanical Analysis of Additive Manufactured Smart Materials with Metamaterials Design(Anisotropic Honeycomb Lattice)

Sandhya[1], Samyuktha[1], Santosh Sampath[1]*

[1]*Programmable Responsive Intelligent Structures and Materials (PRISM) Group, Department of Mechanical Engineering, Sri Sivasubramaniya Nadar (SSN) College of Engineering, Rajiv Gandhi Salai (OMR), Kalavakkam - 603 110, Tamil Nadu, INDIA.*

***Corresponding author e-mail:** sandhyar2410961@ssn.edu.in

ABSTRACT:

This paper aims to study the mechanical and microstructure analysis of additive manufactured materials, containing metamaterials design, (anisotropic honeycomb lattice) integrated with Shape Memory Alloy (SMA) Nitinol. Their unique properties such as negative Poisson's ratio, light weight ratio, stiffness, Shape memory effect and super plasticity made them to be employed in various fields like aerospace, biomedical field and so on. This combined effect leads to 4D printing. The sample is designed using AutoCAD(fusion360), following which additive manufacturing technique of Fused Filament Deposition (FDM) is incorporated for the fabrication of sample. Further, the mechanical strength (tensile test) and microstructural analysis (Field Emission Scanning Electron Microscope) was performed.

Keywords: 4D printing, Metamaterials design, Shape Memory Alloy, Additive manufacturing

References:

1. X. Kuang, D. J. Roach, J. Wu, C. M. Hamel, Z. Ding, T. Wang, M. L. Dunn, and H. J. Qi, 4D printing: Materials and applications, Adv. Funct. Mater., 29(2) (2019) 1805290.
2. Y. Lee, J. An, and C. K. Chua, Two-way 4D printing: A review on the reversibility of 3D-printed shape memory materials, Engineering, 3(5) (2017) 663–674.

AFM-020

Synthesis and Multifunctional Properties of UiO-66 MOF for Palladium (II) Adsorption from Aqueous Solutions

T. Xavier Jerlin Akshaya[1], S. Maria Jenifer[1], D. Prem Anand[1]*

[1]*Department of Physics, Material Research Centre St. Xavier's College (Autonomous), Palayamkottai 627 002, Tamil Nadu, India Affiliated to Manonmaniam Sundaranar University, Abishekapatti 627 012, India.*

***Corresponding author e-mail:** anandhdprem@gmail.com

ABSTRACT:

Palladium (Pd^{2+}) is a precious metal extensively used in nuclear, electronic, and catalytic applications. In this study, UiO-66 (Zr-MOF) was synthesized via a solvothermal method, and its structural, optical, and electrical properties were characterized using FTIR, PXRD, UV–visible spectroscopy, and dielectric measurements. The adsorption behavior of UiO-66 MOF toward Pd^{2+} ions from aqueous solution was investigated under various conditions, including adsorbent dosage, solution pH, and contact time. Dielectric studies revealed frequency-dependent polarization, confirming the multifunctional nature of the material, while the optical band gap obtained from UV– visible analysis indicated its semiconducting behavior. Kinetic analysis showed that the pseudofirst-order model provided the best fit to the experimental data, suggesting favourable adsorption kinetics. The results demonstrate that UiO-66 MOF is a stable and efficient adsorbent for Pd^{2+} recovery from aqueous solutions, with potential applications in nuclear waste remediation and wastewater treatment.

References:

1. C. R. M. Rao and G. S. Reddi, TrAC Trends Anal. Chem., 19 (2000) 565–586.
2. S. Sharma, A. S. K. Kumar, and N. Rajesh, RSC Adv., 7 (2017) 52133–52142.

AFM-021

Design of Porous Superhydrophobic Metakaolin-based Geopolymer for Microplastic Remediation in Water

Saraswathi A[1], Mullaimalar A[1], Jeyalakshmi. R[1]*

[1] *Research Scholar, Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattangulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** jeyalakr@srmist.edu.in.

ABSTRACT

The pervasive presence of microplastic particles (MPs) in aquatic and terrestrial environments has emerged as a critical global concern due to their persistence, bioaccumulation, and potential risks to ecosystems and human health. Effective removal of MPs from contaminated water systems requires advanced materials with high adsorption capacity, durability, and selective wettability. In this context, hydrophobic and superhydrophobic porous materials have attracted increasing attention owing to their ability to repel water while preferentially interacting with hydrophobic pollutants, thereby enhancing separation efficiency and reusability.

In this study, a metakaolin clay–based porous superhydrophobic material was successfully synthesized using an in-situ foaming strategy assisted by poly (methyl hydrogen) siloxane (PMHS). Under the highly alkaline geopolymerization environment, PMHS undergoes hydrolysis and reacts with hydroxyl species, releasing hydrogen gas that acts as an internal foaming agent, leading to the formation of an interconnected porous structure. Simultaneously, the hydrolysed PMHS molecules self-polymerize and chemically bond with aluminosilicate gel phases, forming low–surface-energy silicone microfilms that uniformly coat the pore walls. This dual functionality of PMHS enables synchronized pore generation and intrinsic hydrophobic modification throughout the bulk matrix, rather than being limited to surface treatment.

The resulting porous geopolymer exhibits superhydrophobic network with enhanced structural stability, making it a promising candidate for microplastic removal and environmental remediation applications. The facile synthesis route, utilization of metakaolin clay, and robust hydrophobic architecture highlight the potential of this material as a sustainable and efficient adsorbent for next-generation water treatment technologies.

References:

1. F. Eshghabadi and V. Javanbakht, J. Mol. Struct., 1295 (2024) 136639.
2. Ö. Açışlı, İ. Acar, and A. Khataee, Chemosphere, 295 (2022) 133870.
3.

AFM-022

Hydrogen-Bonded Organic Framework Synthesized via Diffusion Method as Promising Candidate for Water Splitting

P. Ajith Kumar, Surulivel Gokul Eswaran, K. AravinthKumar, C. Raja Mohan*

Nano Structure lab, Department of Physics, The Gandhigram Rural Institute – Deemed to be University, Gandhigram – 624 302, India

***Corresponding author e-mail:** crmohan.gru@gmail.com

ABSTRACT

Water splitting (results in hydrogen production) will likely be the successful solution for the sustainable energy needs. But the need of the hour is catalytic material with low cost, high efficiency along with better stability in synthesis of catalytic material. The structural attributes of Hydrogen-Bonded Organic Frameworks (HOFs) are considered as a suitable candidate, owing to its porosity. The advantages of HOF include, tuneable porosity, high surface area, structural adaptability, and straightforward synthesis in comparison to early reported works. The presence of various functional group along with Hydrogen bonds results in efficient water adsorption, proton transfer and charge transport, which plays an important role for hydrogen and oxygen evolution reactions. HOFs as photocatalyst or hosts for catalytic active sites yield an improvement in light capture and catalytic performance in aqueous surroundings. Though there seems to be a few challenges in relation to stability and charge mobility, the few characteristics such as continued molecular design and hybrid strategies highlight the strong potential of HOFs in sustainable water splitting and green hydrogen production.

References:

1. J. Tang, X. Hu, X. Zhu, B. Xu, and M. Li, J. Mater. Chem. C, 13 (2025) 18031–18042.
2. R. Gao, R. Shen, C. Huang, K. Huang, G. Liang, P. Zhang, and X. Li, Angew. Chem. Int. Ed., 64 (2025) e202414229.
3. P. Li, M. R. Ryder, and J. F. Stoddart, Acc. Mater. Res., 1 (2020) 77–87.

AFM-023

Study on the Synergistic Effect of Iron-Rich Copper Slag as a Binder and Aggregate in Alkali Activated Geopolymer for Thermal Resistance Application

M Krishnavenia, T Rithikaa, A Mullaimalara, M Manivannana, R Jeyalakshmib*

Department of Chemistry, CET, SRMIST, Kattankulathur, 603203

***Corresponding author e-mail:** jeyalakr@srmist.edu.in

ABSTRACT

This study provides a comprehensive exploration of the potential use of geopolymer technology for the sustainable recycling of non metallurgical wastes, iron rich Fayalite mineral containing copper slag. In this study the production of alkali activated geopolymer by the use ground copper slag (75 micron) as a raw feed stockand finer particles (4 mm) as an fine aggregate(FA) in (1:3 ratio) in the mixer design of mortar as CS100 (100% copper slag ,FA), MS100 (100% M-sand as FA), and CM50 (50% copper slag + 50% M-sand). Subsequently the thermo-mechanical properties of these mortars were tested by exposing them to various temperatures as 200,400,600, 800°C , Additionally, to understand the material behavior , a detailed analysis carried out using X-ray diffraction (XRD), thermogravimetric analysis (TGA) for thermal stability and decomposition patterns, and scanning electron microscopy (SEM) offered insights into microstructural development, pore structure. The usage of the copper slag aggregate in the geopolymer enhanced the compressive strength compared to river sand and retained the strength of 50% at elevated temperature exposure. The phase change of fayalite mineral into Hematite phase after 600 °C temperature exposure acted as pore filler trade off the strength loss. The micro structural study results allow for agreater understanding of copper slag binder -aggregate interactions at ambient and elevated temperature andoffers an innovative solution to combat solid waste disposal.

Keywords: geopolymer technology, non-metallurgical waste copper slag, thermal endurance

AFM-024

Effect on Structural and Electrical Properties of Gd and Zr Co-Doped $La_2Ce_2O_7$ for LT-SOFC

Abhishek Dhalaskar[1]*, Arshiya A. A. Ali[1]*, Smita Acharya[1]*

[1]*Advanced Materials Research Laboratory, Department of Physics, R.T.M. Nagpur University, Nagpur-440033, M.S., India*

***Corresponding author e-mail:** dhalaskarabhishek12@gmail.com, aliarshiya69@gmail.com, saha275@yahoo.com

ABSTRACT

A-site and B-site co-doped pyrochlores have emerged as promising electrolytes for low-temperature solid oxide fuel cells (LT-SOFCs). This study investigates the effects of Gd^{3+} A-site and Zr^{4+} B-site co-doping in $La_2Ce_2O_7$ (LCO) on its structural and electrical properties. Materials were synthesized via a sol-gel route and characterized by X-ray diffraction (XRD), Raman spectroscopy, and Electrochemical Impedance Spectroscopy (EIS). X-ray diffraction confirmed a single-phase disordered fluorite structure, with lattice contraction attributed to the substitution of La^{3+} by smaller Gd^{3+} ions and Ce3+ by Zr4+, Raman spectroscopy revealed coexisting F-type and C-type phases, along with local structural distortions influenced by Gd and Zr doping. Electrochemical impedance spectroscopy (EIS) studies were performed to explore ion dynamics in the systems at operating conditions of LT-SOFCs with increasing Zr doping concentration, surpassing undoped LCO by up to 2 orders of magnitude at 450°C. Distribution of relaxation times (DFRT) analysis deconvoluted bulk, grain boundary, and electrode contributions, attributing improvements to synergistic vacancy engineering and lattice expansion from Zr^{4+} substitution. These results position Gd/Zr co-doped LCO as a tunable LT-SOFC electrolyte, with optimal compositions balancing phase stability and low activation energies.

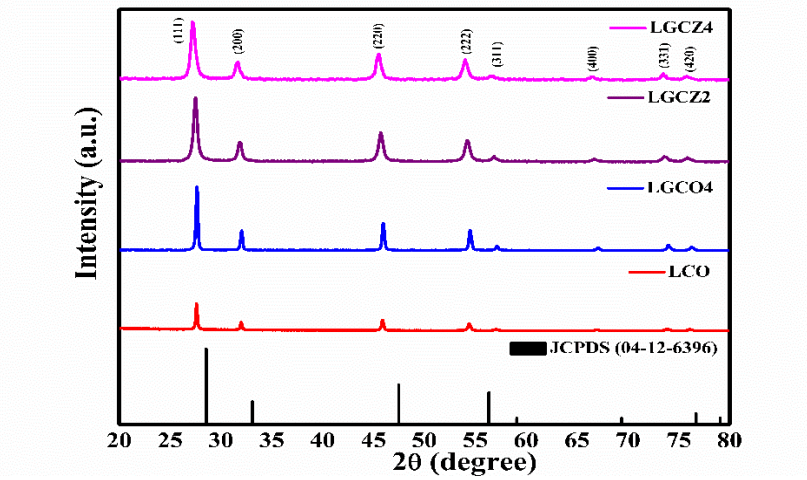


Fig. The XRD patterns of Pure LCO, Gd-doped LCO, and Gd/ Zr CO- doped LCO samples

Keywords: LT-SOFC; Impedance; $La_2Ce_2O_7$; ionic conductivity; DFRT

References:

1. N. M, A. B, A. G, S. Omar, and K. Balani, Prog. Mater. Sci. 72 (2015) 141–337
2. L. M, C.A. F, M.S. I, Chem. Soc. Rev. 39 (2010) 4370–4387

AFM-025

AI-Powered Medical Chatbot for Early Detection and Explanation of Infectious Diseases Using Generative AI and Streamlit

Singaraju Ramya [1]*, G.Diana Kamal [1]

[1]*Vishnu Institute of Technology, Bhimavaram, Andhra Pradesh, India*

***Corresponding author e-mail:** ramya.s@vishnu.edu.in

ABSTRACT

Infectious diseases remain a major global health concern, causing high mortality and significant strain on healthcare systems, where early diagnosis is often hindered by limited resources and delayed access to medical services. This study presents a Smart AI-Based Medical Chatbot that predicts infectious diseases using Google Generative AI, EasyOCR, and machine learning techniques through an interactive Streamlit-based interface. The system interprets user-reported symptoms using natural language processing and extracts relevant information from medical images such as prescriptions and diagnostic reports to enable a multimodal prediction approach. Machine learning models analyze both textual and visual inputs to generate accurate predictions, while explainable AI methods, including SHAP and LIME, provide transparent and interpretable diagnostic explanations, enhancing user trust and reliability.

References:

1. S. Sivasamy, Int. J. Adv. Res. Sci. Commun. Technol., 2025 (2025) 772.
2. R. Bansal, A. K. Vangipurapu, S. S. Satav, N. Nag, and R. Phalnikar, Indian Sci. J. Res. Eng. Manag., 8 (2024) 1.
3. V. Srivastava, R. Kumar, M. Y. Wani, K. M. Robinson, and A. Ahmad, Infect. Dis., 2024 (2024) 1.
4. P. Agarwal, Indian Sci. J. Res. Eng. Manag., 8 (2024) 1.
5. S. Kirubakaran, J. Wilsie, G. M. Kanaga, M. Raja, R. G. Singh, and E. Yuvaraajan, Proc. IEEE Int. Conf. Inf. Commun. Technol., (2024) 10544639.
6. S. Hacking, JMIR Bioinform. Biotechnol., (2024) 52700.
7. A. B. Isiaka, V. N. Anakwenze, C. R. Ilodinso, C. G. Anaukwu, C. M.-V. Ezeokoli, S. M. Noi, G. O. Agboola, and R. M. Adonu, Int. J. Innov. Res. Dev., 13 (2024).
8. R. Ashreen, Int. J. Sci. Technol. Eng., 12 (2024) 1627.

AFM-026

Anion-Driven Tuning of Ferroelectric and Optoelectronic Properties in Chalcogenide–Oxide Perovskites

Hansika Vardhini N[1], Sathiyamoorthy Buvaneswarn[1], Saurabh Ghosh[2]*

[1] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2] *Centre of Advanced Computational and Theoretical Sciences (SRM-ACTS), SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** saurabhs@srmist.edu.in

ABSTRACT

We explore how chalcogen–oxygen mixed-anion chemistry can be used to engineer ferroelectricity and optoelectronic response in Zn–Sn–based perovskites of the form $ZnSnX_3$ (X = S, Se, O). Using density functional theory combined with Berry-phase polarization calculations, lattice-dynamical analysis, and simulations of the optical response, we systematically assess how anion substitution controls structural distortions, spontaneous polarization, and the electronic band structure. The sulfide and selenide end members display comparatively weak polar instabilities and moderate band gaps, whereas oxygen incorporation markedly strengthens polar distortions and stabilizes a robust ferroelectric ground state. Notably, mixed S/O compositions emerge as a particularly attractive regime in which large spontaneous polarization coexists with visible-range band gaps and enhanced optical absorption, highlighting their promise for ferroelectric photovoltaic and photoferroic applications. Mode-resolved distortion analysis shows that anion substitution selectively reshapes the balance between polar distortions and octahedral rotations/tilts, establishing a direct mechanistic link between local bonding environments and macroscopic polarization. In addition, mixing-enthalpy calculations indicate that S/O solid solutions are thermodynamically stable across a broad composition range, supporting their experimental viability. Overall, these results provide practical structure–property design guidelines and demonstrate that chalcogen–oxygen anion mixing is an effective strategy for achieving coupled ferroelectric and optoelectronic functionality in Zn–Sn–based perovskites.

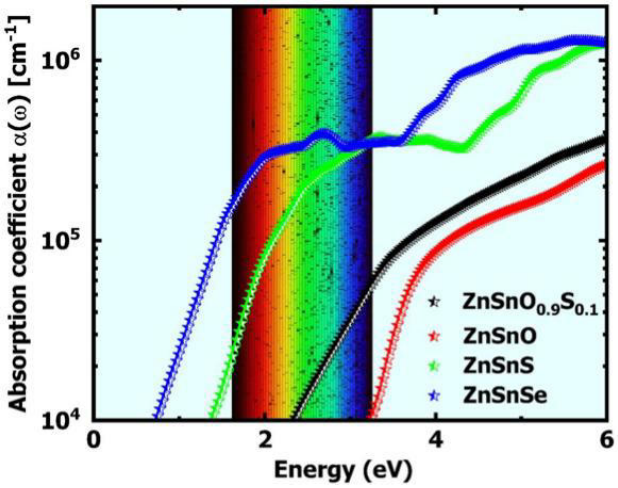


Fig. Calculated absorption spectrum of α(ω) of $ZnSnO_{0.1}S_{0.9}$ in comparison with $ZnSnX_3$ (X = O, S, Se)

AFM-027

Investigation of Mechanical Performance of 3D Printed Lattice Structures for Next-Gen Mechatronic Devices

Revathi K, Vijayaraj P, Aruna V*, Ram Prakash S*

Department of Mechanical Engineering, Centre of Excellence for Additive Manufacturing, Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India, 600119

***Corresponding authors' e-mail:** arunaveer@gmail.com, ramprakashnec@gmail.com

ABSTRACT

Increased demands for lightweight yet high strength components within mechatronic systems have driven the wider adoption of AM technologies. In addition to reduce material waste, lattice structured architectures built through AM can significantly reduce production cost while retaining mechanical properties. This work investigates the impact of lattice strut thickness on the mechanical properties of AM parts through the consideration of three design variants, namely lattice structures with strut thickness of 0.5 and 0.8mm and a solid model. The specimens were designed using the CREO CAD platform and then AM using SLS technology. Mechanical properties such as, tensile strength, compressive strength and shore D hardness were investigated for both lattice and solid configuration systematically. Furthermore, the quality of the material was before and after processing by SEM, XRD and Raman spectroscopy. Comparisons revealed that the strength to weight ratio optimized lattice structures is high, hence very suitable for lightweight application like drone frames and robotics. The outcomes highlight the role that could be played by lattice-based AM designs in pursuing structural efficiency and cost economy in state-of-the-art mechatronic systems.

Keywords: Additive Manufacturing, lattice struts, strength to weight ratio, mechatronic applications.

AFM-028

Kilogram-Scale Flash Synthesis of Waste-Derived Graphene for High-Performance Concrete Applications

Stanleydhinakar M[1], Ramesh R[1]*

[1]*Periyar University, Periyar Palkalai Nagar, Salem, India, 636011*

***Corresponding author e-mail:** rameshphys@gmail.com

ABSTRACT

Graphene is a promising nanomaterial for advanced concrete applications; however, scalable and economical production remains a key limitation. In this study, we report a pulsed flash synthesis method for the kilogram-scale production of graphene from waste-derived carbon sources, including biomass, using an indigenously developed pulsed capacitive discharge system. The process employs millisecond-scale Joule heating, enabling rapid conversion of waste carbon into graphene without chemical reagents or complex preprocessing. The method demonstrates high batch-to-batch repeatability, low energy consumption, and significantly reduced production cost, making it suitable for large-scale deployment.

The flash-synthesized graphene was incorporated at low dosages into cementitious composites to assess its mechanical performance. Graphene-modified concrete exhibited a marked improvement in compressive strength compared to conventional mixes. The enhancement is attributed to improved dispersion, strengthened interfacial bonding, pore refinement, and accelerated cement hydration.

Overall, this work establishes a scalable, low-cost, and repeatable route for converting waste into high-value graphene and demonstrates its effectiveness as a performance-enhancing additive for ultra-high-strength and sustainable concrete applications.

Keywords: Graphene enhanced concrete, Flash graphene, Nano-reinforcement

References:

1. Chen, Weiyin, et al. ACS Nano (2021), 15.1, 1282-1290.
2. Raj, Rishi et al. J. European Ceramic Society (2012), 32.10, 2293-2301.

AFM-029

Magnetic and Magnetocaloric Property Study of Nanocrystalline Gadolinium Hydride

Malaya Chandra Jena[1], Dame La-ai Wankhar Sutnga[1], Abhaya Prasada Mohapatra[1], S. Ramaprabhu[1], J. Arout Chelvane[2], A. V. Morozkin[3] and R. Nirmala[1]*

[1]*Department of Physics, Indian Institute of Technology Madras, Chennai 600 036, India*

[2]*Defence Metallurgical Research Laboratory, Hyderabad 500 058, India*

[3]*Department of Chemistry, Moscow Lomonosov State University, Moscow, 119992, Russia*

***Corresponding author e-mail:** nirmala@physics.iitm.ac.in

ABSTRACT

Study of rare earth metal hydrides is important in the context of both fundamental physics and technological applications. Recently it has been found that hydrogen insertion in rare earth intermetallic compounds leads to nanocrystallization [1]. Therefore, in the present work, rare earth metal Gadolinium is hydrogenated using a Sieverts-type apparatus at 26 bar pressure. Volumetric estimation suggests having 0.7 at. Hydrogen per Gd. Powder X-ray diffraction shows broadened Bragg peaks suggesting presence of nanosized sample. The sample has largely CaF_2-type fluorite structure. Using Scherrer formula, the average crystallite size is found to be ~17 nm. Magnetization of GdH0.7 has been measured as a function of temperature in 5 kOe applied magnetic field in the temperature range of 5 K to 300 K [Fig. 1a] and these data overlap with each other. Although elemental Gd is known to order ferromagnetically at around 293 K, there is no magnetic order observed in the $GdH_{0.7}$ sample down to 5 K. Magnetization-field isotherms of the $GdH_{0.7}$ have been measured between 5 K and 33 K at intervals of 2 K in fields ranging from 0 to 70 kOe. From the M-H data, the isothermal magnetic entropy change has been computed and this value is found to be large at temperatures below 10 K and therefore could be useful in cryogenic applications.

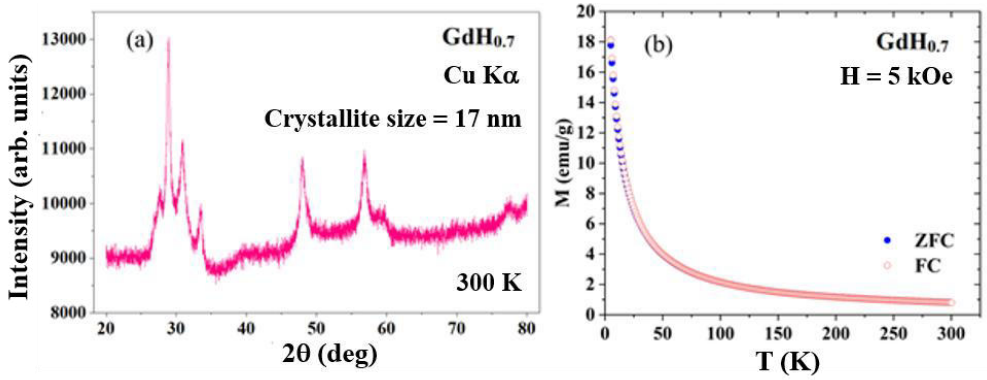


Fig. (a) Powder X-ray diffractogram of $GdH_{0.7}$ and (b) temperature dependence of magnetization in zero-field-cooled (ZFC) and field-cooled (FC) states in magnetic field of 5 kOe.

Keywords: Rare-earth hydrides; magnetic properties; magnetocaloric effect.

Reference:

1. P. Mohapatra, D. A. R., J. A. Chelvane, A. V. Morozkin, S. Ramaprabhu, and R. Nirmala, AIP Adv., 15 (2025) 035305.

AFM-030

Magnetism in multicomponent rare-earth intermetallic compound RAl (R = $Gd_{0.2}Tb_{0.2}Dy_{0.2}Ho_{0.2}Er_{0.2}Al$)

B. Manikanta[1], J. Arout Chelvane[2], A. V. Morozkin[3] and R. Nirmala[1]*

[1]*Department of Physics, Indian Institute of Technology Madras, Chennai 600 036, India*

[2]*Defence Metallurgical Research Laboratory, Hyderabad 500 058, India*

[3]*Department of Chemistry, Moscow Lomonosov State University, Moscow, 119992, Russia*

***Corresponding author e-mail:** nirmala@physics.iitm.ac.in

ABSTRACT

High-entropy alloys initiated a new paradigm in magnetic materials search [1]. Multiple magnetic elements at a particular lattice site could result in exotic magnetic properties that could be rewarding for potential applications. Recently equiatomic GdAl has been found to be a potential low temperature magnetocaloric material [2]. In the present study, Polycrystalline RAl (R = rare earth) intermetallic compound with equal amounts of Gd, Tb, Dy, Ho, and Er elements at R-site has been prepared using the electric arc-melting. Powder X-ray diffraction experiment at 300 K reveals parent orthorhombic crystal structure (space group Pbcm) [Fig. 1a]. The elemental composition is confirmed by energy dispersive analysis of X-rays and the elemental homogeneity is also verified. Magnetization study suggests possible magnetic transitions at 61 K and 89 K. The fit of the paramagnetic susceptibility to Curie-Weiss law yields the effective moment as 10.5 μB/f.u. A field-induced metamagnetic behaviour has been observed at 5 K, as in parent DyAl and ErAl compounds. The present study could be useful in designing potential low temperature magnetocaloric materials.

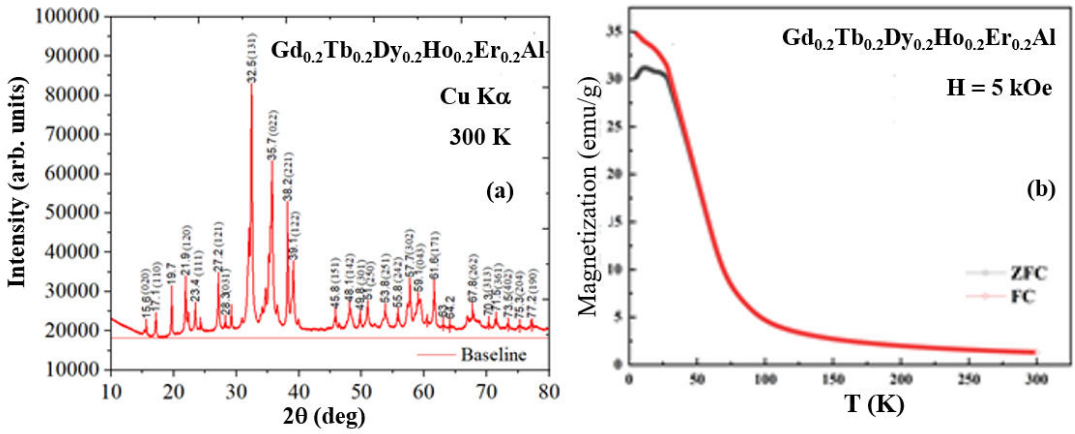


Fig. (a) Powder X-ray diffractogram of RAl (R = $Gd_{0.2}Tb_{0.2}Dy_{0.2}Ho_{0.2}Er_{0.2}$) and (b) temperature dependence of magnetization in zero-field-cooled (ZFC) and field-cooled (FC) states in magnetic field of 5 kOe.

Keywords: Rare-earth intermetallics; high-entropy alloys; magnetic properties.

References:

1. P. E. George, D. Raabe and Robert O Ritchie, Nature Reviews Materials 4 (2019) 515.
2. G. Yao et al, Phys. Chem. Chem. Phys., 27 (2025) 4419.

AFM-031

Studies of Microstructure and Electromagnetic Properties of $Li_{0.5}Zn_{0.1}Ti_{0.1}Fe_{2.3}O_4$ Spinel Ferrites with Ytterbium (Yb^{3+}) Substitution

Athikho Hriishu, Thongam Ningthouba Singh, Mamata Maisnam*

Department of Physics, National Institute of Technology Manipur, Langol, Imphal, India, 795004

***Corresponding author e-mail:** mamata@nitmanipur.ac.in

ABSTRACT

Rare-earth Ytterbium (Yb^{3+}) substituted Li-Zn-Ti ferrites with the chemical formula $Li^{+}_{0.5}Zn^{2+}_{0.1}Ti^{4+}_{0.1}Yb^{3+}_{x}Fe^{3+}_{2.3-x}O^{2-}_{4}$ (where x = 0.00, 0.02, 0.04, 0.06, 0.08, 0.10) were synthesized via the solid-state reaction method and sintered at 1050°C for 6h. The influence of Yb^{3+} substitution on the structural, microstructural, and dielectric properties have been systematically investigated. X-ray diffraction studies confirmed the formation of a single-phase cubic spinel structure, with the lattice parameter increasing linearly from 8.341 Å to 8.361 Å with increasing Yb^{3+} content, verifying the successful incorporation of the larger Yb3+ ion into the crystal lattice. Scanning electron microscopy (SEM) revealed a dramatic reduction in average grain size from 3.855 µm to approximately 1.8 µm, indicating that Yb3+ acts as a potent grain growth inhibitor. Frequency-dependent dielectric properties revealed the dispersion behaviour of dielectric constant and dielectric loss and their temperature dependence showing relaxation behavior around 350ºC, which shift to higher temperature with Yb3+ substitution. Complex impedance spectroscopy elucidated the contributions of grain boundaries to the overall electrical response, which were significantly modified by the Yb-induced microstructural refinement. These findings establish that Yb^{3+} substitution as an effective strategy for tailoring the microstructure and electromagnetic performance of Li-Zn-Ti ferrites.

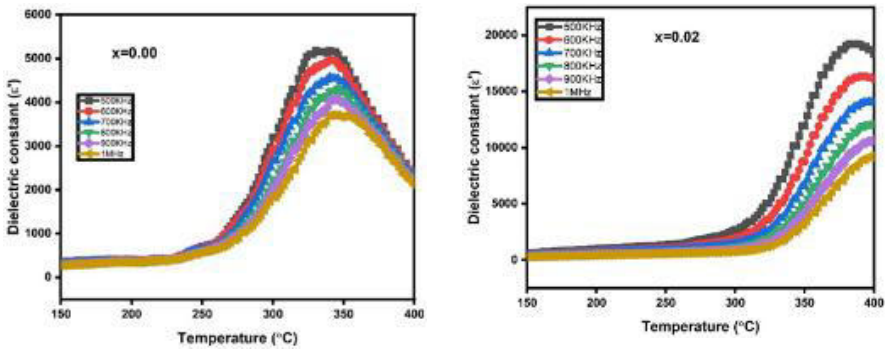


Fig. (a) Temperature dependent dielectric constant of of $Li_{0.5}Zn_{0.1}Ti_{0.1}Yb_xFe_{2.3-x}O_4$ where x = 0.00 and 0.02

Keywords: Spinel Ferrite, Ytterbium, Microstructure, Dielectric Properties, Impedance Spectroscopy

References:

1. Goldman,. Modern ferrite technology. Boston, MA: Springer US (2006).
2. S. E. Jacobo, S. Duhalde, and H. R. Bertorello, J. Magn. & Magn. Matr., 272 (2004) 2253.

AFM-032

Flexural Performance of Metakaolin – Enhanced Concrete Beams Reinforced with Basalt Fiber Reinforced Polymer Bars

B. Priyadharshini[1], M. Pon Karpagaa[2]*

[1] *Sathyabama Institute of Science and Technology, Chennai, Tamilnadu, India, 600119*

[2] *Sathyabama Institute of Science and Technology, Chennai, Tamilnadu, India, 600119*

***Corresponding author e-mail:** karpagaamr02@gmail.com

ABSTRACT

This study investigates the flexural performance of concrete beams enhanced with metakaolin as a partial replacement of cement and reinforced with Basalt Fiber Reinforced Polymer (BFRP) bars. Metakaolin, a highly reactive pozzolanic material with a specific gravity of 2.5 and an average particle size of 3µ, was used to partially substitute cement at 2.5%, 5%, 7.5% and 10% replacement levels. The mechanical and chemical composition of metakaolin contributed significantly to the improved matrix density and interfacial bonding. BFRP bars, characterized by an ultimate tensile strength of 1200 MPa, elastic modulus of 50 GPa, ultimate strain of 0.0375 and elongation at break of 1.6%, were used as longitudinal reinforcement, offering a corrosion – resistant, lightweight alternative to conventional steel.

Analytical studies were conducted using ANSYS Workbench 19.2 to simulate and validate the experimental findings. The concrete beam models incorporating varying metakaolin content and BFRP reinforcement were analyzed under static loading to evaluate stress distribution, deflection behavior and crack patterns. The integration of advanced material characterization with computational modeling provided a comprehensive understanding of the structural behavior, showcasing the potential of metakaolin and BFRP bars in developing high – performance, durable and sustainable concrete structural elements.

References:

1. A. Ahmed and A. Tabatabaeian, J. Build. Eng., 108 (2025) 112864.
2. M. M. Keshta, M. M. Y. Elshikh, and A. M. Elkerany, Next Sustain., 6 (2025) 100107.
3. A. S. Albidah, Eng. Struct., 275 (2023) 115271.
4. A. El Refai, W. Alnahhal, A. Al-Hamrani, and S. Hamed, Compos. Struct., 288 (2022).
5. H. Li, L. Hong, M. Li, B. Zhan, and Q. Yu, Case Stud. Constr. Mater., 22 (2025).

AFM-033

Investigation of Flexural and Crack Behaviour of Hybrid Fibre-Reinforced Concrete Beams Using Banana and Polyester Fibre

Y.Arokiya Telena[1]*, R.Nirmala[1]

[1] *Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India,600119.*

***Corresponding author e-mail:** teletelena@gmail.com

ABSTRACT

This experimental study investigates the mechanical performance of hybrid fibre-reinforced concrete (HFRC) incorporating alkali-treated banana fibres and polyester fibres at varying volume fractions. The primary objective of this research is to enhance the ductility, tensile strength, flexural performance, and crack resistance of conventional concrete through the optimized use of hybrid fibre reinforcement. Banana fibres, obtained from agricultural waste, were chemically treated using an alkali solution to improve fibre–matrix bonding and durability, while polyester fibres were incorporated to enhance tensile capacity and crack-bridging efficiency.

Concrete mixes were prepared by combining banana fibre volume fractions of 0.5%, 1.0%, 1.5%, and 2.0% with polyester fibre volume fractions of 0.25%, 0.5%, 0.75%, and 1.0%. The mix design was carried out in accordance with IS 10262:2019, with fibres incorporated based on volume fraction to ensure uniform dispersion within the concrete matrix. Comprehensive mechanical testing was conducted, including compressive strength, split tensile strength, and flexural strength tests, to evaluate the influence of fibre dosage on the mechanical behaviour of concrete. The experimental results were statistically analysed to identify the optimum hybrid fibre combination.

In addition to the experimental investigation, analytical modelling was performed using ANSYS software to simulate the flexural behaviour of selected hybrid fibre-reinforced concrete beams. Finite element analysis was used to validate the experimental findings and to study stress distribution, deflection behaviour, and crack propagation mechanisms under loading conditions.This study highlights the potential of hybrid fibre-reinforced concrete as a sustainable and high-performance construction material for structural applications.

References:

1. M. M. M. Attia and S. M. Shymma, N. Y. Sci. J., 14 (2020) 48–57.
2. Ranjani, K. Keerthana, and N. K. Amudhavalli, Int. Res. J. Eng. Technol., 3 (2016) 1031–1038.
3. M. H. Nensok, M. A. O. Mydin, and H. Awang, Rev. Constr., 20 (2021) 491–511.
4. J. S. Abolarin, R. O. Rahmon, G. A. Ogunkunbi, and K. J. Olaleye, J. Res. Inf. Civ. Eng., 14 (2017) 1465–1475.5.
5. S. I. Anowai and O. F. Job, Int. Res. J. Eng. Technol., 4 (2017) 1168–1172.

AFM-034

DFT study on enhancing conductivity in alkali metal adsorbed AGNR

Himanshu Pundir, Gaurav Sapra, Preetika Sharma*

UIET, Panjab University, Chandigarh, India

***Corresponding author e-mail:** preetika.uiet@gmail.com

ABSTRACT

This study uniquely demonstrates that lithium adsorption on pristine armchair graphene nanoribbons (AGNRs) yields a remarkably higher current output of 4.5 μA at 2.7% concentration compared to sodium (0.5 μA) and potassium (0.25 μA) as well as pristine AGNRs which exhibit near zero current. Pristine AGNRs are semiconducting but adsorption of alkali ions induces metallic behavior enhancing conductivity. Each alkali ion imparts distinct electronic properties that enable targeted applications: Li-adsorbed AGNRs, with their superior conductivity show exceptional promise for high-performance Li-ion battery anodes, fast-charging and nanoelectronics. Na-adsorbed AGNRs exhibiting moderate current levels are well suited for flexible electronics while K-adsorbed AGNRs despite lower current output demonstrate enhanced metallicity making them viable for low power devices and sensing applications. The pronounced enhancement in current with Li adsorption highlights its superior charge transfer efficiency and carrier mobility establishing a highly promising anode material. Unlike previous studies that predominantly examine adsorption energies and structural stability, this work prioritises current output as a critical performance metric providing novel insights into the electrochemical functionality of alkali-ion-adsorbed AGNRs.

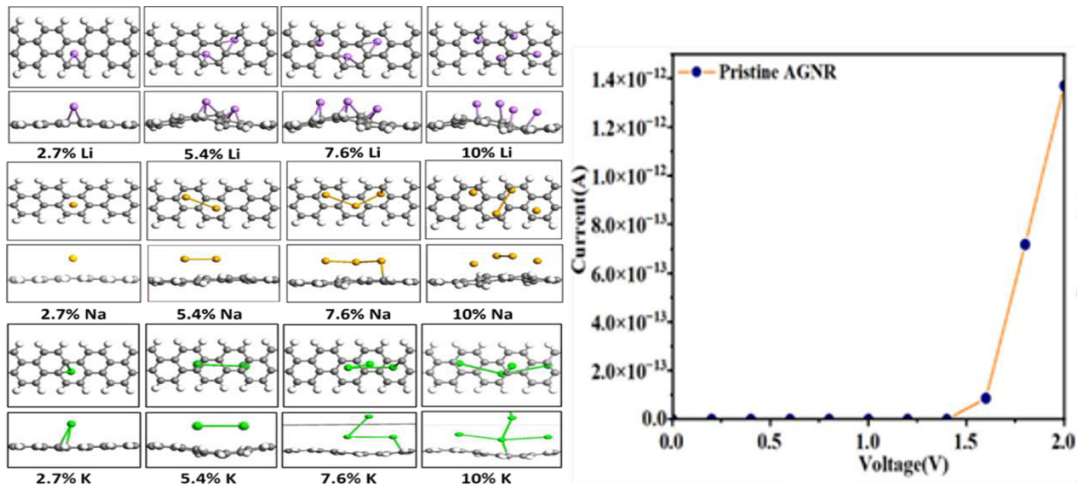


Fig. (a) Schematic of optimized structures of Li, Na and K ions adsorbed on AGNR in varying concentrations of 2.7%,5.4%,7.6 and 10% and I-V characteristics of pristine AGNR

Keywords: Alkali Metal Ions Adsorbed AGNR, DFT, I-V characteristics, Output current.

References:

1. M. R. Kumar et al., J. Power Sources, (2023) 232256.
2. B. Dunn, H. Kamath, and J.-M. Tarascon, Science, 334 (2011) 928–935.

AFM-035

Tribological Characterization of LPBF Processed SS316L Pins Fabricated on a Self-Developed Indigenous Metal 3D Printer

Arun Prakash S*, Praveen Kumar S, Parameshwaran R, Senthil SM, Sai Sanjay M K, Santhosh P, Hariharan G

Kongu Engineering College, Perundurai, Erode, Tamilnadu, India, 638060

***Corresponding author e-mail:** arunprakashsingaravel@gmail.com,

ABSTRACT

Laser Powder Bed Fusion (LPBF) is one of the most advanced metal additive manufacturing techniques, through which complex geometrical shapes are manufactured by layer upon layer of materials with high precision. Customers specific products can be printed making this technology suitable for biomedical and dental applications; also, topology optimization in aerospace and automotive components can also be achieved. This study depicts the development of an indigenous 3D metal printer by adopting a fuzzy integrated Failure Mode and Effects Analysis (FMEA) and Quality Function Deployment (QFD) framework, ensuring product reliability and systematic optimization during the development process. Through an extensive literature review, SS316L cylindrical pins were fabricated with the process parameters, Laser Power (P) = 150 W, Scanning Speed (v) = 600 mm/s, Hatch Spacing (h) = 50 µm, and Layer Thickness (t) = 50 µm for achieving best quality printed parts. Pin-on-disc tests were conducted for both wet and dry friction conditions with varying loads of 5, 10, and 15 N, with rotational speeds of 500, 1000, and 1500 RPM, and track radii of 50, 60, and 70 mm. Experimental results indicates distinct differences in wear behaviour under wet and dry conditions, with variations in coefficient of friction, wear resistance, and surface morphology. Overall, this study highlights the influence of LPBF process parameters and tribological testing conditions on the performance of SS316L, demonstrating the potential of the developed indigenous printer for reliable production of functional AM components.

References:

1. Zhang, Y.; Sanchez, M. V.; Li, X.; Peng, Z. J. Tribol. 148 (2026) 024201.
2. Pathania, A.; Subramaniyan, A. K.; B. K., N. Prog. Addit. Manuf. (2025) 1–29.
3. Vinothraj, U. T.; Xavior, M. A. J. Appl. Sci. (2024).

AFM-036

MOFs-derived and Chitosan-based Photocatalysts for Scalable VOCs Degradation in Photocatalytic Fluidized Beds

Ming-Wei Chen[1], Duo-Syuan Lin[1], Wei-Lun Huang[1], Yu-Che Hsiao[1], and Chao-Wei Huang[1]*

[1] *National Cheng Kung University, Department of Engineering Science, Tainan City, Taiwan*

***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

Photocatalytic fluidized beds (PFBs) synergistically couple photocatalysis with fluidized dynamics to enhance the degradation of volatile organic compounds (VOCs). By maintaining photocatalysts in suspension, PFBs improve light penetration and mass transfer, thereby overcoming the common limitations of fixed-bed systems such as light shielding and catalyst fouling. However, large-scale deployment remains constrained by catalyst attrition, loss, and insufficient mechanical stability. In this work, we introduce a MOFs-derived [1] and chitosan-based photocatalyst designed to address these challenges. Chitosan, a biodegradable and renewable biopolymer derived from natural biomass, provides low-cost, environmentally friendly, and mechanically robust support. Active photocatalytic particles were uniformly dispersed within a chitosan solution and solidified into spherical granules in an alkaline bath. These spheres exhibited superior abrasion resistance and maintained catalytic activity through progressive surface renewal as the outer layer eroded, continuously exposing fresh active sites. Our findings demonstrate that this chitosan-derived photocatalyst delivers long-term durability and scalability in fluidized bed operations, offering a sustainable pathway to practical VOC abatement. This approach provides both environmental and engineering benefits, establishing a promising strategy for advancing photocatalytic air pollution control technologies.

References:

1. Hsiao, Y.-C., Lin, D.-S., Wang, T.-Y., Chen, M.-W., & Huang, C.-W. (2025).

AFM-037

Structural, Morphological and Dielectric Properties of Cerium (IV) Oxide Nanoparticles Prepared Via Co-Precipitation Method

Tanu Pawar[1], Jyoti Shrivastava[1], Abhishek Sharma[2]*

[1] *Department of Chemistry, Rani Durgwati University, Jabalpur M.P. 482001 India*

[2]*Department of Chemistry, Dr. C.V. Raman University, Bilaspur C.G. 495113 India*

***Corresponding author e-mail:** abhisheksharma@cvru.ac.in

ABSTRACT

Cerium oxide (CeO_2) nanoparticles were synthesized through a straight forward and economical co-precipitation technique, chosen for its simplicity and ability to produce phase-pure nanomaterials. A complete set of characterization techniques was employed to evaluate the structural, optical, morphological and dielectric properties of the synthesized material. The crystalline phase and morphology were examined using X-ray diffraction (XRD), confirming the formation of cubic fluorite CeO_2 and allowing estimation of crystallite size. UV–visible spectroscopy was used to investigate the optical absorption behaviour. Fourier Transform Infrared (FTIR) spectroscopy verified the existence of characteristic Ce–O vibrations and the removal of residual precursor related species. The surface morphology and particle distribution were evaluated using Scanning Electron Microscopy (SEM), while Transmission Electron Microscopy (TEM) provided detailed information on particle size and shape at the nanoscale. The dielectric properties of the CeO_2 nanoparticles were investigated over a wide frequency range 1 to 105 Hz. Dielectric permittivity and capacitance of CeO_2 nanoparticles increase continuously with frequency. The dielectric permittivity of CeO_2 pellets enhances to 3 mm thickness and subsequently drops, possibly due to an increase in resistivity. The electrical conductivity of CeO_2 boosts exponentially with frequency. As per to the dielectric studies, the dielectric permittivity and electrical conductivity of CeO_2 are heavily rely on the thickness and level of frequency. The dielectric impedance of CeO_2 pellets has also been examined as a function of frequency.

Keywords: Dielectric permittivity, conductivity, impedance, frequency.

References:

1. Farahmandjou, M., Zarinkamar, M., & Firoozabadi, T. P. Rev. Mex. Fis, 62(5), (2016). 496-499.
2. Arooj, Y., Karim, R., Maqsood, S., Farhan, A., Kahlid, A., Erum, A., & Qamar, M. A.J. OvonicRes.Vol, 21(3),(2025)307-318.
3. Sravanthi,M.N.,&Sudagar,J .ES Mater. Manuf. 28,(2025)1493.
4. Muduli, S.,& Sahoo, T. R. Mater. Today Proc, 67,(2022).1147-1151
5. Srinivasan, M. P., Uthiram, C., Ayeshamariam, A., Kaviyarasu, K.,& Punithavelan, N.J.King Saud Univ. Sci 35(2), (2023). 102508.

AFM-038

A Table-Like Structured Magnetocaloric Effect in (1-x)PBMO-xPSMO

K.Sai Teja[1], N, Pavan Kumar[2]

[1]*Department of Physics, University College of Science, Telangana University South Campus Bhiknoor, kamareddy District, 503102, India*

[2]*Department of Sciences and Humanities, Matrusri Engineering College, Hyderabad - 500059, India*

ABSTRACT

The current investigation describes the structural, optical, vibrational, surface morphology, and magnetic attributes of the composites $(1–x)Pr_{0.5}Ba_{0.5}MnO_3 – xPr_{0.7}Sr_{0.3}MnO_3$ at x-values of 0, 0.25, 0.5, and 0.75. The synthesized composites have been observed through X-ray diffraction analysis (XRD), UV-visible spectroscopy, Fourier transforms infrared analysis (FTIR), atomic force microscopy analysis (AFM), and vibrating sample magnetometer analysis (VSM). The structural properties confirm the formation of a polycrystalline phase with a good level of crystallinity. The optical band gaps have been measured from UV-visible spectrograms. The FTIR analysis shows peaks due to Mn-O bonds. These bonds confirm the presence of MnO_6 groups. This further bifurcates into perovskite structures. The atomic force micrographs display rough surfaces. Additionally, ferromagnetic properties and magnetocaloric properties show large magnetic changes. Moreover, magnetic entropy variation, a plot against temperature TASm(T), displays a tail-like variation. This variation can be described due to magnetic transitions for broadening. The PBMO-PSMO composites exhibit magnetic entropy variation over a wide temperature range. This makes the composites a better candidate for magnetic cooling properties.

AFM-039

Experimental and Phy-X Based Assessment of Radiation Shielding (γ-ray & X-ray) and Optical Properties of Pb-Doped Rare-Earth Orthoferrite Ceramics ($Pb_xRe_{1-x}FeO_3$ where Re = Gd^{3+} & Pr^{3+})

Jasvinder Singh[1], Shaili Rani[1], Sunil Kumar[2]* and Sunil K. Dwivedi[1]

[1]*Department of Sciences, SAS, Om Sterling Global University, Hisar, Harayna-125001*

[2]*Department of Applied Physics, Sardar Beant Singh State University, Gurdaspur, Punjab, India-143521*

***Corresponding author e-mail:** sunil_nano@yahoo.com

ABSTRACT

Rare-earth orthoferrite perovskites ($REFeO_3$; RE = Pr & Gd, etc.) have emerged as multifunctional ceramic oxides owing to their robust structural stability, high density, tunable electronic structure, and rich defect chemistry. These materials crystallize in a distorted orthorhombic perovskite structure, offering a versatile platform for tailoring physical properties through cationic substitution and defect engineering. In recent years, increasing attention has been directed toward exploiting $REFeO_3$ perovskites for radiation shielding and luminescent applications, driven by the growing demand for advanced materials capable of simultaneously attenuating ionizing radiation and providing optical functionality.

AFM-040

Hybrid Organic-Inorganic Flame Retardant - Non-isocyanate polyurethane

Evangeline David[1], Senthil A. Gurusamy Thangavelu[1]*

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India. 603203*

***Corresponding author e-mail:** senthilt1@srmist.edu.in

ABSTRACT

The recent development of flame-retardant polyurethane coatings with multifunctional properties such as corrosion resistance, self-healing, and hydrophobicity has become an emerging area of research. Non-isocyanate polyurethanes (NIPU) have emerged as sustainable alternative to traditional polyurethane (PU) by eliminating toxic substrates from the synthetic pathway. The intrinsic flammability of PU material limits their performance, therefore, a novel flame-retardant NIPU (FR-NIPU) system with hybrid organic-inorganic framework has been developed and has gained interest. Phosphorous and nitrogen tend to enhance fire retardancy when incorporated into polymeric backbones. Cyclotriphosphazene (CTP) substituents exhibit excellent flame-retardant properties along with other applications. In this work, a CTP based diamine was reacted with bio-derived castor oil cyclic carbonate to obtain flame retardant NIPU. The structural confirmation of urethane linkage was achieved using FTIR and NMR spectroscopy. Thermogravimetric analysis demonstrated an increase in thermal stability and char yield, while flame-retardant performance evaluated using LOI, and UL-94 vertical burning tests confirmed a significant improvement in flame resistance. This behavior was due to the synergistic action of phosphorous-induced condensed-phase char formation and nitrogen assisted gas-phase flame inhibition. The mechanical and thermomechanical analysis of the FR-NIPU indicated that the incorporation of flame-retardant component did not compromise the structural integrity of the material. Overall, this study highlights the potential of CTP-modified bio-based NIPU as promising materials for flame retardant materials and high-performance applications.

References:

1. Lv, M.; Yao, C.; Yang, D.; Zeng, H. J. Appl. Polym. Sci. 2016, 133(25), 43555.
2. Usri, S. N. K.; Jamain, Z.; Makmud, M. Z. H. Polymers 2021, 13, 2916.
3. Li, X.; Xu, K.; Wu, J.; Pan, Y.-T.; Li, X.; He, J.; Yang, R. RSC Appl. Interfaces 2025, 2, 1527.
4. Rayung, M.; Abd Ghani, N.; Hasanudin, N. RSC Adv. 2024, 14, 9273.
5. Chelike, D. K.; Thangavelu, S. A. G. ChemistrySelect 2023, 8(26), e202300921.

AFM-041

Temperature-Engineered Hierarchical Porous Biochars derived from Invasive Biomass for Energy Storage Applications

C. Praveena and V. Sridevi*

Department of Chemistry, Lady Doak College, Madurai, 625002, Tamilnadu, India

***Corresponding author e-mail:** sridevi@ldc.edu.in

ABSTRACT

In this study, Mucuna bracteata, a highly invasive leguminous biomass, is converted into a series of temperature engineered biochars via slow pyrolysis in the range of 300–700 °C. The influence of carbonization temperature on the physicochemical properties of the resulting biochars is systematically investigated to establish a temperature–structure–property relationship relevant to energy related applications. Proximate analysis (moisture, volatile matter, fixed carbon, and ash content) and ultimate analysis (C/H/N/S/O elemental composition) are employed to quantify bulk composition and degree of carbonization as a function of temperature. Complementary characterization using thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR), X ray diffraction (XRD), Raman spectroscopy, Brunauer–Emmett–Teller (BET) surface area and pore size analysis, and electron microscopy provides detailed insight into thermal stability, surface functional groups, structural ordering, textural parameters, and morphology. With increasing pyrolysis temperature, the biochars exhibit higher fixed carbon content, increased C/O ratio, larger specific surface area, and enhanced aromatic/graphitic ordering, arising from progressive devolatilization, condensation, and hierarchical pore development. In parallel, a decrease in biochar yield and oxygen containing surface functionalities (O–H and C=O) at higher temperatures (600–700 °C) accompanies the growth of more ordered sp^2 carbon domains, thereby enhancing electronic conductivity and facilitating more efficient electrochemical interfaces. Thermal (TGA) and structural (Raman, XRD, BET) trends indicate that biochars produced between 500 °C and 700 °C offer an optimal balance between material yield, porosity, and structural organization, making them promising low cost carbon platforms for energy storage and electrochemical energy conversion studies. Thus, in alignment with the United Nations Sustainable Development Goal 15 ‘Life on Land’ (15.8: reducing the impact of invasive alien species through their controlled utilization) this work demonstrates the effective conversion of the aggressive invasive species Mucuna bracteata to a functional carbon material towards energy storage applications.

Keywords: Mucuna bracteata, biochar, pyrolysis temperature, porous carbon, electrochemical energy conversion, sustainable functional materials.

AFM-042

Broadband spectral responsive $PtSe_2$/n-type GaN heterojunction photodetector ranging ultraviolet-visible-near-infrared wavelengths

K. Anushree[1], V. Janardhanam[1]*, I. Jyothi[2], Chel-Jong Choi[2]

[1]*Department of Physics, School of Engineering, Dayananda Sagar University, Bengaluru 562112, India.*

[2]*School of Semiconductor and Chemical Engineering, Semiconductor Physics Research Center (SPRC), Jeonbuk National University, Jeonju 54896, Republic of Korea.*

***Corresponding author e-mail:** janardhanam-phy@dsu.edu.in

ABSTRACT

A broadband $PtSe_2$/n-type GaN heterojunction photodetector was fabricated by integrating a large-area two-dimensional $PtSe_2$ layered film onto a three-dimensional GaN. The synthesized $PtSe_2$ film consists of four layers having thickness of 2.29 nm and an interlayer spacing of 0.54 nm [1-3]. The A1g/Eg band intensity ratio from Raman spectra is obtained to be 0.69 reveals the thickness of $PtSe_2$ film is 2.0 nm [4,5]. The $PtSe_2$/GaN photodetector exhibits strong photoresponse in the ultraviolet region with a responsivity of 0.305 mA/W at zero bias under 365 nm wavelength, demonstrating self-powered operation. Under illumination of 365 nm, the photodetector showed responsivity of 38.9 mA/W, detectivity of 2.323×1010 $cm \cdot Hz^{1/2} \cdot W^{-1}$ and noise-equivalent power of 6.808×10^{-13} $p \cdot W \cdot Hz^{-1/2}$ with rise and decay times of 544/831 ms at −3 V bias. The photodetector demonstrated a broad spectral response effectively detecting light across wavelengths of 250-900 nm highlighting its sensitivity spanning ultraviolet, visible, and near infrared regions. Furthermore, the operating mechanism and charge carrier transport behaviour of the photodetector was systematically analysed using an energy band diagram.

References:

1. R. Zhuo et al., Nano Res., 2019, 12, 183–189.
2. D. Wu et al., ACS Photonics, 2018, 5, 3820–3827.
3. V. Janardhanam et al., Vacuum, 2023, 218, 112597.
4. M. O'Brien et al., 2D Mater., 2016, 3, 021004.
5. K. Bhorkar et al., ACS Appl. Electron. Mater., 2022, 4, 4814–4822.

AFM-043

In Situ Engineering of MOF on Zeolite Hybrid Architectures for Precision Acid Base Tuning and Enhanced Ethanol to Butadiene Selectivity

Duo-Syuan Lin[1], Ching-Chun Chang[1], Yi-Cyun Liu[1], Chao-Wei Huang[1]*

[1]*Department of Engineering Science, National Cheng Kung University, Tainan, Taiwan, 701401*

***Corresponding author e-mail:** huangcw@gs.ncku.edu.tw

ABSTRACT

Sustainable butadiene production via the Ethanol-To-Butadiene (ETB) process is a vital response to the shifting landscape of shale gas feedstocks [1]. However, achieving high selectivity remains a significant challenge. We report a synergistic catalyst design featuring an in-situ grown MOF template on a dealuminated Beta zeolite support [2]. By integrating zinc impregnation, we achieved tailor-made acid-base sites, effectively overcoming the selectivity barriers that have long hindered conventional ETB catalysts.

In contrast to conventional IWI catalysts, our engineered material features diminished silanol-based acidity, resulting in a significant drop in ethylene byproduct formation. We also observed that butadiene selectivity is sensitive to the MOF morphology; larger MOF particles tend to decrease selectivity, presumably because the active catalytic centers are masked by the bulky framework, reducing their accessibility for the ETB reaction.

Under optimal conditions at 350 °C, the engineered catalyst delivered a remarkable performance, achieving 97.7% ethanol conversion and 65.8% butadiene selectivity—significantly eclipsing the benchmarks set by conventional reference catalysts [3-5]. This superior catalytic activity is rooted in the precise orchestration of acid-base sites; the synergy between MOF-derived oxides and zinc species, combined with an exceptionally high surface area, creates an ideal environment for the ETB reaction.

References:

1. Pomalaza, G., et al., Catalysis Science & Technology, 2020. 10(15).
2. Payam, A.F., S. Khalil, and S. Chakrabarti, Small, 2024. 20(32): p. 2310348.
3. Wang, K., et al., Chemical Engineering Journal, 2024. 479: p. 147780.
4. Zhao, Y., et al., Chemical Engineering Journal, 2025. 519: p. 164837.
5. Zhou, B.-C., et al., Chinese Journal of Catalysis, 2024. 56: p. 166-175.

AFM-044

BCZT Nanocomposites as a High-Performance Lead-Free Piezoelectric Energy Generator

Priya Ranjan[1], Anuja Datta[1,2]*

[1]*School of Applied and Interdisciplinary Science, Indian Association for the Cultivation of Science, Jadavpur Kolkata,India, 700032*

[2] *SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** anujad@srmist.edu.in

ABSTRACT

Lead free non-toxic materials are targeted to replace commercially available lead based PZT for ferroelectric (FE) devices and piezoelectric (PE) transducers. Polycrystalline FE ceramics are widely used in commercial piezoelectric devices since they exhibit a high PE response (voltage generation due to external force due to non-centrosymmetric structure, used for harvesting mechanical energy) and tailored polarization orientation (switching of dipoles for memory applications). In this direction, we report on PE energy harvesting performance of lead-free polycrystalline perovskite $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$[BCZT] nanocomposites, due to its comparable reported PE coefficient with that of PZT (BCZT -620pC/N, PZT-5H -590pC/N]) and the presence of morphotropic phase boundary similar to PZT. Polycrystalline BCZT being environmental-friendly, and biocompatible, have potential for use in commercial devices due to its low-cost synthesis as compared to single crystals. Here we synthesize dimensional composite of polycrystalline BCZT nanorod and nanoparticle and measure the piezoelectricity. A maximum open circuit voltage of 15 V and a maximum short circuit current of 0.6 µA is obtained from a single device due to a pressure of 8N at frequency 6Hz and a maximum power obtained around 9µW. the increase in polarization is arising due to pressure-induced and cooperative alignment of dipoles on nanorods and surrounding nanoparticles in a dense nanocomposite. Polarization enhancement is reported along the pressure axis, producing a strong, highly anisotropic electric field in the surrounding nanocomposite matrix. The results are highly encouraging towards designing new generation self-powered electronics for sustainable energy applications.

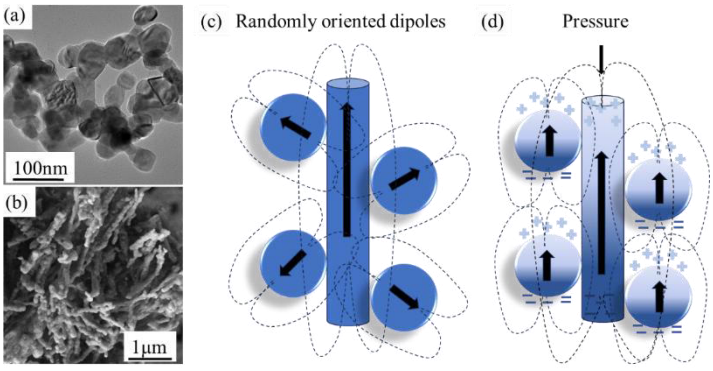


Fig. 1(a)TEM image of nanoparticle. (B)SEM image of nanorod. (c) Schematic of interaction between randomly oriented dipoles of nano rod and nanoparticle in nanocomposite. (d) partial alignment of surrounding dipoles under sufficiently high pressure due to increase in rod dipole along its axis.

Keywords: Nano rod, nanoparticle, nanocomposite, piezoelectricity

AFM-045

Defect-Engineered Trap Dynamics in $SrAl_2O_4$: Eu^{2+}, Dy^{3+} Functional Oxides via Glass Network Modification

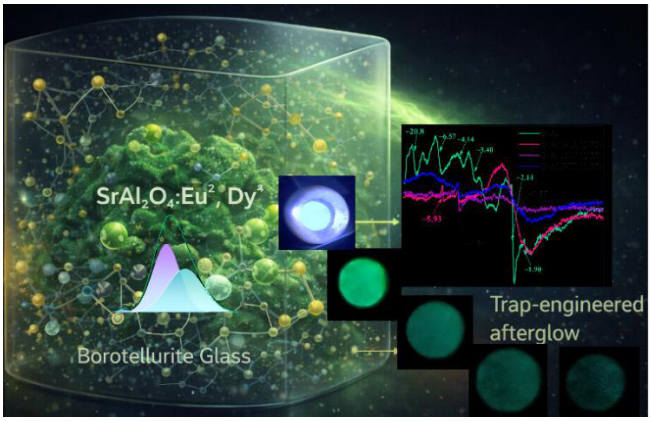
Kiran Kalkal, Yashashchandra Dwivedi*

Department of Physics, National Institute of Technology Kurukshetra, India

***Corresponding author e-mail:** yashjidwivedi@nitkkr.ac.in

ABSTRACT

Defect-mediated trap engineering plays a central role in governing the persistent luminescence performance of functional oxide phosphors. In this work, we report a systematic strategy to tailor trap dynamics and luminescence behavior in the prototypical persistent phosphor $SrAl_2O_4:Eu^{2+},Dy^{3+}$ through controlled glass network modification. $SrAl_2O_4:Eu^{2+},Dy^{3+}$ phosphor particles were embedded within borotellurite glass matrices with varying B_2O_3 content, enabling modulation of the local lattice environment and defect landscape without compromising phosphor crystallinity. Structural and microscopic analyses confirm uniform phosphor dispersion and strong interfacial coupling between the oxide phosphor and the glass matrix. Optical studies reveal matrix-induced modification of the Eu^{2+} local environment, leading to bandgap tuning and subtle emission shifts. Thermoluminescence investigations demonstrate effective control over trap depth (0.65–0.98 eV) and trap distribution, resulting in a significantly prolonged afterglow lifetime of up to ~8000 s. Electron paramagnetic resonance measurements further confirm defect-induced changes in local symmetry and crystal field effects around Eu^{2+} centers, evidencing matrix-driven lattice perturbation. The observed enhancement and stabilization of persistent luminescence are attributed to boron-induced formation of non-bridging oxygen defects and optimized trap-assisted charge storage and release processes. This study establishes glass-assisted defect engineering as a powerful route to tune trap dynamics in functional oxide phosphors, offering promising opportunities for persistent lighting, optical data storage, security marking, and advanced photonic applications.



References:

1. T. Matsuzawa, Y. Aoki, N. Takeuchi, Y. Murayama, J. Electrochem. Soc., 143 (1996) 2670–2673.
2. D. Poelman, D. Van der Heggen, J. Du, E. Cosaert, P. F. Smet, J. Appl. Phys., 128 (2020) 240903.
3. R. Kabe, N. Notsuka, K. Yoshida, C. Adachi, Adv. Mater., 28 (2016) 655–660.

AFM-046

Investigating the Potential of Zn Incorporated $CoFe_2O_4$/ α -Fe_2O_3 Nano-Composite Hetero-Structure for RRAM Application

Chandraprakash[1]*, B. K. Sahoo[1]

[1]*National Institute of Technology Raipur, Raipur, Chhattisgarh, India, 492010*

***Corresponding author e-mail:** chandraprakash.phd2024.phy@nitrr.ac.in

ABSTRACT

Resistive Random Access Memory (RRAM) is an emerging non-volatile memory technology that utilises resistance modulation of a switching layer (SL) by formation and rupture of oxygen vacancy conductive filament. In this study, we propose $Co_{1-x}Zn_xFe_2O_4$/α-Fe_2O_3 (x = 0, 3) heterostructure as a potential candidate for active SL for RRAM application. The influence of Zn on switching property were systematically investigated. XRD results confirm the decrease in crystallite size from 70 nm to 40 nm, enhancing grain boundary density for easier filament formation. FESEM along with EDX elemental mapping is employed for symmetric operation across multiple switching cycle. Raman reveals a significant redshift (~28 cm-1) in vibrational frequency on Zn-doping, indicating enhanced oxygen ion mobility required for low power SET/RESET operation. Magnetic property analysis shows a clear difference in magnetic response between undoped and Zn-doped systems. Initial I-V characteristics of the bulk pellet sample shows near ohmic semiconducting behavior with slight reduction in average resistance from 10.12 MΩ to 9.27 MΩ upon Zn incorporation. These results indicate the enhanced endurance and stable retentivity (>104) which is comparable to other industry standard metal oxides. These findings suggest that Zn-doped CFO/hematite nanocomposites is a promising candidate for RRAM application.

References:

1. M. M. El-Masry, A. E.-R. Mahmoud, H. Y. Morshidy and R. Ramadan, J. Mater. Sci.: Mater. Electron., 2023, 34, 383.
2. M. F. Ahmed, A. Yasmin, B. Biswas, M. L. Rahman and J. Khanam, Mater. Adv., 2025, 6, 6724–6741.
3. K. Gayakvad, K. Somdatta, V. Mathe, T. Dongale and M. W., Emergent Mater., 2024, 7, 103–131.

AFM-047

Sustainably Produced, Low-Cost Graphene for High-Performance Concrete at Ultra-Low Loading

Krishnaja P V[1], *Binitha N Narayanan*[1, 2]*

[1]*Department of Chemistry, University of Calicut, Malappuram, Kerala, India, 673635*

[2]*Inter University Centre for Hydrogen & Energy Storage, University of Calicut, Malappuram, Kerala, India, 673635*

***Corresponding author e-mail:** binitha@uoc.ac.in

ABSTRACT

The incorporation of graphene into cementitious materials offers a promising route toward next-generation high-performance concrete; however, large-scale application is limited by poor dispersion, high cost, and environmentally intensive processing. This work presents a sustainable, low-cost concrete-strengthening strategy using edge-specifically functionalized graphene synthesized through an eco-friendly process that preserves graphene's intrinsic aromatic π-conjugated network. Selective edge functionalization enables the formation of a highly stable dispersion in green solvents, ensuring uniform distribution within the cement matrix without surfactants or harsh chemical treatments. Remarkably, an ultra-low graphene loading of 0.02 wt% achieves an approximately 67% improvement in mechanical strength compared to pristine concrete. This enhancement arises from synergistic mechanisms, including efficient stress transfer through the preserved basal plane, strong interfacial bonding via functionalized edges, effective crack bridging, and microstructural densification of the cement matrix. The findings demonstrate that strategic edge engineering combined with electronic structure preservation enables significant performance gains at drastically reduced graphene dosages, providing a scalable, sustainable, and economically viable pathway for graphene-enabled concrete in durable and thus low-carbon infrastructure applications.

References:

1. Md. Habibur Rahman Sobuz, Rahat Aayaz ,Arifur Rahman SM, Faiz Uddin Ahmed Shaikh , Md. Kawsarul Islam Kabbo, Md. Munir Hayet Khan, J. Mater. Res. Technol, 36, (2025), 1409–1430.
2. A. H. Alateah, Case Stud. Constr. Mate., 19, (2023), e02653.
3. Babatunde Abiodun Salami, Faisal Mukhtar, Saheed Ganiyu A., Saheed Adekunle, Tawfik Saleh A. , Constr. Build. Mater., 396, Sep. (2023), 132296.
4. R. Zhang et al., Constr. Build. Mater., 415, (2024), 135019.
5. Reddy P. V. R. K., Ravi Prasad D., J. Build. Eng., 63, (2023), 105481.

AFM-048

Tuning Resistive Switching Performance of Nickel Ferrite RRAM Through Annealing Temperature

Payodhara Namdeo[1]*, B.K. Sahoo[1], S.M. Saini[1]

[1]*National Institute Technology Raipur, Raipur, Chhattisgarh, India, 492010*

***Corresponding author e-mail:** pnamdeo.phd2024.phy@nitrr.ac.in

ABSTRACT

Resistive random access memory (RRAM) comes out as the most promising candidates among varied non-volatile memory devices. Resistive Switching mechanism plays the key role in the memory storage. In this work, NiFe2O4(NFO) were synthesized by sol-gel auto combustion method. In order to study the improved resistive switching, prepared material was annealed at 625℃, 725℃ and 825℃. X-ray diffraction (XRD) confirms the cubic spinel structure with lattice parameter ~ 8.33Å to 8.34Å. Fourier transform infrared spectroscopy (FTIR) shows the presence of octahedral and tetrahedral stretching. Using FTIR data, elastic parameters, phonon velocity, Debye temperature and thermal conductivity were calculated via modified Callaway-Klemens model to examine sample's thermal stability. The Debye temperature was found to be decreasing from 596K to 587K as annealing temperature was increased. In addition, Energy dispersive X-rays (EDX) confirmed the presence of nickel, iron and oxygen elements. Field emission scanning electron microscopy (FESEM) images suggest spherical morphology of the samples with increasing grain size as the synthesis temperature was increased. X-ray photoelectron spectroscopy (XPS) findings indicate the concentration of oxygen vacancies present in the samples that are responsible for RS mechanism. To find the correlation between dielectric parameters and resistive switching of RRAM device, a dielectric study was performed. I-V characteristics study of the sample shows semiconducting nature with hysteresis type trend which indicates the presence of RS.

References:

1. Ling Du, Jiacheng Li, Yu Zhang, Ni Qin, Dinghua Bao, Current Applied Physics, 48(2023) 123-133.
2. Dae Yun Kang, Won-Yong Lee, No-Won Park, Yo-Seop Yoon, Sang-Kwon Lee, Journal of Alloys and Compounds, 790(2019) 992-1000.

AFM-049

A Novel Electrospun Taurine-Doped Polyaniline (TPANI)/ Hydroxypropyl methylcellulose (HPMC)–Curcumin Nanofibrous Composite with Enhanced Functional Properties.

Archana M S[1], Jiya Jose[2], Deepa S[1]*

[1]*Department of Physics, Mar Athanasius College (Autonomous) Kothamangalam, Kerala, India,686666*

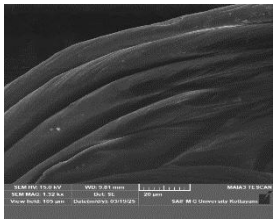
[2]*Department of Biosciences, Rajagiri College of Social Sciences (Autonomous), Cochin, Kerala, India,683104*

***Corresponding author e-mail:** sdeepa@macollege.in

ABSTRACT

Electrospun conducting polymer based nanofibers have attracted considerable interest due to their tunable electrical, optical, and biofunctional properties, making them promising candidates for multifunctional biomedical materials. In this work, a novel electrospun nanofibrous composite based on taurine-doped polyaniline (T-PANI) blended with hydroxypropyl methylcellulose (HPMC) and incorporated with curcumin was successfully fabricated to investigate its structural, physicochemical, electrochemical, and biological properties. The addition of HPMC improved spinnability, mechanical integrity, and moisture retention, while curcumin imparted bioactive functionality.

X-ray diffraction analysis confirmed the semi crystalline nature of the T-PANI/HPMC composite nanofibers, and Fourier transform infrared spectroscopy verified the successful incorporation of taurine, curcumin, and HPMC through characteristic vibrational features and intermolecular interactions. Field emission scanning electron microscopy revealed uniform, bead-free nanofibrous morphology resembling extracellular matrix architecture, while thermogravimetric analysis demonstrated enhanced thermal stability due to synergistic interactions among the composite components. UV–Visible spectroscopy showed characteristic polaron-related absorption, and photoluminescence analysis indicated modified emission behavior arising from molecular-level interactions. Electrical conductivity measurements exhibited frequency-dependent AC conductivity consistent with hopping-dominated charge transport, and electrochemical studies revealed enhanced redox activity and charge transfer capability. Preliminary biostudies indicated favorable biointeraction and cytocompatibility, highlighting the multifunctional nature of the developed nanofibers.



References:

1. Li, X., Wang, Y., Zhang, H., Nano Today, 57 (2024) 102397.
2. Zhang, Y., Liu, S., Chen, M., Eur. Polym. J., 178 (2022) 111490.
3. Yadav, P., Sharma, R., Singh, A., Carbohydr. Polym., 259 (2021) 117640.

AFM-050

NiO Nanoparticles from a mer-Ni (II) Pyrazole-Carboxylate Complex

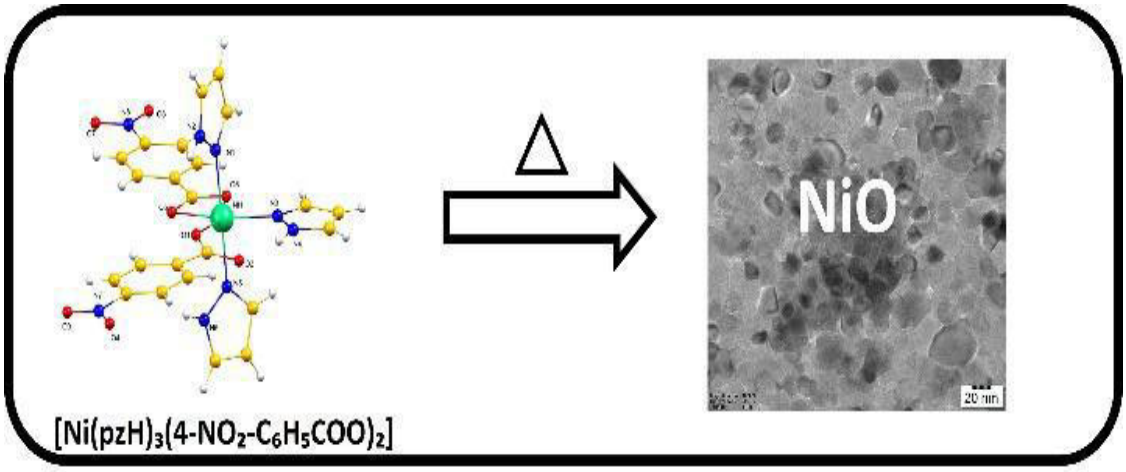
Devika M, Dharshini V, Logesh Mathivathanan*

Vellore Institute of Technology, Vellore, Tamilnadu, India, 632014

***Corresponding author e-mail:** logesh.m@vit.ac.in

ABSTRACT

NiO is a versatile material with applications across numerous disciplines. We report the synthesis of a mononuclear Ni complex with three pyrazoles in a mer-arrangement and its calcination to yield NiO nanoparticles. NiO thus prepared shows uniform particles and a 2.5 eV band gap, indicating their suitability for semiconductor-based applications.



Keywords: Nickel pyrazole complex, molecular precursor, Nickel oxide, Nanoparticle, Semiconductor

References:

1. A. C. Colson and K. H. Whitmire, Chemistry of Materials, 23, 3731 (2011).
2. T. Mandal et al., Chemistry of Materials, 23, 4158 (2011).
3. L. Mathivathanan, M. Rivera-Carrillo, and R. G. Raptis, Inorganica Chimica Acta, 391, 201 (2012).

AFM-051

Waste Thermocol–Derived Polymer Nanofibrous Membranes via Electrospinning for Sustainable Water Filtration

Mukesh Kumar, Yashashchandra Dwivedi

National Institute of Technology, Kurukshetra, Haryana, India, 136119

***Corresponding author e-mail:** yashjidwivedi@nitkkr.ac.in

ABSTRACT

The growing accumulation of waste thermocol (expanded polystyrene, EPS) and the increasing demand for clean water necessitate the development of sustainable polymer-based materials for environmental remediation. In this work, waste thermocol is upcycled into functional polymer nanomaterials for water filtration through electrospinning by blending recycled EPS with poly (methyl methacrylate) (PMMA) and related polymer systems. Volatile solvent systems comprising tetrahydrofuran (THF), chloroform, and dimethylformamide (DMF) were employed to achieve effective polymer dissolution and stable jet formation during electrospinning. The influence of polymer blending and solvent composition on fiber morphology, porosity, and structural integrity was systematically investigated.

The optimized polymer/EPS solutions yielded uniform, bead-free nanofibrous membranes with high porosity and interconnected pore networks, as confirmed by morphological analysis. The incorporation of PMMA significantly improved spinnability, mechanical robustness, and long-term membrane stability, overcoming the intrinsic limitations of electrospinning recycled thermocol alone. Owing to their nanoscale fiber diameter, large surface area, and tunable porous architecture, the fabricated membranes exhibit characteristics well suited for microfiltration and hybrid sustainable water treatment systems.

This study demonstrates a circular-economy-driven approach for converting plastic waste into value-added polymer nanofibrous membranes, contributing to the broader framework of polymer-based sustainable materials. The findings highlight the future potential of integrating recycled polymers with biochar or bio-derived fillers to further enhance adsorption capacity, mechanical performance, and environmental sustainability, positioning electrospun polymer membranes as promising materials for next-generation water filtration and environmental remediation technologies.

References:

1. B. H. Arrosyid, A. Zulfi, ACS Omega, 8 (2023) 23664–23672.
2. A. Rajak, D. A. Hapidin, Waste Management, 103 (2020) 76–86.
3. Liao, A. G. Fane, Prog. Polym. Sci., 77 (2018) 69–94.
4. P. S. Suja, A. Sujith, Polymer Reviews, 57 (2017) 467–504.

AFM-052

Microstructural Evolution and Graphitization Trajectory of Carbon Derived from Diverse Biomass Materials

Abhijith C S[1], C.N. ShyamKumar[1]*

[1]*Department of Materials Science and Engineering, National Institute of Technology, Calicut, Kerala, India, 673601*

***Corresponding author e-mail:** shyam@nitc.ac.in

ABSTRACT

The dependency on fossil-based carbon can be reduced by utilizing the carbon derived from biomass, as it is a sustainable alternative. However, understanding the properties of carbon derived from such sources is crucial for using this carbon as an alternative to the fossil-based counterpart. For that, systematic comparisons of graphitization behaviour and properties across different biomasses under identical pyrolysis conditions are required. This work is a comparative study to understand the temperature-dependent evolution of graphitic carbon from five lignocellulosic biomasses: teak wood, sugarcane bagasse, banana fibre, rice husk, and bamboo fibre. All the materials were pyrolyzed at 600 °C, 800 °C, and 1000 °C under a nitrogen atmosphere. The carbon obtained was systematically characterized to evaluate changes in chemical functionality, morphology, porosity, and structural ordering.

SEM imaging and BET surface area analysis indicated enhanced pore development and increased porosity with temperature rise across all biomasses. FTIR analysis reveals that carbon produced at 600 °C retains a higher concentration of oxygen-containing functional groups, which progressively diminish with increasing temperature. The structural evolution across temperature is evident from changes in the ID/IG ratio. In the case of sugarcane bagasse, an increase from 0.66 (600 °C) to 1.22 (1000 °C) was observed, while for teak wood, it is from 0.33 to 1.10. Banana fibre exhibits a rise from 0.52 to 0.81, followed by near saturation at higher temperatures. In contrast, rice husk shows a gradual increase from 0.48 to 0.67, and bamboo fibre displays a sharp rise from 0.42 to 1.27.

Although all biomasses follow similar temperature-driven trends, the extent of graphitization varies significantly and is strongly influenced by intrinsic biomass composition, particularly lignin content. The findings from this study provide clear design guidelines for selecting biomass feedstocks for targeted applications of graphitic carbon.

References:

1. Mohammed Mudassir, Bushair Ali K, Ali Ahmadian, C.N. Shyam Kumar, Biomass Bioenergy, 191 (2024) 107479.
2. Ferrari A.C, Robertson J, Physical Review B, 61 (2000) 14095-14107.

AFM-053

Controlled Defect Dynamics in MoS_2 Using a Splicing-Inspired Computational Framework

Kushpu M[1], D. K. Sheena Christy[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** sheenac@srmist.edu.in

ABSTRACT

Defects strongly influence the electronic and functional properties of two-dimensional nanomaterials such as molybdenum disulfide (MoS_2). Understanding how these defects form, migrate, and heal is essential for designing materials with tailored performance. In this work, we present a simple and interpretable computational approach inspired by splicing concepts, where defects are treated as bond-breaking and bond-reforming events governed by clear, physically meaningful rules. Using this framework, we track how defect populations evolve over time and examine their effect on material behaviour. The simulations show that defects tend to cluster or spread depending on the applied rules, and these patterns directly influence trends in electronic properties such as effective bandgap and defect density. The results demonstrate that rule-based modelling can provide controlled insight into defect evolution while remaining computationally efficient and interpretable. This framework can also be adapted to other two-dimensional nanomaterials, offering a practical tool for studying defect engineering in nanotechnology.

References:

1. T. Head, Bull. Math. Biol. 49 (1987) 737–759.
2. L. Kari, T. Neary, Int. J. Found. Comput. Sci. 32 (2021) 685–711.
3. G. Păun, Discrete Appl. Math. 70 (1996) 57–79.

AFM-054

Report on Extended Infrared Absorption Spectrum in Cobalt Activated Erbium Aluminium Garnet Nanocrystals for Opto-thermal and Infrared Sensing Applications

Archisha Singh, Y. Dwivedi*

Department of Physics, National Institute of Technology Kurukshetra, Haryana, 136119, India

***Corresponding author e-mail:** yashjidwivedi@nitkkr.ac.in

Cobalt-doped erbium aluminium garnet (Co:$Er_3Al_5O_{12}$) has been examined as a promising material for infrared absorption [1] and photophysical applications. $Er_3Al_5O_{12}$ (ErAG) provides a thermally stable, low-phonon-energy garnet host that supports sharp f–f transitions of Er^{3+}, while the incorporation of Co^{2+} introduces broad d–d absorption bands arising from crystal-field-driven electronic transitions. In this work, $Er_3Al_5O_{12}$:Co nanophosphors were synthesized through a combustion synthesis method. X-ray diffraction confirmed the successful formation of a single-phase ErAG structure with cobalt incorporated into the lattice, while SEM–EDS analyses revealed a porous network of interconnected grains and agglomerated nanoparticles, a morphology conducive to enhanced optical interaction.

UV–visible–NIR absorption spectra exhibited extended broadband absorption in the infrared region (), attributed to Co^{2+} and Er^{3+} electronic transitions at 1450 nm & 1550 nm and 1.54 μm emission attributed to the 4I15/2→4I13/2 transitions, respectively. This establishes the material's potential as an effective infrared absorber and functional nanophosphor for infrared devices including optical amplifiers, lasers, and IR sensing technologies. Moreover, its temperature-dependent luminescence and absorption behaviour enable optical temperature sensing, while the broadband and intensity-dependent absorption make Co:ErAG a suitable saturable absorber for pulsed laser cavities operating in the near-infrared telecommunication window.

Reference:

1. V. Singh et al., Appl. Phys. B 101 (2010) 631–638.

AFM-055

Modulating Energy Harvesting Performance of PVDF Piezo-Polymer based Flexible Triboelectric Nanogenerator by Incorporation of Ferroelectric Ceramic Filler

Ankita K[1], Gifty Godson P.[1] and P. Murugavel[1]

Department of Physics, IIT Madras, Chennai, Tamilnadu, India, 600036

***Corresponding author e-mail:** k123ankita@gmail.com

ABSTRACT

The modulation of energy-harvesting performance in piezoelectric polymers via ceramic filler incorporation has proven to be an effective strategy for low-frequency mechanical energy harvesting applications namely PENGs and TENGs. In this work, flexible PVDF–BCZT composite films were studied, where ferroelectric $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (BCZT) nanoparticles are embedded within a poly(vinylidene fluoride) (PVDF) matrix to enhance electromechanical energy conversion. The BCZT nanoparticles were dispersed in a PVDF matrix, and the composite films were formed using a scalable doctor-blade process. The presence of BCZT nanoparticles effectively modulates polarization behaviour and interfacial charge dynamics, leading to a significant enhancement in triboelectric output. When operated in contact–separation mode, the composite-based device exhibits ~1.5× higher open-circuit voltage than pristine PVDF. The device demonstrated stable performance over prolonged cycling and after one month of operation, and was capable of powering small electronic devices, highlighting its potential for flexible self-powered systems.

References:

1. Y. S. Choi, S. W. Kim, S. Kar-Narayan, Adv. Energy Mater., 11 (2021) 2003802.
2. J. Wang, C. Wu, Y. Dai, Z. Zhao, A. Wang, T. Zhang, Z. L. Wang, Nat. Commun., 8 (2017) 88.
3. P. Bera, S. Sen, S. Kundu, S. Sen, ACS Appl. Energy Mater., 7 (2024) 11834.

AFM-056

High-Strength Poly (Vinyl Alcohol) Physical Eutectogels: Effects of Polymer Molecular Weight, DES Composition, and Heat Treatment

Ruei-Min Chuang[1], Trung Hieu Vo[1], Heng-Kwong Tsao[1]*, Yu-Jane Sheng[2]

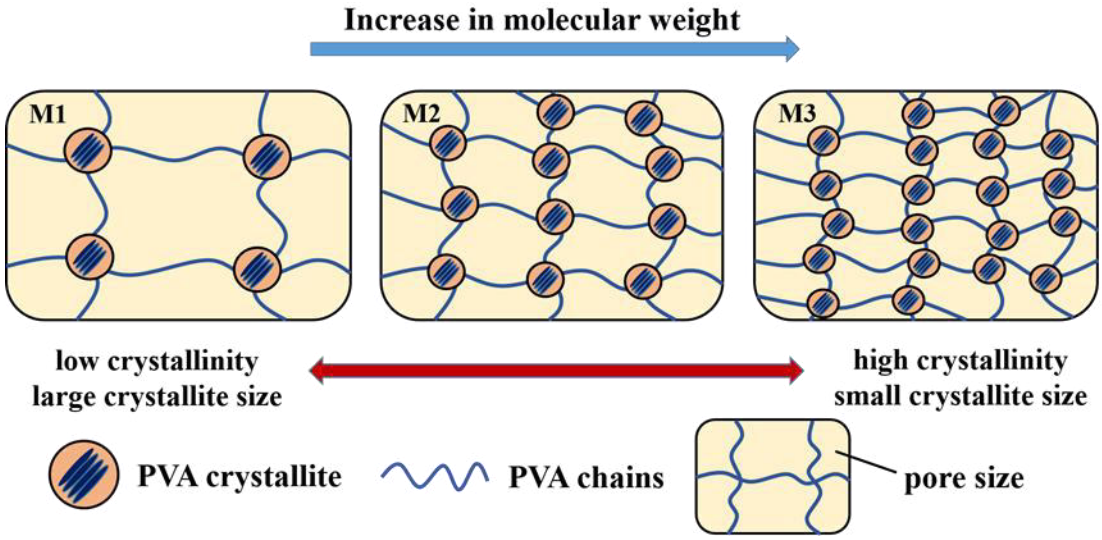
[1]*Department of Chemical and Materials Engineering, National Central University, Taoyuan 32001, Taiwan, ROC*

[2]*Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan, ROC*

***Corresponding author e-mail:** hktsao@cc.ncu.edu.tw

ABSTRACT

A one-step manufacturing process is employed to fabricate stretchable physical eutectogels. It involves directly mixing polyvinyl alcohol (PVA) with choline chloride as a hydrogen bond acceptor and either ethylene glycol or glycerol (Gly) as a hydrogen bond donor. This process results in the formation of numerous crystallite domains of PVA within the deep eutectic solvent (DES), which act as physical crosslinking points in the eutectogel. The study systematically investigates the effects of PVA molecular weight, DES composition, and various heat treatments on the mechanical properties of eutectogels. The stress-strain curves demonstrate that a higher PVA molecular weight, the addition of Gly to the DES, and repeated freeze-thaw cycles can enhance the mechanical properties of the PVA physical eutectogel. Finally, scanning electron microscopy and X-ray diffraction are used to examine and analyze the polymer networks and crystallite domains in terms of pore size, crystallinity, and crystallite domain size.



AFM-057

Electrostatic Self-Assembly of Carbon Nanotubes for Next-Generation Functional Materials – A Review

Rupinder Kaur, Sławomir Boncel*

Silesian University of Technology, Gliwice, Silesia Poland 44-100

***Corresponding author e-mail:** slawomir.boncel@polsl.pl

ABSTRACT

Carbon nanotubes (CNTs) have been recognized as quintessential materials for their remarkable electrical, thermal, and mechanical properties. However, they exhibit inherent hydrophobicity due to strong van der Waals interactions, thereby inhibiting practical application. To overcome these limitations, electrostatic self-assembly has emerged as a powerful and adaptable modification technique. This non-covalent route to construct layered nanoarchitectures and self-assemblies, without disrupting the sp^2-network, has been explored to understand the underlying assembly mechanism. The key charge-imparting strategies are anionic (e.g., acid oxidation) and cationic (e.g., amination) functionalization. Assembly mechanisms include different strategies such as layer-by-layer (LbL) deposition for ordered multilayers, solution self-assembly for scalable composites, and interface-directed methods for patterned structures [1]. These electrostatic interactions can construct interconnected pathways such as 1D-1D (CNT-nanowire/dot systems enhancing transport), 1D-2D (CNT-graphene with intimate contacts), and 3D (hydrogels/porous films) networks. Electrostatic self-assembly can optimise interfaces to enhance performance in applications such as bio-sensing and energy storage. This approach yields devices like the MXene/NH_2-CNTs sensor, which is characterized by a high sensitivity of 10.8 kPa^{-1}, short response/recovery time, i.e., 40/60 ms, an ultra-low 4.6 Pa detection limit, and reliable performance across 5000 cycles [2]. Moreover, hydrogels formed via electrostatic crosslinking achieve a conductivity of ~30 S m–1 within an interconnected 3D conducting network, which is considerably higher than that of most conventional conductive hydrogels [3]. Key challenges, such as scalable precision, material heterogeneity, and environmental sensitivity, are being met with innovative strategies including permanent charge motifs. The integration of responsive, multifunctional components promises to further expand the impact of electrostatically assembled CNTs [4].

References:

1. B. Sun, K. Huang, X. Qi, X. Wei, J. Zhong, Adv. Funct. Mater. 2015, 25, 5633.
2. Z. Xu, D. Zhang, Z. Li, C. Du, Y. Yang, B. Zhang, W. Zhao, ACS Appl. Mater. Interfaces 2023, 15, 32569.
3. M. Yang, X. Ren, T. Yang, C. Xu, Y. Ye, Z. Sun, L. Kong, B. Wang, Z. Luo, Chem. Eng. J. 2021, 418, 129483.

AFM-058

Effective Anti-Cancer Therapeutics Using Piezoelectric BCZT Nanostructures

Shobanadoss.K[1], Priya Ranjan[2], Oishi Mukherjee[3], Anuja Datta[1], Koustav Sarkar[3]

[1]*Department of Physics and Nanotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[2]*School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata, West Bengal, India, 700032*

[3]*Department of Biotechnology, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** anujad@srmist.edu.in

ABSTRACT

The advancement in oxide-based lead-free perovskite materials research in self-powered technology now offer realistic and exciting alternatives to lead-based materials (ex. lead zirconium titanate) because of their low toxicity from the "green" constituent elements. The reports on (Barium Calcium Zirconium Titanate) BCZT serves as a strong illustration of how the pursuit of sustainable electroceramic materials can result in innovations that not only compete with but also surpass the effectiveness of their harmful predecessors.[1] The optimal composition of BCZT ceramic exhibits superior piezoelectric property (d33 ~ 600 pC/N), and a suitable tri-critical morphotropic phase boundary (MPB), showing excellent piezoelectricity at R-T(Rhombohedral to Tetragonal) phase transition, dependent on the composition, crystal structure, domain structure, and ceramic microstructures. The application areas therefore widely vary from sensors, to transducers and biomedical fields. Piezoelectric nanotherapeutics, focusing on whether the biophysical properties of piezoelectric nanomaterials can be used to design effective nanotherapy approaches for challenging tumours, has potential application in cancer therapy and being lead-free and biocompatible, BCZT is highly suitable. Here, our study investigates the anti-tumor agent of BCZT on various cell lines as a preliminary biological study to further assess its tumor therapy potential. We treated the cell lines with varying compositions and nanostructures of BCZT with the help of a portable electroporation device operated at low, medium, and high frequency. The results demonstrate concentration-dependent effects on cell viability, supporting the potential of BCZT for further tumor therapy studies. The research focuses a futuristic concept that uses the piezoelectric effect to initiate or accelerate chemical reactions. We envision to create a wireless bioelectronic oncology platform wherein low intensity focused ultrasound remotely actuates implanted or tumor targeted BCZT piezoelectric nanoparticles to generate localized electric fields, depolarizing cancer cell membrane potentials and thereby modulating voltage gated ion channel conductance to suppress proliferative signaling and enhance therapeutic response.

Keywords: BCZT (Barium Calcium Zirconium Titanate), Piezoelectric Properties, Anti-Cancer Therapy.

References:

1. Zuo et al. Journal of Experimental & Clinical Cancer Research (2025) 44:171
2. Marzia Mureddu et al. Elsevier (2025) 6 4:100434
3. José Eduardo Garcia et al. J. Appl. Phys. (2020) 127, 131102

AFM-059

Engineering a Core–Shell Ta-Doped $SrTiO_3$@PTC Structure for High Frequency Capacitor Applications

Deepesh Kumar, Jitendra Singh, Shivani Sangwan, Gagan Sharma, and Deshraj Meena*

Clean Energy Research Laboratory, Department of Applied Physics, Delhi Technological University, Delhi, 110042, Delhi, India

***Corresponding author e-mail:** deshrajmeena@dtu.ac.in

ABSTRACT

In this study, Ta-doped $SrTiO_3$ was synthesized using the solid-state reaction method, and the formation of the phase was confirmed by XRD and FTIR analyses. The dielectric behavior was systematically investigated. The Ta-doped $SrTiO_3$ exhibited a pure cubic perovskite phase with an average crystallite size of 64 nm, calculated using the Scherrer formula. To suppress grain growth during sintering, a novel approach was adopted by utilizing a titanium precursor solution known as Peroxo Titanium Complex (PTC). The PTC solution was employed to form an ultra-thin amorphous shell layer on the Ta-doped $SrTiO_3$ nanoparticles, resulting in a core–shell structure in which the nanoparticles act as the core and the PTC layer serves as the shell. The formation of this core–shell structure was confirmed by TEM analysis. The dielectric properties of the synthesized core–shell structure were measured and demonstrated excellent stability of the dielectric constant over a wide frequency range. The Ta-doped $SrTiO_3$@PTC core–shell structure exhibited a very low dielectric loss (0.01–0.1) within the frequency range of 1 kHz to 1 MHz Owing to its low dielectric loss at high frequencies, the synthesized material shows strong potential for microwave and other high-frequency applications.

References:

1. L. Zhang et al., J. Eur. Ceram. Soc., 43 (2023) 5713–5747.
2. D. A. Elalfy et al., Energy Strategy Rev., 54 (2024) 101482.
3. Y. Yu et al., J. Mater. Sci. Technol., 84 (2021) 10–15.
4. B. Wang et al., J. Am. Ceram. Soc., 103 (2020).
5. D. Lee et al., Ceram. Int., 51 (2025) 37525–37532.

AFM-060

Fabrication of Copper-Reinforced Aluminum Alloy Processed by Friction Stir Processing with Statistical Data Analytics

Krishnakumar K[1,2*], Senthil Saravanan M. S[3,4], Mohammad Israr[5]

[1]*APJ Abdul Kalam Technological University, Thiruvananthapuram*

[2]*Department of Mechanical Engineering, Rajdhani Institute of Engineering & Technology, Thiruvananthapuram*

[3]*Lincoln University college, Malaysia*

[4]*Department of Mechanical Engineering, Sree Buddha College of Engineering, Alappuzha*

[5]*Maryam Abacha American University of Nigeria, Kano, Federal Republic of Nigeria*

***Corresponding author e-mail:** krishnakumark@rietedu.in

ABSTRACT

Friction Stir Processing (FSP) is an advanced solid-state technique widely employed for micro-structural modification and surface property enhancement of metallic materials. In the present work, copper-reinforced aluminum alloy surface composites were fabricated using friction stir processing. The influence of copper reinforcement on microstructure, micro-hardness, and tensile strength was experimentally investigated. To improve the scientific rigor and reproducibility of the study, statistical data analytics using Analysis of Variance (ANOVA) was carried out to quantify the significance of reinforcement on mechanical properties. The results revealed substantial grain refinement in the stir zone and statistically significant improvement in hardness and tensile strength of Al–Cu composites compared to unprocessed aluminum. The integration of experimental metallurgy with data-driven statistical validation strengthens the reliability of the reported findings.

Keywords: Friction stir processing, Aluminum–copper composite, Microhardness, Tensile strength, ANOVA, Data analytics

AFM-061

Structural and Optical Properties of Gd^{3+}-Doped $Sm_2Ti_2O_7$ Pyrochlore Nanomaterials for Solid-State Lighting

R. Antonette Divya Faustina[1], T. Jose Antony[1,2], K. Ramachandran[1]*

[1]*Department of Physics, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Vadapalani Campus Chennai-600026, Tamil Nadu, India.*

[2]*Sree Balaji Institute of Science and Technology (SBIST), Chrompet, Chennai-600044, Tamil Nadu, India.*

***Corresponding author e-mail:** *ramachak1@srmist.edu.in*

ABSTRACT

The increasing demand for the rare earth activated phosphors have intrigued the research for advanced nanomaterials for LED applications. In particular, pyrochlore based nanomaterials have emerged as promising host lattices due to their structural stability and rare-earth accommodation ability. In this work, pure and Gd^{3+} doped $Sm_2Ti_2O_7$ nanomaterials were synthesized using solid state reaction. The synthesized nanomaterials were employed for various characterization techniques to understand their characteristic behavior. The XRD analysis confirmed successful synthesis of pure and Gd^{3+} doped $Sm_2Ti_2O_7$ nanomaterials having a single-phase pyrochlore structure without secondary impurities. The HRSEM images depicted an agglomerated and homogeneous morphology. The EDX analysis revealed the presence of desired elements. The XPS indicated the elemental composition and oxidation states of the pure and Gd^{3+} doped $Sm_2Ti_2O_7$ nanomaterials. The optical studies revealed strong absorption in the UV region with a calculated band gap ranging from 3.6 to 3.85 eV, indicating wide band gap semiconducting behavior. The FTIR analysis demonstrated the characteristic metal–oxygen vibrational modes such as Sm-O, Ti-O, Gd-O. The chromaticity coordinates derived from the CIE 1931 diagram suggest that the prepared materials are promising candidates for blue-emitting LED applications.

Keywords: $Sm_2Ti_2O_7$; Pyrochlore; Gd^{3+}-doping; Photoluminescence; Solid-state lighting.

AFM-062

Self – Sterilizing Nanofiber Air Filter for PM2.5 Filtration

Anitha Christy A, Raveena P V, Logamithrai D, Debabrata Sarkar*

Applied Nanophysics Laboratory, Department of Physics and Nanotechnology,

SRM Institute of Science and Technology, Kattankulathur– 603203, Chennai, India.

***Corresponding author e-mail:** ramachak1@srmist.edu.in

ABSTRACT

Air pollution from fine particulate matter (PM) is a pressing public health concern, linked to respiratory illnesses, cardiovascular diseases, and environmental degradation[1,2]. The integration of superior particulate removal with reliable antimicrobial functionality within one filtration medium continues to be a demanding task[3,4]. In this work, a self-sterilizing multifunctional nanofiber network was fabricated via electrospinning method. Polyvinylpyrrolidone (PVP) was coupled with organic titanium salt to enhance structural stability while maintaining high porosity, ensuring both durability and breathability. The resulting membrane exhibited exceptional performance, achieving ~95% filtration efficiency for [1,2]$PM_{2.5}$ with a low pressure drop of ~36 Pa, corresponding to an excellent quality factor[1]. To prevent microbial growth on the filter surface, a photosensitizer dye was incorporated into the nanofiber matrix. Under visible light, the dye generated reactive oxygen species (ROS), enabling rapid bacterial inactivation and imparting self-sterilizing functionality. This dual-purpose system integrates mechanical filtration, environmental stability, and light-activated antimicrobial activity within a single flexible platform. Preliminary antibacterial tests confirmed substantial bacterial reduction under illumination, validating its effectiveness. The developed nanofiber network shows strong potential for next-generation filtration applications, including personal protective equipment, indoor air purification, and industrial systems, where prolonged service life and combined particulate–microbial protection are critical.

Keywords: Electrospinning; PM particles; Air filtration; Anti-bacterial activity;

References:

1. A. Lakshmanan, P. P. Sarngan, D. Sarkar, 2022, *286*.
2. S. Yeon, J. Hak, I. Ho, D. Yun, D. Uk, G. Byoung, B. Han, S. Bok, D. Song, I. Park, J. Hee, 2025, *266*.
3. F. Ayaydin, 2014, 129.
4. S. K. Sehmi, S. Noimark, J. C. Bear, W. J. Peveler, M. Bovis, E. Allan, J. Macrobert, I. P. Parkin, 2015.

AFM-063

Influence of Operating Parameters on the Surface Properties of SiOx-Coated PET Films via Ar/O_2 Glow Discharge Plasma for Improving Cytocompatibility

M. Karuppusamy, K. Navaneetha Pandiyaraj*

Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore-641020, Tamil Nadu, India

***Corresponding author e-mail:** dr.knpr@gmail.com

ABSTRACT

Polyethylene terephthalate (PET) is extensively used in biomedical applications, especially in cardiovascular and peripheral vascular devices, owing to its physio-chemical properties. However, a major limitation of PET is its inherently poor surface properties, which can restrict its biological performance and limit its effectiveness in certain biomedical applications. Hence, surface modification of polymers is therefore essential to enhance biocompatibility, ultimately improving the functionality and longevity of medical implants. The aim of this investigation was to enhance the biocompatibility of PET film surfaces through the formation of SiOx-like coatings deposited via low-pressure Ar+O_2 plasma-assisted polymerization, using hexamethyldisiloxane (HMDSO) as a gaseous precursor in vapour form. The surface coatings were carried out as a function of applied voltage and gas flow. The impact of the operating parameter on the surface properties of SiOx-like coatings were comprehensively examined by means of X-ray photoelectron spectroscopy (XPS), Scanning Electron Microscopy (SEM), atomic force microscopy (AFM) and Contact angel analysis. The active species generated in the plasma during the SiOx were identified and characterized using optical emission spectroscopy (OES). Furthermore, the durability of the SiOx coating was assessed by measuring water contact angle values 15 days after storage under air atmosphere. The characterization results clearly demonstrated that SiO-containing functional coatings were successfully deposited onto the surface of PET films surfaces. Moreover, the retention of characteristic functional groups could be effectively controlled by adjusting the plasma operating parameters. Finally, the viability of the SiOx coated PET film surfaces films was also evaluated in vitro analysis including assessments of cell adhesion and cytotoxicity. The antibacterial activity of the SiOx coatings was evaluated against two representative bacterial strains: Gram-positive Bacterium *Staphylococcus aureus* (S. aureus) and the Gram-positive bacterium *Escherichia coli* (E. coli).

Keywords: Glow discharge Plasma, SiOx Coating, operating parameter, *In vitro* analysis.

AFM-064

Rational Design of Coordination-Modulated NiCo MOFs as High-Efficiency Electrodes for Next-Generation Supercapacitors

Jaya Shree K S[1], Ajay Rakkesh R[2] and Balakumar S[1*]

[1]*National Centre for Nanoscience and Nanotechnology, University of Madras, Chennai-600 025.*

[2]*Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, India-603 203.*

***Corresponding author e-mail:** balasuga@yahoo.com

ABSTRACT

In the current era of rapid population growth and technological advancement, global energy demand necessitates the development of sustainable energy storage systems to reduce dependence on fossil fuels. Among emerging materials, metal-organic frameworks (MOFs) have gained attention owing to their surface area, tunable porosity, structural diversity, and design flexibility. These attributes render MOFs promising candidates for supercapacitor applications. However, practical utilization is often limited by poor electrical conductivity, structural instability, and insufficient cycling durability. Consequently, numerous strategies have been explored to improve MOF electrochemical performance, yet the incorporation of coordination modulators during synthesis remains underexplored. This work employed a coordination modulation (CM) strategy to tailor the coordination environment of a bimetallic NiCo MOF, leading to enhanced electrochemical performance. The study investigates how CM influences organic linker deprotonation, nucleation and correlates these effects with electrochemical behaviour. By varying the modulator concentration, NiCo MOFs with different pH values were synthesized, producing distinct morphologies and revealing the role of pH in governing surface charge and electrochemical properties. Notably, the NiCo MOF synthesized at pH 6.0 delivered a specific capacitance of 576.4 F g^{-1} at 1 A g^{-1}, with energy and power densities of 24.2 Wh kg^{-1} and 275 W kg^{-1}, respectively. Furthermore, an asymmetric supercapacitor device assembled using the pH 6.0 NiCo MOF and activated carbon retained 87.50% capacity with a Coulombic efficiency of 92.75% after 2,500 cycles. Overall, this study identifies the NiCo MOF at pH 6.0 as an electrode material for advanced supercapacitors.

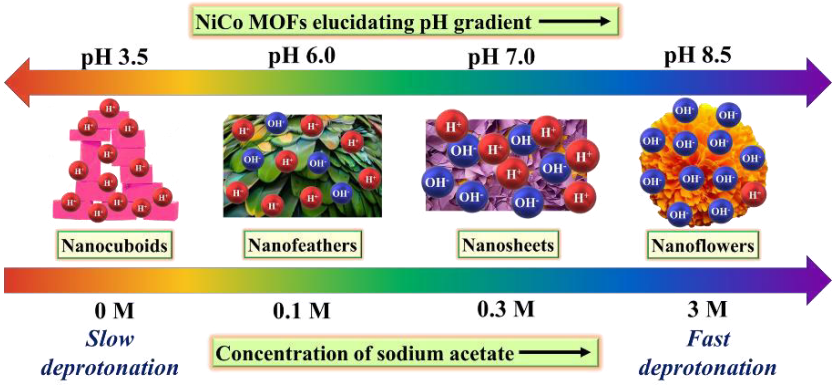


Fig. 1. Schematic representation of the effect of pH on NiCo MOFs for supercapacitor application

References:

1. Guo, H.; Zhu, Y.; Wang, S.; Su, S.; Zhou, L.; Zhang, H. Chem. Mater. 2012, 24 (3), 444–450.
2. Korapatti Selamayya, J. S.; Rajendran, A. R.; Subramanian, B. Langmuir 2025, acs.langmuir.5c03749.
3. Wang, Y.; Liu, Y.; Wang, H.; Liu, W.; Li, Y.; Zhang, J.; Hou, H.; Yang, J. ACS Appl. Energy Mater. 2019, 2 (3), 2063−2071.

AFM-065

Investigation of Room-Temperature Poling in $LiNbO_3$-Based Sol–Gel Composite Films

Mako Tanaka, Makiko Kobayashi*

Graduate School of Science and Technology, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto, Japan, 860-8555

***Corresponding author e-mail:** kobayashi@cs.kumamoto-u.ac.jp

ABSTRACT

High-temperature facilities require ultrasonic sensors capable of stable operation at elevated temperatures. Sol–gel composite ultrasonic transducers, consisting of ceramic powders dispersed in a sol–gel matrix, possess a porous structure that enables operation without backing or couplant materials, making them promising for ultrasonic measurements in harsh thermal environments [1]. Lithium niobate ($LiNbO_3$) exhibits a high Curie temperature of approximately 1200 °C and is considered an excellent candidate for high-temperature piezoelectric applications. However, polycrystalline $LiNbO_3$ remains difficult to pole due to its high coercive field. Previous studies proposed $LiNbO_3/TiO_2+SrCO_3$ (LN/TO+Sr) sol–gel composite transducers composed of $LiNbO_3$ powder and a TiO_2+SrCO_3-based sol–gel solution [2]. The TO+Sr sol–gel phase has a relatively higher dielectric constant than Pb (Zr, Ti) O_3 and $Bi_4Ti_3O_{12}$ phases. This facilitates effective electric-field distribution within the composite, enabling poling at approximately 200 °C. In contrast, LN/Pb (Zr,Ti)O_3 and LN/$Bi_4Ti_3O_{12}$ systems require poling at 550 °C [3] and 900 °C [4], respectively. LN/TO+Sr composites also exhibit high thermal stability during thermal cycling up to 700 °C [2], and ultrasonic responses have been confirmed at 1050 °C. However, elevated-temperature poling increases fabrication complexity. In this study, the powder-to-sol ratio was modified to further reduce the poling temperature. Successful room-temperature poling was achieved while maintaining sufficient thermal stability. Further optimization and X-ray diffraction (XRD) analysis are ongoing to clarify the mechanism of room-temperature poling.

References:

1. M. Kobayashi and C.-K. Jen, Ultrasonic Transducers, ed. K. Nakamura (Woodhead Publishing, 2012), pp. 408–443.
2. N. Kambayashi, N. Zaito, H. Akatsuka, and M. Kobayashi, Jpn. J. Appl. Phys. 61 (2022) SG1060
3. D. Maeda, M. Furukawa, N. Shohei, and M. Kobayashi, Proc. USE (2019) 1P1-6.
4. M. Kobayashi, C.-K. Jena, J.F. Bussiere, and K.-T. Wu, NDT & E Int. 42 (2009) 157.

AFM-066

Cage Charge Modulation in C12A7 Through Alkali Metal Substitution for Enhanced Ionic Transport

Jagadeeswaran K S[1], Kyosuke Ban[2], Yusuke Kishi[2] Takahiko Kawaguchi[2], Naoki Wakiya[1,2,3], Naonori Sakamoto[1,2,3]*

[1]*Graduate School of Sci. and Tech., Shizuoka Univ., 3-5-1 Johoku, Naka-ku, Hamamatsu-shi, 432-8561, Japan*

[2]*Dept. Eng., Graduate School of Integrated Sci. and Tech., Shizuoka Univ., 3-5-1 Johoku, Naka-ku, Hamamatsu-shi, 432-8561, Japan*

[3]*Research Institute of Electronics, Shizuoka Univ., 3-5-1 Johoku, Naka-ku, Hamamatsu-shi, 432-8561, Japan*

***Corresponding author e-mail:** sakamoto.naonori@shizuoka.ac.jp

ABSTRACT

Mayenite type calcium aluminate $12CaO \cdot 7Al_2O_3$, abbreviated as C12A7, consists of a cage structured framework with twelve sub-nanometer cages per unit cell. These cages can host anions or electrons, enabling control of lattice charge and ionic transport. While anion and electron substitution are well studied [1], systematic tuning of cage charge through alkali metal cation substitution remains limited. This study examines lithium, sodium, and potassium substitution in C12A7, focusing on lattice evolution and cage charge modification. Lithium and sodium show limited effectiveness for stable cage charge control. Lithium incorporation is strongly restricted due to its small ionic radius and charge mismatch, which introduce lattice strain and promote secondary phase formation even at low concentrations [2]. Sodium substitution at Ca^{2+} sites is more compatible because of its closer ionic size to Ca^{2+}, leading to gradual lattice expansion while preserving the cubic structure at low to moderate contents. However, sodium solubility remains limited, and higher substitution levels reduce structural stability, resulting in only partial modification of the cage charge environment. In contrast, potassium substitution exhibits the highest structural tolerance and the most significant impact on lattice and charge. Replacement of Ca^{2+} by larger K^+ ions causes a clear and systematic lattice expansion at low to intermediate substitution levels, confirming effective incorporation into the framework. At higher potassium contents, the lattice parameter approaches saturation, indicating a balance between framework expansion and internal charge compensation within the cages. Potassium substitution reduces the net positive framework charge leading to weakening and partial removal of cage O^{2-} species and effective cage charge neutralization. These results show that alkali metal substitution in C12A7 is governed by ionic size and charge compatibility. Lithium and sodium provide limited control, whereas potassium enables stable lattice expansion and substantial cage charge modulation. Potassium substituted C12A7 therefore represents a promising platform for enhanced ionic transport and advanced solid-state ionic applications

Keywords: Alkali substitution, cage charge control, lattice expansion, ionic transport

References:

1. K. Hayashi, et al., OPTRONICS, 10 (2004) 140-147.

AFM-067

Nanoclay Composites in Human Immunodeficiency Virus Pharmaceuticals Sensors

Sapokazi Timakwe[1], Sizwe Ngcobo[1] and Randall Smith[1] Mangaka Matoetoe[1]*

[1]*Cape peninsula university of Technology, Department of Chemistry, , P.O. Box 1906, Bellville, South Africa*

***Corresponding author e-mail:** lellangm@gmail.com

ABSTRACT

Nanoclays' are nanofillers phyllosilicates made up of SiO_4 tetrahedra attached to $(Mg,Fe,Al,O,OH)_6$ octahedra thin sheets. Clays are accessible, cheap, have high surface area, stable, resistant to extreme temperature with excellent intercalation properties and environmentally friendly hence, why there are constantly researched. However, their usage in electrochemical sensors is limited due to poor conductivity. Metal, metal oxide and bimetallic nanoparticles functionalization (figure 1) of nanoclay improves their electrochemical properties and widens their applicability in electrochemical devices. The composites changes in morphology and conductivity were studied using FTIR, XRD, SEM and Cyclic voltammetry. The nano films of the composites were found to adopt functionalizing metals/oxide electrochemical properties. All composites depicted a slight negative potential shift from the metal/oxides potentials with currents that are inversely proportional to the concentration of the nanoclay. There was a noticeable change in electron transfer rates, diffusion values and surface area for the composites. The electrochemical efficiency trend was Ag >Ag-Au>ZnO nanoclay composites when comparing Q , electron transfer rates. The nanofilms of the composites sensors fabrication for analysis of nevirapine, zidovudine and efavirenz showed good linearity and acceptable limit of detection. These devices were used in analysis of commercial tables/capsules successfully.

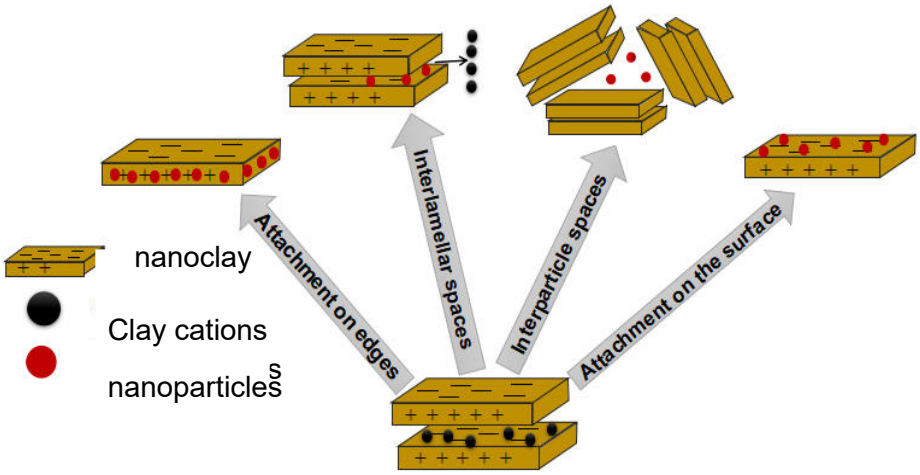


Fig. 1 Different sites on clay for metal/metal oxides functionalization.

AFM-068

Free-Standing GaP/MWCNT Composite Film as an Efficient Cathode Material for Li–O_2 Batteries

Inhan Kang[1], Shanmugasundaram Kamalakannan[2], Muhamma[4] Hilmy Alfaruqi[3] Mani Navaneethan[4], Sungjin Kim[1]*and Jungwon Kang[1]*

[1]*Department of Advanced Materials Science and Engineering, Mokpo National University, 61dorim-ri, 1666 Yeongsan-ro, Cheonggye-myeon, Muan-gun, Jeonnam, South Korea.*

[2]*Center of Excellence in Materials for Advanced Technologies (CeMAT), SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India.*

[3]*Department of Materials Science and Engineering, Chonnam National University, 300 Yongbong-dong, Bukgu, Gwangju, South Korea–61186.*

[4]*Nanotechnology Research Centre, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India*

***Corresponding author e-mail:** jwkang17@mokpo.ac.kr, ksj840711@gmail.com

ABSTRACT

A free-standing gallium phosphide/multi-walled carbon nanotube (GaP/MWCNT) film was fabricated via a simple vacuum filtration method and investigated as a cathode catalyst for Li–O_2 batteries. SEM and EDS analyses verified the uniform deposition of GaP and homogeneous elemental distribution throughout the MWCNT network. The GaP/MWCNT cathode demonstrated enhanced catalytic activity toward both the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), exhibiting stable redox peaks in cyclic voltammetry across scan rates ranging from 0.1 to 2 mV s^{-1}. Electrochemical impedance spectroscopy revealed a significantly lower charge-transfer resistance compared to pristine MWCNT electrodes. Galvanostatic charge–discharge tests conducted at 100 mA g^{-1} with a fixed capacity of ~500 mAh g^{-1} showed a reduced charging overpotential (3.8 V for GaP/MWCNT versus 4.1 V for MWCNT) and a higher energy efficiency of 73–74% over 20 cycles. Ex situ characterization confirmed the reversible formation and decomposition of Li_2O_2 with suppressed parasitic reactions. Furthermore, density functional theory (DFT) calculations were employed to support the experimental findings and elucidate the enhanced catalytic activity of the GaP/MWCNT composite. These results demonstrate that the GaP/MWCNT free-standing film is a promising cathode material for high-performance Li–O_2 batteries.

Keywords: Li–O_2 batteries; GaP/MWCNT composite; Free-standing cathode; Oxygen electrocatalysis; Energy efficiency

AFM-069

Theoretically and Experimentally Assessment of Foldable Lightweight Sheet of Ceramic-PU-PMMA IPN for γ ray Shielding and Light Emitting

Paramjit Singh[1*], Viney Sharma[1], Vipan Sohapl[1], Vikas Anand[2], Manpreet Kaur[3] , Nrip Jit[1], Sunil Kumar[1*]

[1] *Department of Applied Chemistry, Sardar Beant Singh State University, Gurdaspur, Punjab, India-143521*

[2] *Department of Nano Science and Materials, Central University of Himachal Pradesh-176206*

[3] *Department of Physics, AMITY University, Mohali, 140306, India*

***Corresponding author e-mail:** sunil_nano@yahoo.com

ABSTRACT

The increasing use of ionizing radiation in medical, nuclear, space, and industrial applications demands efficient, lightweight, and flexible shielding materials. Conventional heavy-metal and cement-based shields are limited by toxicity, brittleness, and poor processability, making polymer–ceramic composites attractive alternatives. PU/PMMA interpenetrating polymer networks (IPNs) with high-density ceramic fillers offer tunable functional, mechanical, and radiation-shielding properties for advanced multifunctional composites. Among ceramic fillers, Hexaferrite especially M-type ceramic oxides modified with trivalent substitution have gained significant attention owing to their high density, excellent chemical stability, magnetic characteristics, and strong photon interaction capability. These materials can effectively attenuate X-rays and γ-rays through photoelectric absorption, Compton scattering, and pair production mechanisms, depending on the photon energy range. The present study reports a comprehensive investigation of the radiation shielding performance, photoluminescence (PL) behavior, and FTIR spectroscopic characteristics of hexaferrite ceramic oxide (Zn^{2+}) reinforced PU/PMMA interpenetrating polymer network (IPN) composites based on polyurethane (PU) and Polymethyl-Methacrylate (PMMA). Gamma-ray shielding parameters such as linear attenuation coefficient (μ), mass attenuation coefficient (μ/ρ), half value layer (HVL), and mean free path (MFP) were evaluated, demonstrating enhanced shielding efficiency with increasing hexaferrite content due to higher effective atomic number and improved photon–matter interaction probability. Photoluminescence studies reveal defect-mediated emission originating from oxygen vacancies, Fe^{3+}–O^{2-} charge transfer transitions, and interface-induced trap states created at the ceramic–polymer boundary. FTIR analysis verifies the formation of the PU/PMMA interpenetrating polymer network and the effective dispersion of hexaferrite ceramic fillers. Shifts and variations in the intensity of vibrational bands corresponding to urethane, ester, and metal–oxygen functionalities reflect strong interfacial interactions and potential coordination between the polymer chains and hexaferrite surfaces.

Keywords: Polymer composites, Gamma-ray shielding, PU/PMMA interpenetrating polymer networks, hexaferrite fillers

AFM-070

Thermal Shielding Performance of Geopolymer Composite Syntactic Foams

M. Edwin Vines Raj[1], Umamaheshwari Ravikumar[1], V. K. Bupesh Raja*[1,2], J. Baalamurugan[1,3], B. Sheela Rani[4], V. Ganesh Kumar[1,3], R. Padmapriya[1,5], B. Kanimozhi[2]

[1]*Steel Research Facility, Sathyabama Research Park, Sathyabama Institute of Science and Technology, Chennai - 600119, Tamil Nadu, India.*

[2]*School of Mechanical Engineering, Sathyabama Institute of Science and Technology, Chennai - 600119, Tamil Nadu, India*

[3]*Materials Chemistry Lab, Centre for Ocean Research, Sathyabama Research Park, Sathyabama Institute of Science and Technology, Chennai - 600119, Tamil Nadu, India*

[4]*Centre for Quality Assurance and Nondestructive Evaluation, Sathyabama Research Park, Sathyabama Institute of Science and Technology, Chennai - 600119, Tamil Nadu, India*

[5]*Department of Civil Engineering, Sathyabama Institute of Science and Technology, Chennai - 600119, Tamil Nadu, India*

***Corresponding author e-mail:** bupesh.v.k@gmail.com

ABSTRACT

The growing demand for lightweight, environmentally friendly, and high-performance thermal protection systems has expedited the development of innovative materials for aerospace, automotive, energy, and fire-resistant infrastructure applications. In this study, geopolymer composite syntactic foams were synthesized by combining fly ash and steel slag with polystyrene balls. The fabricated geopolymer foams with controlled porosity structures were tested for its thermal shielding capability. Geopolymer samples were prepared with varying proportions of fly ash and steel slag (100:0, 90:10, 80:20, 70:30, 60:40, 50:50) and cured for 7, 14, 21, and 28 days to optimize the compressive strength. The geopolymer containing 70% fly ash and 30% steel slag demonstrated superior mechanical performance, achieving a maximum compressive strength of 51.4 kN at 28 days air curing, indicating enhanced geopolymerization and structural integrity. This optimized composition was used in creating lightweight syntactic foams for enhancing thermal insulation performance by adding polystyrene balls (1%, 2%, and 5%) into the geopolymer matrix. In thermal studies ranged from -20°C to 1000°C, the polystyrene melted at 240°C, creating a porous structure that decreased heat transfer via phonon scattering and air entrapment. Composites with a lower polystyrene content were stronger, the sample with a 1% polystyrene content had a greater compressive strength. The optimized geopolymer syntactic foam demonstrated appropriate compressive strength for semi structural applications, possessing low density, superior insulation, and excellent heat shock resistance.

Keywords: Geopolymer, Steel Slag, Fly ash, Polystyrene balls, Aluminosilicate Syntactic foams, Thermal shielding

References:

1. Hajimohammadi, A., Ngo, T. Compos B Eng, 173 (2019).
2. Zhang, L., Zhang, F. Chem. Eng. J, 313, (2017), 74-82.
3. Hashem, F. S., Salam. JERA 72, (2024), 117–134.
4. Ji, Y., Ren, Q., Li, X., Zhao, P., Vandeginste, V. Polym. J, 15, (2023), (15).

AFM-071

Effect of g-C_3N_4 Nanoparticles on the Mechanical, Thermal, and Fracture Behavior of Jute Fiber Reinforced Polymer Composites

Himanshu Athya[1], M. Ananda Rao[2], Syam Kumar Chokka[1]*

[1] *Department of Mechanical Engineering, PDPM-IIITDM Jabalpur, India.*

[2] *CSIR National Metallurgical Laboratory, Chennai, India.*

***Corresponding author e-mail:** skc.iiit@gmail.com

ABSTRACT

This study reports the effect Graphitic Carbon Nitride (g-C_3N_4) Nanoparticles on thermal, mechanical, and fracture performance in Jute fiber-reinforced polymer (JFRP) Composites. A hybrid adhesive system containing structural & non-structural epoxy adhesives was used to manufacture JFRP's under optimised vacuum bagging processes; g-C_3N_4 Nanoparticles were added to JFRP at varying concentrations to determine suitable levels for maintaining or enhancing thermal stability, tensile strength, flexural strength, and Mode I fracture energy of hybrid JFRP composites. Results of the mechanical tests indicated that the 2% g-C_3N_4 additive significantly improved the mechanical properties of the hybrids, producing approximately 62.5% increase in tensile strength relative to neat JFRP composites with a 55.7% increase in Mode I fracture energy. Above the 2% g-C_3N_4 concentration, the mechanical properties decreased due to particle agglomeration and increased brittleness of the polymer matrix. Thermogravimetric Analysis (TGA) results indicated that g-C_3N_4 modified composite demonstrated improved thermal stability. Overall, the results of this study illustrate that g-C_3N_4 Nanoparticle fillers are an effective multifunctional Nanofiller to improve sustainable natural fiber Composites.

References:

1. P. P. Naidu and G. Raghavendra, J. Appl. Polym. Sci., 136 (2019) 48413.
2. H. Li, J. Dai, Y. Hu, H. Zheng, X. Ge, Y. Guo, S. Gao, and C. Liu, J. Appl. Polym. Sci., 139 (2022).
3. W. Dong Zeng, F. Yao Wang, J. Jie Shen, P. Fu, Z. Dong Lin, and Chen, J. Appl. Polym. Sci., 143 (2026).

AFM-072

Development of Al–Cr_2AlC MAX Phase Coating on AA2024 Alloy via HVOF Method

K. Sai Kumar[1], G. Chandra Mouli[1], Meenu Srivastava[2]*, Siju[2], R.P.S Chakradhar[2], Sheela Singh*[1]

[1] *Department of Mechanical Engineering, School of Engineering and Applied Sciences, SRM University AP, Amaravati, Andhra Pradesh, India, 522502*

[2] *Surface Engineering Division, Council of Scientific and Industrial Research - National Aerospace Laboratories, HAL Airport Road, Bengaluru, Karnataka, India, 560 017*

***Corresponding author e-mail:** sheela.s@srmap.edu.in

ABSTRACT

Aluminium alloys are used in aerospace components because of their strength, thermal conductivity, and corrosion resistance. However, they have poor wear resistance and are not ideal for applications in extreme environments. The paper aims to develop a composite (Al-Cr_2AlC) coating for lightweight aluminium alloys to enhance their tribological performance in both dry and lubricated conditions. An aluminium powder (Al, > 99.00% pure and ~ 35±5 microns)-based, Cr_2AlC (~ 40±5 microns) particle–reinforced composite coating was deposited onto AA2024 alloy substrates by a high-velocity oxy-fuel (HVOF) spray process. The additions of Cr_2AlC in the feedstock were 10, 20, and 30 wt.%. The as-sprayed coatings were characterized by X-ray diffraction (XRD), field emission scanning electron microscope (FESEM), micro-hardness tester, and pin-on-disk wear tester, respectively. The coatings exhibit a dense microstructure, less porosity, and the least surface roughness with an increase in the amount of Cr_2AlC. A hardened steel ball with a diameter of Ø 6 mm was used as the counter material for the ball-on-disc tests. For lubrication tests, high-performance synthetic gas engine oil (Mobil Pegasus-1) was used. Al-30 wt.% Cr_2AlC coating possesses the least coefficient of friction under dry conditions and with lubrication conditions 0.25 ± 0.03 and 0.08 ± 0.01 were obtained, respectively, as compared to others. And also, Al-30 wt.% Cr_2AlC coatings show a lower wear rate under dry conditions and with lubrication conditions 4.97 x 10-6 (± 0.14) and 2.35 x 10-7 (± 0.09) mm3N-1m-1 were obtained, respectively. This results in about an 80% reduction in wear loss and nearly a 68% reduction in the coefficient of friction (COF) compared to dry sliding conditions. The worn surface contains regions rich in carbon and oxygen. The layered structure of the Cr_2AlC compound and the formation of tribo-film consisting of elements rich in carbon and oxygen were responsible for reducing the coefficient of friction.

References:

1. Davis, D., Singh, S., Chakradhar, R.P.S., J Thermal Spray Tech. 29, 1763–1783 (2020).
2. Li Z., Bradt R.C., J. Mater. Sci. 1986; 21:4366–4368
3. T.S. Sidhu, S. Prakash, and R.D. Agrawal, Mater. Sci., 2005, 41(6), p 805-823.

AFM-073

Disorder Driven Triphenylamine based Monolithic Covalent Organic Framework for the Efficient Removal of Toxic Oxo-anions from Water

Arjun Warrier, Pampa Jhariat, Mebin Varghese, Tamas Panda*

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu-632014, India.

***Corresponding author e-mail:** *arjun.warrier4539@gmail.com*

ABSTRACT

Covalent Organic Frameworks (COFs) have garnered significant attention for environmental remediation due to their ordered porosity, high surface area, and exceptional contaminant removal properties. However, the synthesis of pure-phase monolithic COFs and their application in water remediation is still in the infancy stage. Herein, an industrial-friendly and eco-friendly ball-mill-assisted in-situ gas forming approach is developed for the synthesis of pure phase monolithic COF, named BPTP Foam, that efficiently removes the toxic oxoanions from water. This approach induces a hierarchical porous structure, providing high adsorption capacities of 961.54 mg g^{-1} for MnO_4^- and 448.09 mg g^{-1} for CrO_4^{2-}, with rapid removal times of 1 and 3 min, respectively. Notably, the adsorption capacity for MnO_4^- is the highest among all porous materials reported to date. Density Functional Theory (DFT) and adsorption studies reveal that strong non-covalent interactions between the peripheral oxygen atoms of metal anions and the triphenylamine moieties within the framework contribute to enhancing removal kinetics. The simplicity and scalability of the synthesis method, combined with the high performance of BPTP Foam, make it a promising candidate for large-scale environmental remediation applications.

References:

1. A.Warrier, P.Jhariat,M.Varghese,T.Panda, *Small*, **2025**,e06837.
2. P.Jhariat,A.Warrier.M.Varghese, T.Panda, *J. Mater. Chem. A*, **2025**,13, 23893-23901
3. P. Jhariat, A. K. U., A. Warrier, A. P. Sunda, S. Das, S. Sarfudeen, V. M. Dhavale, T. Panda, *ACS Appl. Mater. Interfaces*, **2024**, 16, 23387.
4. P. Jhariat, A. Warrier, A. Sasmal, S. Das, S. Sarfudeen, P. Kumari, A. K. Nayak, T. Panda, *Nanoscale*, **2024**, 16, 5665.
5. S. Paul, M. Gupta, K. Dey, A. K. Mahato, S. Bag, A. Torris, E. B. Gowd, H. Sajid, M. A. Addicoat, S. Datta, R. Banerjee, *Chem. Sci*. **2023**, 14, 6643.

AFM-074

Defect-Stabilized, Urbach-Energy–Controlled UV-to-Visible down Conversion in Bi^{3+} Doped $Y_2Zr_2O_7$ Disordered Pyrochlore-like Phosphors

Ashok Kumar Srivastava[1], D. Anand[2], K. Ramachandran[1]*

[1,2]*Department of Physics, SRM Institute of Science and Technology, Vadapalani Campus, Chennai- 600 026, Tamil Nadu, India*

[2]*Department of Physics, Prathyusha Engineering College, Aranvoyalkuppam, Tiruvallur - 602025, Tamil Nadu, India*

***Corresponding author e-mail-** ramachak1@srmist.edu.in

ABSTRACT

Cost effective, defect stabilized, Lanthanide-free and stable down conversion UV-Visible phosphors plays an important role in solid-state lightning and optoelectronic application. It transforms intense UV light into visible emission. The development of defect stablized phosphor is challenging because it is commonly seen in many reported UV-Visible phosphor, disorder increases with dopant concentration, resulting in the creation of Coulombic traps and scattering centres that impede electron and hole transport. To overcome these challenges Bi^{3+} doped $Y_2Zr_2O_7$ disordered pyrochlore-like phosphors were synthesized by a straightforward and affordable conventional high-temperature solid-state reaction method. In this system Bi^{3+} was substituted in $Y_2Zr_2O_7$ at the Y^{3+} site of the host matrix. X-ray diffraction confirms the formation of disordered pyrochlore-like phosphor with monotonic lattice expansion and Williamson–Hall analysis shows local compressive microstrain. Optical band gap and Urbach energy analysis, derived from UV diffuse reflectance spectroscopy, revealed a narrowing bandgap with increasing dopant concentration. In contrast to traditional rare-earth phosphors, this produces broadband visible light under 350 nm excitation by enabling UV-to-visible down-conversion via defect-stabilized host emission facilitated via $6s^2$ to Y^{3+} site metal to metal charge transfer (MMCT) mechanism. Chromaticity analysis reveals stable CIE coordinates near standard coordinates with high Correlated Color Temperature (CCT) value which is the characteristic of a cyan-blue emission. Overall, the results show that Bi^{3+} doped $Y_2Zr_2O_7$ disordered pyrochlore-like phosphors had good UV to visible down conversion capabilities, which could be useful for optoelectronic and solid-state lighting applications.

Keywords: Phosphor Material, Disordered Pyrochlore, Band gap engineering, Down Conversion Phosphor

References:

1. B. M. Jaffar, H. C. Swart, H. A. A. Seed Ahmed, A. Yousif, and R. E. Kroon, Heliyon, 10 (2024) e27247.
2. B. V. N. Kumar and R. E. Kroon, Opt. Mater., 167 (2025) 117274.
3. M. He, Z. Lyu, D. Sun, T. Tan, S. Shen, and H. You, Mater. Today Chem., 41 (2024) 102301.

AFM-075

Influence of Ca Substitution on the Structural and Dielectric Properties of $Ba_{1-x}Ca_xTiO_3$ Ceramics.

Soubhagya Panda, Dr. susmita Rabha

National Institute of Technology Silchar, Silchar, Assam, India, 788010

***Corresponding author e-mail**: spanda_jrf@phy.nits.ac.in, susmita@phy.nits.ac.in

ABSTRACT

In this study, we synthesised $Ba_{1-x}Ca_xTiO_3$ (BCT) ceramics with varying calcium concentrations (x = 0.1, 0.2, 0.3, 0.4, and 0.5) via conventional solid-state sintering. Structural analysis by X-ray diffraction revealed that all compositions crystallised in a perovskite solid-solution structure, featuring a combination of $BaTiO_3$ (BTO) phases. Rietveld refinement further confirmed the formation and transformation from the BT tetragonal to the BT cubic phase at higher concentration. We observed a pronounced reduction in the average crystallite size as calcium content increased from 0.1 to 0.5 in BTO ceramics. Optical analysis through UV–Vis spectroscopy showcased that the substitution of Ca^{2+} leads to a notable narrowing of the optical band gap, decreasing from 3.29 eV for pure $BaTiO_3$ to 3.24 eV for BCT5. Furthermore, the reduction of defect concentration has obtained from the Pl analysis. Dielectric study has shown an increase in dielectric constant for 0 to 0.2 concentration, and the maximum dielectric constant obtained is 1177 for x = 0.2. These insights into the structural, optical and dielectric properties provide a deeper understanding of the compositional effects on BCT ceramics.

References

1. M. Rawat and K. L., Mater. Chem. Phys., 148 (2014) 655–663.
2. M. T. Buscaglia, V. Buscaglia, M. Viviani, P. Nanni, and M. Hanuskova, J. Eur. Ceram. Soc., (2000).
3. S. Pattipaka, Y. Lim, Y. H. Son, Y. M. Bae, M. Peddigari, and G. Hwang, Adv. Mater., 17 (2024).
4. M. H. Khedhri, N. Abdelmoula, H. Khemakhem et al., Appl. Phys. A, 125 (2019) 193.

AFM-076

Robust Superhydrophobic $V_2O_5/CoFe_2O_4@SiO_2$/PDMS Composite Membranes for Membrane Distillation

Swarnamayee Behera[1], Kalyan Raidongia[2*] and K. K. R. Datta[1*]

[1]*Functional Nanomaterials Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603203, Tamil Nadu, India*

[2]*Department of Chemistry, Indian Institute of Technology, Guwahati, Assam 781039, India*

***Corresponding author e-mail**: sb2544@srmist.edu.in, kumarard@srmist.edu.in

ABSTRACT

Membrane distillation (MD) is a promising technology for water desalination. The widespread application of MD requires membranes with improved wettability, durability, fouling resistance, precise selectivity, and high efficiency. Composite MD membranes with a superhydrophobic makeover, tailored porosity, and robust textures are emerging as advanced sieves enroute toward improved flux and exceptional salt rejection. Herein, a fluorine-free dual-layer composite membrane with superhydrophobic-hydrophilic characteristics is fabricated using a layer-by-layer assembly route. The importance of our design lies in tailored wettability-gradient across the composite membrane with heterogeneous textures functioning as manifold sites for condensation and hierarchical pores for efficient vapor transportation. The resulting dual-layer membrane featured a re-entrant surface with WCA ~168° and physicochemical durability in extreme environments, including acidic (pH=1), basic (pH=14), surfactant (SDS), hot saline water, rust, and sonication. In a direct-contact-membrane-distillation (DCMD) set-up, the membrane displayed a water flux of 87 $LM^{-2}H^{-1}$ with separation efficiency up to ~ 99.6% over 12 h operation. Additionally, it demonstrated a strong antifouling property, stable water flux, and salt rejection ability during desalination of saline solution containing surfactant and rust as foulants. Notably, the membrane maintained a stable flux and high salt rejection during the usage of seawater further validating its robustness and suitability for long-term use in harsh saline environments.

Keywords: Layer-by-layer, Hydrophobic membrane, Vanadium pentoxide, Membrane Distillation, Desalination Membranes.

Reference:

1. Deshmukh, C. Boo, V. Karanikola, S. Lin, A. P. Straub, T. Tong, D. M. Warsinger and M. Elimelech, Energy Environ. Sci., 2018, 11, 1177–1196.

AFM-077

Superhydrophobic Carbamodithioate Functionalized Fluorinated Graphene Nanosheet Composite Membrane for Sea Water Desalination

Akhina Roshin, Swarnamayee Behera, Iniya Prasanthi, K.K.R. Datta*

Functional Nanomaterials Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603203, Tamil Nadu, India

***Corresponding author e-mail**: kumarard@srmist.edu.in, kkrdatta@gmail.com

ABSTRACT

Membrane distillation (MD) is emerging as a sustainable desalination technology owing to its ability to employ low-grade heat to treat high-saline feedwater. The innovation in designing high performance membranes include improvements toward desalination efficiency parameters concomitant to high water flux with absolute salt rejection, while maintaining membrane's stability under continuous operation. Herein, a dual-layer composite membrane (GSFP) was strategically assembled via layer-by-layer route over nylon substrate with coatings of hydrophilic GO nanosheets and SiO_2 particles followed by carbamodithioate functionalized fluorinated graphene nanosheet blended with PDMS yielding superhydrophobic top layer. This hierarchical architecture imparts the optimized composite membrane GSF (0.5)P with a water contact angle of 151º and a surface free energy of 7 mJ/m^2, making it resistant to wetting by distilled water (~ 1 µS/cm), NaCl solution (~ 5000 µS/cm) and seawater (~ 47,000 µS/cm). Furthermore, GSF(0.5)P acts as a functional strainer in direct contact membrane distillation (DCMD) to desalinate feed water containing 3.5 g/L NaCl with an average water flux of 54 LMH and 99.9 % salt rejection. Importantly, under the condition of salinity enhanced seawater (35 g/L, ~ 65,000 µS/cm), GSF(0.5)P demonstrated the highest performance at an elevated temperature of 80 ºC, with an average water flux of 55.6 LMH and 99.9 % salt rejection. Additionally, the membrane maintained an average water flux of 49.8 LMH with 99.9 % salt rejection when tested with the salinity enhanced seawater feed for 100 h at 70 ºC highlighting its durability. Moreover, the regenerated membrane retained its superhydrophobic as well as mechanical stability even after prolonged desalination operation, confirming its physicochemical endurance. These results highlight the potential of functionalized graphene-based composite membranes for efficient and sustainable saline water treatment and upholding water-energy nexus.

Keywords: Fluorinated graphene, Carbamodithioate, Superhydrophobicity, Layer-by-layer composite membrane, Desalination, Membrane distillation

References:

1. P. L´opez-Porfiri, S. Ramos-Paredes, P. Nú˜nez, P. Gorgojo, npj Clean Water, 6 (2023)

AFM-078

Flexible PVA-Based KTNT/MXene Nanocomposite Films with Improved Dielectric and Electrical Performance

Ravikiran*[1], Poorvith P G[2], Punith T G[2], Sudhir Ullagaddi[2], Vinay P[2]

[1]*Assitant Professor, Department of Mechanical Engineering, The National Institute of Engineering, Mysuru, Karnataka, India*

[2]*Students, Department of Mechanical Engineering, The National Institute of Engineering, Mysuru, Karnataka, India*

***Corresponding author e-mail:** nayak.ravikiran@gmail.com

ABSTRACT

The new developments in nanotechnology allow us to tune the material properties by being able to control structures on the nanoscale. Material based on titanium is particularly cool since it is chemically stable, and it can be tuned to behave in particular manner electrically. This paper synthesized TiO_2 nanoparticles and converted them into titanium nanotubes (TNT) using a hydrothermal reaction in order to increase the surface area and charge interaction. The addition of potassium ions formed potassium titanate nanotubes (KTNT) thereby enhancing structural stability and dielectric functionality. In order to bring the electrical properties to the extreme, we mixed KTNT with varying quantities of MXene to achieve nanocomposites. We have analyzed the structural, morphological, and bonding characteristics based on XRD, SEM, and FTIR. Through I V tests, voltage response and analysis of dielectric constant electrical and dielectric properties were tested. The findings indicated extreme electrical output and dielectric constant improvement concerning structural modifications and supplementation with MXene, and reached its highest point at mid-level MXene concentrations. We further sandwiched the nanomaterials within a PVA matrix to form flexible nanocomposite films, in which the fillers were dispersed evenly and were mechanically stable, and where the electrical performance was not damaged. In conclusion , the work demonstrates that controlled nano structuring and hybridization have a serious potential to increase electrical and dielectric characteristics which is promising high results in energy harvesting, sensing, and flexible electronics.

References:

1. S. Malik, K. Muhammad, and Y. Waheed, Molecules, 28 (2023) 661.
2. M. Nasrollahzadeh, S. M. Sajadi, M. Sajjadi, and Z. Issaabadi, Interface Sci. Technol., 28 (2019) 1–27.
3. G. Zhou, L. Huang, W. Li, and Z. Zhu, J. Sens., 2014 (2014) 815467.
4. R. Nartita, D. Ionita, and I. Demetrescu, Sustainability, 13 (2021) 10217.
5. K. Lee, A. Mazare, and P. Schmuki, Chem. Rev., 114 (2014) 9385–9454.
   X. Wang, Z. Li, J. Shi, and Y. Yu, Chem. Rev., 114 (2014) 9346–9384.

AFM-079

Mechanochemical Solid Solution Formation in Zeolitic Imidazole–Tetrazole Frameworks for Enhanced Oxygen Evolution Reaction

Shafeeq Sarfudeen[1], Abdul Kareem[2], Mebin Varghese[3], Harshini Annadata[4], Sailesh Nithin[5], Swetha Kannan[6], Arjun Warrier[6], Sellappan Senthilkumar [7] and Tamas Panda[8*].

[1] *Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India, 632014*

[2]*Bhabha Atomic Research Center(BARC), Mumbai, India,400085*

***Corresponding author e-mail:** tamaskumarpanda@vit.ac.in

ABSTRACT

Investigating heterometallic frameworks with uncoordinated nitrogen sites in zeolitic imidazole–tetrazole frameworks (ZITFs) offers a distinctive strategy to improve electrocatalytic activity. In this study, a solvent-free mechanochemical alloying method is introduced to simultaneously induce Co–Zn metal mixing and imidazole–tetrazole ligand mixing, forming an amorphous solid solution, aZn$_{0.5}$Co$_{0.5}$ZI$_{0.5}$T$_{0.5}$F-8, from ZnZTF-8 and CoZIF-8 under an argon atmosphere. Exposure of this phase to methanol vapor at 25 °C converts it into a crystalline counterpart, cZn$_{0.5}$Co$_{0.5}$ZI$_{0.5}$T$_{0.5}$F-8. Structural and compositional analyses using X-ray absorption spectroscopy, ICP-MS, HAADF-STEM, and FESEM confirm metal–ligand solid solution formation and abundant defect-associated uncoordinated nitrogen sites in the amorphous phase. Owing to its higher active-site density and structural heterogeneity, the amorphous material exhibits superior oxygen evolution reaction performance, with an overpotential of 338 mV and a Tafel slope of 94.8 mV dec^{-1} compared to parent frameworks. Computational hydrogen electrode calculations evaluating *OH, *O, and *OOH intermediates further validate the enhanced activity. This work demonstrates that mechanochemically induced dual solid-solution formation is an effective and sustainable route for designing non-crystalline MOFs with high electrocatalytic efficiency.

References:

1. H. Furukawa, K. E. Cordova, M. O'Keeffe, and O. M. Yaghi, Science, 341 (2013).
2. Y. Liang, X. Yang, X. Wang, Z.-J. Guan, H. Xing, and Y. Fang, Nat. Commun., 14 (2023) 5223.
3. Y. Wang, B. Liu, X. Shen, H. Arandiyan, T. Zhao, Y. Li, M. Garbrecht, Z. Su, L. Han, A. Tricoli, and C. Zhao, Adv. Energy Mater., 11 (2021).
4. T. Panda, P. Pachfule, Y. Chen, J. Jiang, and R. Banerjee, Chem. Commun., 47 (2011) 2011–2013.

AFM-080

Independent Evaluation of Pyroelectric and Triboelectric Properties in PVDF/PZT Composite Films

Thara Prasannan[1], Soham Kumar[2], Muthuragavan Mahendiran[1], Pranab Mandal[1], Vengadesh Kumara Mangalam Ramakrishnan[1*]

[1] *Functional Materials Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India*

[2] *Department of Physics, SRM University – AP, Guntur, 522 240, Andhra Pradesh, India.*

***Corresponding author e-mail:** pranab.m@srmap.edu.in

ABSTRACT

Nanogenerators based on pyroelectric and triboelectric effects offer excellent output performance and mechanical flexibility, making them promising for self-powered sensing and energy harvesting applications. The novelty of this study is strengthened by the relatively limited prior research addressing these distinct effects separately, emphasizing its potential for advancing multifunctional energy harvesting technologies. In this work, polyvinylidene fluoride/lead zirconium titanate (PVDF/PZT) composite films were fabricated to independently harness thermal and mechanical energy for electrical energy generation. Fourier-transform infrared spectroscopy confirmed enhanced β-phase formation, with the 5 wt % PZT-loaded film (within a 15 wt % PVDF matrix) exhibiting the highest β-phase content and improved crystallinity compared to 10 wt % and 15 wt % PZT compositions. A phase-sensitive method was utilized to evaluate the pyroelectric current of both pristine PVDF and its composite films, where the 5 wt % PZT composite demonstrated a pyroelectric energy conversion figure of merit of 0.416%. Triboelectric testing also showed enhanced charge generation for the same composition, confirming 5 wt % PZT as an efficient hybrid material capable of harvesting thermal as well as mechanical energy. The 5% PZT composite exhibits a peak-to-peak open-circuit voltage (V_{PP}) of 6.8V and an output current (I_{oc}) of 5.6nA.

References:

1. J. Singh, R. Kaur and D. Singh, "*Energy harvesting in wireless sensor networks: A taxonomic survey"*, Int. J. Energy Res., **45**, (2021): 118-140.
2. R. Mondal, M. A. M. Hasan, J. M. Baik and Y. Yang, "*Advanced pyroelectric materials for energy harvesting and sensing applications"*, Mater. Today, **66**, (2023): 273-301.
3. J. Li, M. Zhang, G. Ni, H.-Y. Mi, B. Dong, C. Liu and C. Shen, "*A dynamic supercritical carbon dioxide foaming method for fabricating wrinkled surface to enhance triboelectric nanogenerator performance"*, J. Appl. Polym. Sci., **140**, (2023): e53351.
4. J. Sun, X. Pu, M. Liu, A. Yu, C. Du, J. Zhai, W. Hu and Z. L. Wang, "*Self-Healable, Stretchable, Transparent Triboelectric Nanogenerators as Soft Power Sources"*, *ACS Nano,* **12**, (2018): 6147-6155.

AFM-081

pH-Responsive mPEG-b-PCL-b-PEC Triblock Micelles for Stabilization and Tumor-Selective Delivery of Camptothecin

Rizwana Fathima M Kasim, Kalaivizhi Rajappan*

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Tamil Nadu-603203, India

***Corresponding author e-mail:** kalaivir@srmist.edu.in

ABSTRACT

Camptothecin (CPT) is a powerful anticancer agent limited by poor solubility and rapid inactivation of its lactone form. Herein, we report a pH-responsive triblock copolymer nanocarrier, poly(ethylene glycol)-block-poly(ε-caprolactone)-block-poly(ethylene carbonate) (mPEG-b-PCL-b-PEC), synthesized via sequential ring-opening polymerization to enhance CPT stability and tumor-selective delivery. The copolymer formed stable micelles with a size of ~145 nm and an ultra-low critical micelle concentration of 0.063 mg/mL. CPT-loaded micelles showed high encapsulation efficiency (84.5%) and effectively inhibited burst release under physiological conditions. In vitro release experiments showed sustained drug release at pH 7.4 (≈35% release over 7 days) and accelerated release at acidic pH (≈78% release at pH 5.5), which confirmed the pH-responsiveness. Cytotoxicity experiments showed strong dose-dependent cell killing of MCF-7 breast cancer cells comparable to free CPT, while significantly reducing toxicity to normal VERO cells, which indicated improved therapeutic selectivity. The addition of the surface-eroding PEC block helped to improve the structural stability and controlled release properties. In summary, the mPEG-b-PCL-b-PEC micellar system offers a structurally stable and tumor-responsive platform that improves CPT stability and therapeutic index, and has great potential for controlled breast cancer therapy.

Keywords: Camptothecin, Triblock copolymer, Micelles, Drug Delivery.

References:

1. Kai G, Wu C, Gen L, Zhang L, Cui L, Ni X. Biosynthesis and biotechnological production of anti-cancer drug Camptothecin. Vol. 14, *Phytochemistry Reviews.* Kluwer Academic Publishers; 2015. p. 525–39.
2. Martino E, Della Volpe S, Terribile E, Benetti E, Sakaj M, Centamore A, et al. The long story of camptothecin: From traditional medicine to drugs. Vol. 27, *Bioorganic and Medicinal Chemistry Letters*. Elsevier Ltd; 2017. p. 701–7.
3. Shaw PA, Klausen M, Bradley M. A dual action coumarin-camptothecin polymer for light responsive drug release and photodynamic therapy. *Polym Chem.* 2023 Dec 5;15(2):54–8.

AFM-082

Heterointerface-Driven Electronic Modulation in Bimetallic Sulfide Nanostructures for Accelerated Oxygen Evolution

Barath Ravi, Panneerselvam Perumal*

Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India.

***Corresponding author e-mail:** panneerp1@srmist.edu.in

ABSTRACT

Developing cost-effective and highly efficient electrocatalysts for the alkaline oxygen evolution reaction (OER) remains a critical challenge for the advancement of sustainable energy technologies. Herein, we report a heterostructured bimetallic sulfide electrocatalyst derived from a metal–organic framework precursor through a controlled sulfurization strategy. Structural and morphological analyses confirm the uniform incorporation of sulfur species within the bimetallic domains, leading to the formation of strongly coupled heterointerfaces. The framework-templated approach enables the construction of hierarchically engineered nanoscale architectures that promote interfacial charge redistribution and enhance electron-transfer kinetics during anodic oxidation. In alkaline medium, the optimized catalyst exhibits remarkable OER activity with fast reaction kinetics and excellent long-term stability. Surface area analysis reveals the development of porous channels after sulfur incorporation, which improves electrolyte accessibility and facilitates efficient mass and charge transport. Comprehensive characterization further confirms that the synergistic coexistence of sulfur and oxygen species within the heterostructure plays a decisive role in enhancing intrinsic catalytic activity. Overall, this work demonstrates an effective strategy for designing framework-derived bimetallic sulfide heterostructures with improved interfacial properties for advanced oxygen evolution electrocatalysis.

Keywords: oxygen evolution reaction, Co/Nd-BDC, heterostructure, metal sulfides, electrocatalysts.

Reference:

1. Ma, W., Li, W., Zhang, H., & Wang, Y. (2023). N-doped carbon wrapped CoFe alloy nanoparticles with MoS2 nanosheets as electrocatalyst for hydrogen and oxygen evolution reactions. *International Journal of Hydrogen Energy*, *48*(58), 22032-22043.

AFM-083

Formulation and Characterization of Xanthan Gum-Shea Butter Bigels & Influence of Emulsifiers (SDS, CTAB, SL) on Structure and Properties

Lavanya Jujjuri [1], Sivaranjani E [2], Samarendra Maji [3]*

[1]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

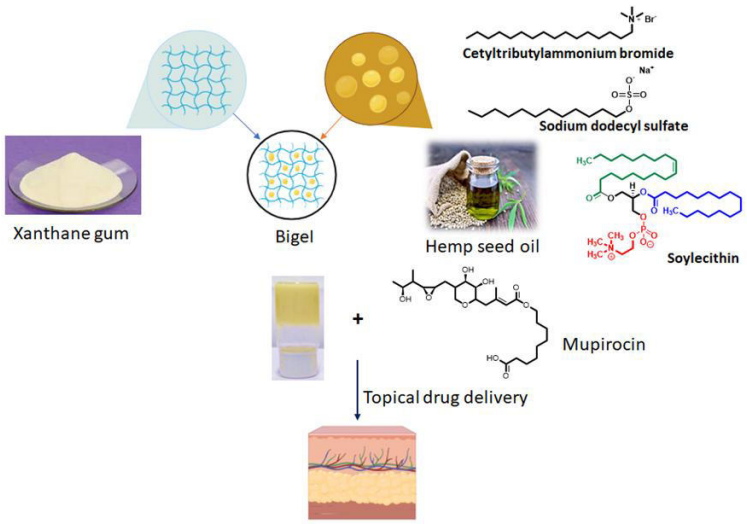
[2]*SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

[3] *Department of Chemistry, Faculty of Engineering and Technology SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:**samarenr@srmist.edu.in

ABSTRACT

Bigels have gained significant interest as versatile semisolid systems capable of immobilising both hydrophilic and lipophilic phases, making them as suitable carriers for drug delivery.[1] The current paper discusses the formulation of bigels by combining xanthan gum hydrogel with shea butter hempseed oil oleogel, and the influence of emulsifier types (CTAB, SDS, SL) and polymer concentration (1-5% w/w) on the physicochemical properties of the bigels was systematically characterised. Microscopic analysis revealed O/W structures of bigels, Fourier-transform infrared spectra confirmed composition-dependent interactions between hydrogel and oleogel phases, while X-ray diffraction patterns showed the predominance of amorphous structures within the bigel matrices. Thermal stability using DSC highlighted improved stability with increasing xanthan gum concentration. The in vitro release of mupirocin was best fitted by Korsmeyer-Peppas and Peppas-Sahlin models, suggesting Fickian diffusion as the principal release mechanism. Furthermore, the mupirocin-loaded bigels exhibited notable antimicrobial activity, confirming their suitability for topical drug delivery.



Reference:

1. Francavilla, M. G. Corradini and I. J. Joye, *Gels*, 2023, **9**, 648

AFM-084

Development and Characterization of Novel Biopolymer-Based Bigels Formulated using Xanthan Gum, K-carrageenan and Agar for the Delivery of Linezolid

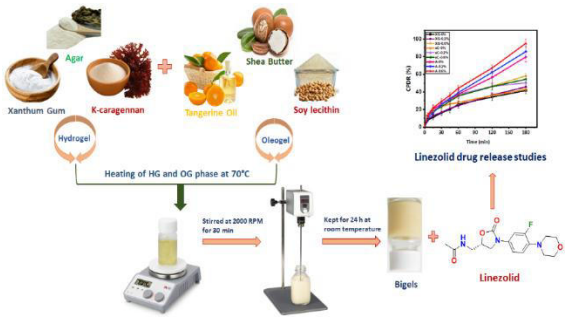
Sivaranjani Elumalai, Lavanya Jujjuri, Samarendra Maji*

Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail:** samarenr@srmist.edu.in

ABSTRACT

The development of a novel biopolymer-based Bigel system (BGs) using Xanthan Gum (XG), K-Carrageenan (κC), and Agar (A) with increasing Soy lecithin (SL) concentration for the drug delivery of linezolid was investigated in this work.[1] The Hydrogel phase was structured with 2% Xanthan Gum (XG), 2% K-Carrageenan and 2% Agar, while the Tangerine oil (TO) Oleogels were structured using 0.6% Shea butter (SB) and Soy lecithin (SL) with concentrations such as (0%, 0.2% and 0.6%). The influence of SL incorporation on the structural, thermal, chemical and rheological properties of the BGs was analysed using a range of characterization techniques, including bright field, polarized, stereozoom microscopy, calorimetry, X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC) and rheological analysis. Calorimetric analysis revealed variations in colour intensity across all the BGs. FTIR data confirms the successful incorporation of the SL into the prepared BG samples.[2] XRD data reveals the semi-crystalline and amorphous characteristics of the BGs, while DSC demonstrated their thermal stability. Rheological data showed the strongest BG with notable differences across the polymer types. The invitro release of linezolid from the BGs was best described by the Korsmeyer-Peppas models, indicating that the drug diffusion occurred via both non-Fickian and Fickian mechanisms and the Zone of inhibition reveals a comparable inhibition zone ranging from 1.5 to 1.8 cm in diameter. Among the analysed data for all the BG samples, agar-based BG demonstrated superior drug delivery performance, indicating its potential suitability for tropical therapeutic applications.



References:

1. D. Dimakopoulou-papazoglou, K. Zampouni and T. Moschakis, *Food Hydrocoll.*, 2025, 166, 111341.
2. C. M. Cholant, F. Ely, M. J. L. Santos, A. Pawlicka, F. C. Tavares, D. S. D and C. O. Avellaneda, 2019, 305, 232–239.

AFM-085

Stabilization of Hybrid Halide Perovskite by Schiff Base – A Colloidal Synthetic Approach

Shebin C K[1], Tarak Nath Mandal[1]*

[1]*Department of Chemistry, SRMIST, Kattankulathur, Tamil Nadu-603203*

Corresponding author e-mail: taraknam@srmist.edu.in

ABSTRACT

Metal halide perovskite have attracted wide attention over recent years due to their outstanding optoelectronic properties, and versatile applications such as photovoltaics, Solid state light emitting diodes (LEDs), and other optoelectronic applications. The Controllable fabrication of highly dispersed, stable, and functionalized perovskite nanocomposites has significant industrial importance. However, the high sensitivity of perovskites hinders their commercialization. Here, we report the synthesis of hybrid perovskites by incorporating a Schiff base ligand derived from salicylaldehyde and ethylenediamine. The strategic use of the Schiff base provides effective capping by coordinating to the nanocrystal surface, thereby reducing crystal defects and yielding highly stable, bright green luminescent superstructures. The composite maintains its structural integrity for prolonged periods under varying temperature and humidity conditions. Furthermore, the Schiff base is readily synthesized, highly stable, and obtained in high yield from in expensive precursors, making the composite preparation both simple, cost effective and scalable.

References:

1. Teunis, M. B.; Jana, A.; Dutta, P.; Johnson, M. A.; Mandal, M.; Muhoberac, B. B.; Sardar, R. Chem. Mater. 2016, 28, 5043–5054
2. Mollick, S.; Mandal, T. N.; Jana, A.; Fajal, S.; Desai, A. V.; Ghosh, S. K. ACS Appl. Nano Mater. 2019, 2, 1333–1340
3. Suneetha, G.; Ayodhya, D.; Manjari, P. S.. Results Chem. 2022, 4, 100688
4. Zhang, F.; Zhong, H.; Chen, C.; Wu, X.-g.; Hu, X.; Huang, H.; Han, J.; Zou, B.; Dong, Y.. ACS Nano 2015, 9, 4533–4542
5. González-Carrero, S.; Schmidt, L. C.; Rosa-Pardo, I.; Martínez-Sarti, L.; Sessolo, M.; Galian, R. E.; Pérez-Prieto, J. ACS Omega 2018, 3, 1298–1303

AFM-086

Fullerene (C60) Endowing Antistatic Properties to the Industrially Viable Biodegradable Polyurethane Nano-Composites

Moumita Mukherjee[1,2], R.Yasmin Sulthana[5], R. Mohan[3] and Senthil Andavan G. T[4]*

[1]*Ministry of Defence, Department of Defence Production, Directorate of Ordnance(C&S), Kolkata-700001, India*

[2] *SPDC, CSIR-Central Leather Research Institute, Adyar, Chennai 600020, India*

[3] *Centre for Analysis, Testing, Evaluation& Reporting Services, CSIR-Central Leather Research Institute, Adyar, Chennai 600020, India*

[4] *Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603203 Tamil Nadu, India*

[5] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203 Tamil Nadu, India*

***Corresponding author e-mail:** senthilt1@srmist.edu.in

ABSTRACT

Electrical and electronic engineering plays a vital role in transforming the global economy, energy system, resources management and manufacturing process within the framework of Industry 4.0 revolution. Electrostatic control is critically necessary in many industrial sectors such as mining industry, explosive handling and pyrotechnics where stray static electricity can lead to severe consequences including damage to the equipment or accidental ignition due to electric spark [1] Present work is mainly focus on development of novel antistatic composites suitable for industrial applications shows anti-static or electrical resistance properties under two-probe method and surface resistivity meter. The present work not only focuses on industrial development but also providing an environmentally friendly solution [2] To address the issue, for the first time about the successful synthesis of novel commercial biodegradable polyurethane-fullerene (PU-C60) composites is achieved via *in-situ* synthesis of trifunctional polyol [polycaprolactone (PCL; CAPA 3201; M.W 2000)], along with isophorone diisocyanate (IPDI) based the fullerene (C60) are designated as PUF. The intrinsic characterization of the control and PU-C60 nanocomposites based on physicochemical, morphological, electrical and mechanical properties may pave the route to develop prospective polymeric materials with promising anti-static features. The structural analysis includes ATR-IR, 13C NMR and UV-vis DRS, the thermal characteristics TGA, DSC and the physical parameters like hardness, compression set, density and tensile strength. Through optimization, the present biodegradable PU foam may lead for potential application of high-performance antistatic additives for EMI shielding in electronics industry and in other field where conductive polymers are imperative. This will also lead the reduction of the enormous waste from the e-plastic generation from the eminent field while balancing Industry 4.0 with environmental impact causes from the enormous waste disposal.

AFM-087

Quest for Designing PLA-based Engineered Toughened Nanocomposites for Packaging Applications

Nirmala Devi*, Y. Alotoli Achumi

Department of Chemistry, Girijananda Chowdhury University, Guwahati 781017, Assam, India

***Corresponding author e-mail:** nirmaladevi2040@gmail.com

ABSTRACT

Food packaging is one of the most important areas where enormous amounts of synthetic petroleum-based plastics are used every day.The escalating concerns regarding the non-biodegradability, environmental impacts, human health and several limitations of these materials which have motivated scientists and engineers to develop new generation of bioresource based polymer nanocomposite materials that finds application in sustainable packaging and contributes to the circular economy.

This talk highlights on the Polylactide (PLA) based nanocomposite packaging materials and films designed and developed through the process of spinning followed by melt extrusion technique. Bentonite clay was used for preparing the PLA-Clay nanocomposites. The prepared PLA nanocomposite materials and films were characterized by the following tests: Tensile and Flexural strength by UTM, Thermogravimetric analysis (TGA), Differential scanning calorimetry (DSC), Dynamic mechanical analysis (DMA), Gel permeation chromatography (GPC), X-ray diffraction (XRD), Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). The disappearance of d_{100} basal peak was used to confirm the formation of exfoliation. Furthermore, a significant improvement in mechanical and thermal properties was observed in the nanocomposites. The new material was used to prepare final packaging product (Fig.1) by thermoforming.



Fig. 1. Packaging material and boxes

Keywords: PLA; Engineered; Nanocomposite; Packaging

AFM-088

Metal-organic Framework Composite Incorporated PVDF UF Membranes for Efficient Wastewater Treatment

Jagadeesh Kumar Alagarasan*

[1]*Department of Chemistry, Manipal University Jaipur, Jaipur 303007, Rajasthan, India*

***Corresponding author e-mail:** jaga.jagadeesh1987@gmail.com, jagadeesh.alagarasan@jaipur.manipal.edu

ABSTRACT

Metal-organic framework (MOF)-integrated polyvinylidene fluoride (PVDF) membranes provide a viable approach for advanced water treatment as they exhibit improved hydrophilicity and permeability as well as antifouling characteristics. PVDF-based UF (ultrafiltration) selective membranes were modified with (zeolitic imidazolate framework) ZIF and ZIFAE (alkali-etched zeolitic imidazolate framework) MOFs in this study. Incorporating ZIFAE MOF membranes demonstrated substantially lowered contact angle, enhanced porosity, and improved flux than ZIF and PVDF membranes. Among them, the pure water flux and bovine serum albumin (BSA) rejection of ZIFAE2 were as high as 951 ± 11 $L \cdot m^{-2} \cdot h^{-1}$ and 99 ± 0.5%, respectively. Cross-sectional and top-surface SEM images confirmed that the ZIFAE membranes showed increased pore density and uniform nanoparticle distribution which resulted in their better hydrophilicity due to the hydroxyl (-OH) and amino (-NH) functional groups. Results of secondary effluent filtration evaluations indicated less fouling resistance and more extended operational lifespan of the ZIFAE2 membrane. Such benefits establish ZIFAE-modified membranes as sustainable, real-world, and efficient candidates for wastewater treatment and compact alternatives to traditional tertiary treatment technologies.

Keywords: UF membranes, MOF, Cobalt, antifouling, advance wastewater treatment

AFM-089

Advancing Hydrogen Storage with Functionalized Carbon Nanoribbons

Rubika Kumar[1], Puspamitra Panigrahi [1*], Sujoy Kumar Ghosh[1*]

[1*]*Centre for Clean Energy and Nano Convergence, Hindustan Institute of Technology and Science, Chennai 603103, India.*

***Corresponding author e-mail:** puspamitrap@hindustanuniv.ac.in, sujoykug@srmist.edu.in

ABSTRACT

This work investigates the hydrogen (H_2) storage potential of recently synthesized carbon nanoribbons (CNRs) using first-principles density functional theory (DFT) simulations. The weak interaction of H_2 with pristine CNRs is significantly enhanced upon functionalization with light metals (Li, Na, K, Mg, and Ca), all of which form strong bonds with the nitrogen-substituted nanoribbons (N-CNRs). H_2 adsorption energies on metal-functionalized N-CNRs range from -0.597 eV/H_2 (Li) to -0.110 eV/H_2 (Mg). Theoretical gravimetric storage capacities (G_t) reached up to 7.08 wt% (Li), with practical storage (G_p) values of 6.37 wt% (Li), 5.69 wt% (Na), 5.28 wt% (Mg), 5.08 wt% (K), and 3.74 wt% (Ca) under realistic conditions (30 atm, 298.15 K) and desorption (3 atm, 373.15 K) conditions. H_2 desorption temperatures range from 140.68 K (Mg) to 763.54 K (Li), and corresponding H_2 recovery times varied from 7.04×10^{-11}s (Mg) to 1.06×10^{-2} s (Li). Thermodynamic stability analyses have confirmed the negative adsorption enthalpies at 0 K and the retention of stability up to 298 K at 100 atm for most systems. These results demonstrate the potential of metal-doped N-CNRs to meet or exceed the U.S. DOE target of 5.5 wt% H_2 storage at room temperature and moderate pressure, highlighting their practical suitability for solid-state H_2 storage systems.

Keywords: Carbon nanoribbons, Hydrogen storage, Metal functionalization, DFT, Gravimetric capacity

AFM-090

Fe-Doped CoS_2 Nano-octahedra as Electrocatalysts for Hydrogen Evolution Reaction in Acidic Medium

S. Swetha and T. Maiyalagan

Electrochemical Energy Laboratory, Department of Chemistry,
SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India.

***Corresponding author e-mail:** maiyalat@srmist.edu.in & maiyalagan@gmail.com

ABSTRACT

CoS_2 was developed as an effective, noble-metal-free electrocatalyst for the Hydrogen Evolution Reaction (HER), providing excellent conductivity and inherent catalytic activity. We report Fe-doped CoS_2 Octahedron synthesized through controlled hydrothermal sulfidation, as a powerful HER electrocatalyst in acidic conditions. Incorporating Fe^{3+} into the pyrite CoS_2 lattice modifies its electronic structure, optimizes the adsorption energies of HER intermediates, and boosts the density of electrochemically active sites. The optimized 8% Fe-doped CoS_2 achieves a lower overpotential of 57 mV at 10 mA cm^{-2} and a Tafel slope of 56 mV·dec^{-1}, exceeding pristine CoS_2 Octahedron. The material exhibits around 96 hours of stable performance in 0.5 M H_2SO_4, highlighting its durability in acidic condition. This study offers a cost-efficient and scalable technique for the development of transition-metal chalcogenide with modified electronic structures to facilitate effective hydrogen production in acidic environments.

Keywords: Fe-doped CoS_2, Octahedron, acidic medium, Hydrogen evolution reaction, Transition metal chalcogenides

AFM-091

Interface-Engineered Bimetallic LDH/Singlet-MOF Heterostructures for High-Performance Electrocatalytic Water Splitting

Arinsha R, Panneerselvam Perumal*

Department of chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India

Corresponding author e-mail: panneerp1@srmist.edu.in

ABSTRACT

The development of highly efficient and durable electrocatalysts for hydrogen generation and overall water splitting is essential for advancing sustainable energy technologies. In this work, we report the rational design and synthesis of a bimetallic layered double hydroxide (LDH) integrated with a singlet metal–organic framework (MOF) to construct a hierarchical composite heterostructure. The intimate interfacial coupling between the bimetallic LDH nanosheets and the porous MOF matrix enables synergistic modulation of electronic structure, enhanced charge transfer kinetics, and abundant exposure of catalytically active sites. The bimetallic LDH component provides high intrinsic catalytic activity and favorable adsorption/desorption energetics for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), while the singlet-MOF contributes high surface area, tunable porosity, and improved mass transport. The engineered heterointerface facilitates rapid electron migration and optimizes intermediate binding energies, thereby lowering overpotentials and improving reaction kinetics in alkaline media. Electrochemical measurements demonstrate significantly reduced overpotential at practical current densities, small Tafel slopes, and excellent long-term operational stability compared to single-component counterparts. This work highlights the importance of interface engineering between LDHs and MOFs in constructing advanced heterostructure electrocatalysts and provides a promising strategy for cost-effective and high-performance hydrogen production through water splitting.

Keywords: MOF/LDH heterostructure, layered double hydroxide, Metal organic framework, interface engineering, hybrid materials design.

Reference:

1. Kengne Fotso, L.E., Mehmood, S., Jetti, V.R. and Pal, U., 2025. Ta-NiFe-LDH@ La-ZIF-67 Composite Heterostructures for Efficient Electrocatalytic Hydrogen Generation and Overall Water Splitting. *ACS Applied Energy Materials*, *8*(24), pp.17970-17988.

AFM-092

Light-Responsive Functionalized Dendritic Fibrous Nano-Silica for Crop Protection and Management

Ezhili Ethirajan [1], Sumithaa Chezhiyan [1], Ganeshpandian Mani [1]*

[1]*SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** ganeshpm@srmist.edu.in

ABSTRACT

Pesticides plays a crucial role in crop protection and management, but due to the overuse of high dosage for a long time period pests and plants have forced to evolve through this condition forming resistance to pesticides, which results decrease in the effect of the pesticides. Also, using high dosage of pesticide leads to the development stress and toxicity. To overcome this challenge wide range of nanomaterials are synthesized and used. In this study we prepared a light-responsive polydiacetylene (10,12-pentacosadiynoic acid, PCDA) functionalized dendritic fibrous nano-silica (PFNS) loaded with glyphosate (herbicide, a type of pesticide) to control the growth of weeds in fields. Dendritic fibrous nano-silica (DFNS) has high loading capacity with huge surface area and polydiacetylene acts as a gatekeeper performing "gate-close" and "gate-open" mechanism using light as trigger. Additionally, the surface of PFNS is hydrophobic because of the long hydrocarbon chain of PCDA, which shows adhesive property in leaf surface. Furthermore, PCDA is known for its emissive nature, which can be used for real-time monitoring of PFNS in the plant. Therefore, the synthesized nanomaterial ensures more loading, real-time monitoring and sustained release of pesticide.

Keywords: Dendritic fibrous nano-silica; pesticides; sustained release; real-time monitoring; agriculture.

References:

1. M. Shaban, & M. Hasanzadeh, Biomedical applications of dendritic fibrous nanosilica (DFNS): recent progress and challenges. *RSC advances*, *10*(61), (2020) 37116-37133.
2. M. Zong, C. Yu, J. Li, D. Sun, J. Wang, Z. Mo, ... & S. He, Redox and near-infrared light-responsive nanoplatform for enhanced pesticide delivery and pest control in rice: construction, efficacy, and potential mechanisms. *ACS Applied Materials & Interfaces*, *15*(35), (2023) 41351-41361.

AFM-093

A Conductive Bimetallic MOF/CNT Hybrid as a Bifunctional Electrocatalyst for Water Splitting Applications

Archanasri Muthusamy, Panneerselvam Perumal*

Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur.

Corresponding author e-mail: panneerp1@srmist.edu.in

ABSTRACT

Developing efficient and cost-effective electrocatalysts for overall water splitting is crucial for sustainable hydrogen production. Herein, we report the synthesis of a nickel–1,2-benzenedicarboxylic acid (Ni–BDC) incorporated with erbium to construct a bimetallic Ni–Er–BDC framework, followed by hybridization with carbon nanotubes (CNTs) to enhance electrical conductivity and structural robustness. The introduction of Er into the Ni–BDC matrix induces synergistic electronic interactions between the metal centres, effectively modulating the local electronic environment and optimizing the adsorption energetics of reaction intermediates for both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER).The optimized catalyst achieves a current density of 100 mA cm^{-2} at an overpotential of 420 mV for OER and 10 mA cm^{-2} at 270 mV for HER, demonstrating promising bifunctional activity. The incorporation of a conductive CNT network forms an interconnected architecture that facilitates rapid electron transport, enhances exposure of active sites, and improves electrochemical durability under prolonged operation. Overall, this work presents a synergistic strategy that integrates bimetallic modulation with conductive carbon hybridization, offering an effective platform for the rational design of high-performance MOF-based electrocatalysts for overall water splitting.

Key words: Bimetallic Organic Framework, Carbon Nanotube, Benzene dicarboxylic Acid Hydrogen evolution reaction, Oxygen evolution reaction.

References:

1. Li, X.; Yang, H.; Zhang, T.; et al. Bimetallic Metal–Organic Frameworks for Efficient Electrocatalytic Water Splitting.*Chem. Eng. J.* 2022, *430*, 132806.
2. Zhang, Y.; Sun, W.; Rui, K.; et al. Hybridization of Metal–Organic Frameworks with Carbon Nanotubes for Enhanced Bifunctional Water Splitting.*J. Mater. Chem. A* 2023, *11*, 14567–14578.

AFM-094

Lead-Free Ceramic-Polymer Nanocomposites for Sustainable Energy Harvesting

Vignesh Murali, Sujoy Kumar Ghosh*

SRM institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail:** sujoykug@srmist.edu.in

ABSTRACT

The growing demand for portable electronics, wearable, wireless sensor networks and IoT systems demands sustainable, maintenance-free power for everyday use. Conventional micro-batteries, often laden with lead and toxins, face short lifespans, environmental risk, replacement difficulties. Other harvesting methods like electromagnetic, thermoelectric, and solar struggle with bulkiness, environmental dependence, low-frequency inefficiency and inflexibility for all-weather, flexible applications. Piezoelectric and triboelectric nanogenerators from lead-free ceramic-polymer nanocomposites stand out as eco-friendly solution, delivering mechanical flexibility, lightweight design, and robust conversion of biomechanical and ambient vibrations. Current technologies power self-sustaining sensors, health wearables, structural monitors, and micro-chargers, yet grapple with durability, output consistency, power density, and scalable production. In this review, an overview of lead-free ceramic polymer nanocomposites and fabricating techniques, mechanisms, and architectures for these flexible nanocomposites in piezo and tribo-harvesting. Future research direction includes High-performance hybrids systems, robust encapsulation strategies, 3D printing, artificial intelligence (AI)-assisted optimization enabled fabrication and as an emerging tool to accelerate the discovery and optimization of high-performance lead-free compounds. Looking ahead, the field is anticipated to move toward the realization of intelligent, flexible, and multifunctional sensing platforms for use in self-powered systems, harsh environments, and advanced energy harvesting technologies, signifying a crucial shift toward sustainable device innovation.

Keywords: piezoelectric, triboelectric, lead-free ceramic, polymer, energy harvesting applications

AFM-095

Percolative $MoSe_2$/rGO Conductive Networks in PVA Enabling Scalable Gel-Free Wearable Biosensing

Arun Karthick S*[1], Harshini I[1], Indra Suresh[1], Janakiraman P[1]

[1]*Feynman Nano Laboratory, Department of Biomedical Engineering,*

Sri Sivasubramaniya Nadar college of Engineering, Kalavakkam, Chennai, Tamilnadu, India, 603110

***Corresponding author e-mail:** arunkarthicks@ssn.edu.in

ABSTRACT

Continuous biosignal monitoring plays a critical role in early disease diagnosis and the advancement of wearable healthcare technologies. However, conventional Ag/AgCl electrodes rely on conductive gels that progressively dehydrate, leading to increased skin–electrode impedance, signal degradation, and reduced user comfort during prolonged monitoring. To overcome these limitations, a flexible, gel-free dry electrode based on a molybdenum diselenide/reduced graphene oxide ($MoSe_2$/rGO) conductive network embedded within a polyvinyl alcohol (PVA) matrix was developed. A homogeneous $MoSe_2$/rGO dispersion was prepared under magnetic stirring at 1250 rpm, followed by PVA incorporation and probe sonication/continuous stirring for 24 h. The composite solution was cast into a precast mould and thermally cured at 55 °C for 8 h, yielding a mechanically compliant and skin-compatible PVA/$MoSe_2$/rGO wearable electrode.

The fabricated electrode was initially validated through galvanic skin response (GSR) measurements to assess skin–electrode interface stability. It was subsequently integrated into a custom-designed electrocardiogram (ECG) acquisition system built around an ESP32-S3 Mini microcontroller, enabling real-time biopotential acquisition, on-board signal processing, and continuous waveform visualization. The system demonstrated stable baseline characteristics and clear waveform morphology. Heart rate estimation showed minimal deviation compared to standard Ag/AgCl electrodes, confirming high signal fidelity without conductive gels. The seamless integration of the dry electrode with compact embedded hardware highlights its feasibility for low-power, wearable biosignal monitoring applications in clinical, remote, and consumer healthcare settings.

References:

1. Y. Zhu, X. Li, H. Chen, J. Wang, ACS Appl. Mater. Interfaces, 17 (2025) 5123.
2. M. S. Lee, A. Paul, Y. Xu, W. D. Hairston, G. Cauwenberghs, Front Electron, 2 (2022) 700363.
3. J. Li, Y. Wang, Y. Wang, J. Liu, Sensors, 20 (2020) 3641.

AFM-096

Synergistic Dual-Anion Vacancy Engineering and Interfacial Charge Modulation in O–MoS_2/NiFe-LDH/MWCNT for Efficient Bifunctional Water Splitting

A. Kalaiselvi, V. Prasanna Kumar and T. Maiyalagan*

Electrochemical Energy Laboratory, Department of Chemistry,

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India

Corresponding author e-mail : maiyalat@srmist.edu.in & maiyalagan@gmail.ccom

ABSTRACT

The rational design of efficient and durable bifunctional electrocatalysts for overall water splitting remains a critical challenge for sustainable hydrogen production. Herein, we report the first systematic construction of a dual anion vacancy-engineered O–MoS_2/NiFe-LDH/MWCNT hierarchical hybrid catalyst, integrating defect modulation, electronic structure reconstruction, and interfacial engineering to achieve exceptional catalytic performance. Controlled oxygen incorporation and heterointerface coupling induce simultaneous enrichment of oxygen and sulfur vacancies, accompanied by pronounced electronic reconstruction characterized by $Ni^{2+} \rightarrow Ni^{3+}$ transformation and defect-rich Mo^{5+}/Mo^{6+} species formation. These synergistic effects significantly optimize reaction intermediate adsorption and accelerate charge-transfer kinetics. Benefiting from the hierarchical nanosheet architecture and conductive carbon framework, the composite exhibits a large electrochemically active surface area and ultralow charge-transfer resistance. As a result, the optimized catalyst delivers outstanding oxygen evolution reaction (OER) activity with a low overpotential of 204 mV at 10 mA cm^{-2} and a small Tafel slope of 57 mV dec^{-1}, along with excellent hydrogen evolution reaction (HER) performance requiring only 159 mV at 10 mA cm^{-2}. Remarkably, the catalyst demonstrates exceptional durability with stable 72 h operation for both OER and HER, and enables efficient overall water splitting at a low cell voltage of 1.58 V for over 100 h of continuous electrolysis. This work establishes a versatile strategy for defect-driven electrocatalyst engineering toward high-performance water splitting.

Keywords: O-MoS_2, NiFe-LDH, MWCNT, Dual Anion Vacancy, Bifunctional electrocatalyst.

Reference:

1. Xie, J., Zhang, H., Li, S., Wang, R., Sun, X., Zhou, M., ... & Xie, Y., Advanced materials, 25(40), 5807-5813 (2013).
2. Wang, S., Ning, X., Cao, Y., Chen, R., Lu, Z., Hu, J., ... & Hao, A., Inorganic Chemistry, 62(16), 6428-6438(2023).
3. Xie, J., Zhang, J., Li, S., Grote, F., Zhang, X., Zhang, H., ... & Xie, Y., Journal of the American Chemical Society, 135(47), 17881-17888(2013)

AFM-097

Defect Engineering of MIL-Derived $VO_x/NiFe_2O_4$/MWCNTs towards Efficient Oxygen Evolution Reaction

Durga sri N[1], Parameshwari[2], T. Maiyalagan*[3]

[1] *Electrochemical Energy Laboratory, Department of Chemistry, SRM institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** maiyalagan@gmail.com

ABSTRACT

The development of efficient and earth-abundant electrocatalysts for the oxygen evolution reaction (OER) is crucial for advancing sustainable hydrogen production. In this work, a high-valent oxide-engineered composite, $VO_x/NiFe_2O_4$/CNT, was synthesized and evaluated as an OER catalyst in alkaline media. The surface incorporation of VO_x onto $NiFe_2O_4$ induces significant electronic modulation within the host lattice. X-ray photoelectron spectroscopy reveals a pronounced increase in the Ni^{3+} content after VO_x introduction, indicating strong electronic interaction between VO_x species and the $NiFe_2O_4$ framework. The stabilization of higher-valent Ni active sites enhances intrinsic catalytic activity, as high-valence Ni species are widely recognized as key contributors to alkaline OER kinetics.Furthermore, the integration of carbon nanotubes (CNTs) provides a conductive network that facilitates rapid electron transport, improves charge transfer efficiency, and enhances structural robustness during prolonged electrochemical operation. The synergistic interplay between VO_x-induced electronic modulation and the conductive CNT scaffold significantly boosts catalytic performance.Electrochemical evaluation demonstrates that the optimized $VO_x/NiFe_2O_4$/CNT catalyst achieves a low overpotential of 265 mV at a current density of 10 mA cm^{-2} in 1.0 M KOH, outperforming pristine $NiFe_2O_4$ and several reported non-noble metal-based catalysts. The reduced Tafel slope confirms improved reaction kinetics, while durability tests indicate stable catalytic activity over 80 hours of continuous operation.Overall, this study highlights the effectiveness of high-valent oxide-induced electronic modulation combined with conductive carbon integration as a promising strategy for designing advanced spinel-based OER electrocatalysts toward scalable and sustainable hydrogen production technologies.

Keywords: Electrocatalyst**,** Oxygen Evolution Reaction (OER), Nickel ferrite, MWCNTs, Spinel oxides.

References:

1. K. Ram Kumar, N. Durga Sri, Vaibhav Namdev Kale, and Thandavarayan Maiyalagan, International Journal of Hydrogen Energy, 101, 2025, 837-847.
2. N. Durga Sri, and Thandavarayan Maiyalagan, Journal of Electroanalytical Chemistry 2025, 119138.

AFM-98

Nitrogen-Doped Borophene: A Metal-free Electrocatalyst for Oxygen Evolution Reaction

Vikram Venkatesan and Anandhakumar Sukeri*

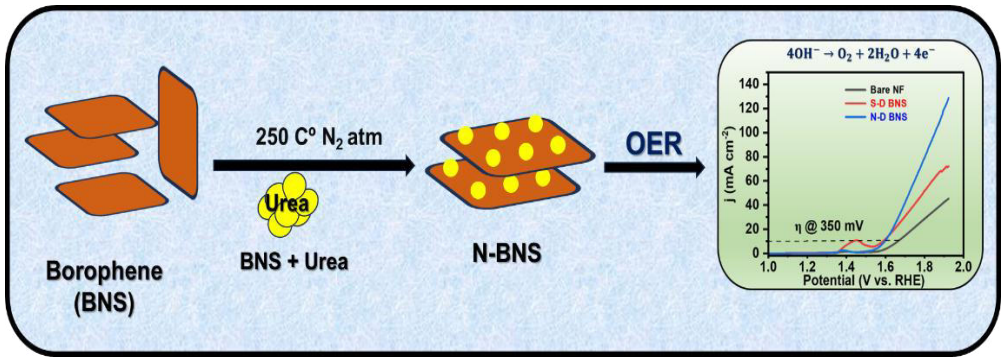
Nanoscale Materials Electrochemistry Laboratory, Department of Chemistry

SRM Institute of Science and Technology, Kattankulathur – 603203, Tamil Nadu, India.

***Corresponding author e-mail:** anandhas2@srmist.edu.in

ABSTRACT

The development of alkaline water electrolyzers relies on the growth of an efficient electrocatalyst that can surpass conventional noble-metal catalysts, which still present challenges in achieving high efficiency and long-term stability. Two-dimensional (2D) borophene has recently emerged as a promising material for several electrochemical applications. Adapting the electronic structure of 2D materials through heteroatom doping has emerged as an effective strategy for enhancing electrocatalytic performances. In this context, nitrogen-doped borophene nanosheets (N-BNS) are proposed as a promising metal-free electrocatalyst for OER. Electrochemical results exhibit enhanced OER activity by achieving the benchmark current density of 10 mA cm^{-2} at ~350 mV overpotential. These results highlight that N-BNS can be a promising metal-free electrocatalyst for durable water oxidation in an alkaline medium.



Reference:

1. H. Jiang, J. Gu, X. Zheng, M. Liu, X. Qiu, L. Wang, W. Li, Z. Chen, X. Ji, J. Li, *Energy Environ. Sci.*, 12 (2019) 322-333.
2. X. Kong, Y. Zhu, H. Lei, J. Wang, *ChemCatChem*, 9 (2017) 846-852.

AFM-99

Sustainable Copper Recovery from Waste Printed Circuit Boards Using Cross-Linked β-Cyclodextrin Polymer for Energy Applications

Muthumari Mariappan and Srinivasarao Kancharla*

Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India.

***Corresponding author e-mail:** srinivak5@srmist.edu.in

ABSTRACT

The increasing generation of electronic waste (e-waste) necessitates environmentally benign and efficient strategies for metal recovery, particularly for copper from waste printed circuit boards (WPCBs)[1]. In this work, an epichlorohydrin cross-linked β-cyclodextrin polymer (EPI-β-CDP) is developed as a multifunctional material for the simultaneous leaching and sorption (leaching-sorption) of copper in aqueous media[2]. The polymer serves a dual role by facilitating oxidative dissolution of metallic copper and concurrently capturing the released Cu (II) ions through coordination with oxygen-rich functional groups. Copper recovery using the EPI-β-CDP system achieves complete extraction efficiency, demonstrating the effectiveness of the integrated leaching-sorption approach. Structural and phase analyses reveal that Cu (II) ions remain highly dispersed within the amorphous cyclodextrin framework after sorption, without the formation of crystalline copper phases[2]. The recovered copper is subsequently stripped and converted into crystalline cuprous oxide nano particle above the polymer substate (Cu_2O@EPI-β-CDP) using mild reducing agent, confirming the feasibility of copper upcycling from e-waste. The formation of well-defined Cu_2O nanoparticles is supported by X-Ray diffraction, SEM and EDS studies. This integrated process avoids the use of aggressive mineral acids and cyanide-based reagents, operating under mild and environmentally friendly conditions while enabling both recovery and value-added transformation of copper[1]. The findings highlight the potential of cross-linked cyclodextrin polymers as sustainable platforms for green metal recovery and circular-economy-driven e-waste management.

Keywords: Waste printed circuit boards; cross-linked β-cyclodextrin polymer; Cu_2O@EPI-β-CDP

References:

1. Mathaiyan, R.; Nechikott, A. A.; Babu M. K., S.; Nayak, P. K.; Kancharla, S. J. Mater. Chem. A Mater. 2024, 12 (41), 28107–28118.
2. Wu, H.; Wang, Y.; Tang, C.; Jones, L. O.; Song, B.; Chen, X.-Y.; Zhang, L.; Wu, Y.; Stern, C. L.; Schatz, G. C.; Liu, W.; Stoddart, J. F. Nat. Commun. 2023, 14 (1), 1284.

AFM-100

Agro-Waste Derived Advanced Biochar for Sustainable Copper Recovery From e-Waste and Subsequent Cu2o Formation Toward Electrochemical Application

Noora Hiyum Ibrahim, and Srinivasarao Kancharla*

Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamil Nadu, India.

***Corresponding author e-mail:** srinivak5@srmist.edu.in

ABSTRACT

The growing volume of electronic waste has intensified the need for sustainable and selective metal recovery technologies. This work presents a green and integrated approach for copper recovery from waste printed circuit boards (WPCBs) using oxidatively modified torrefied biochar derived from banana peels, followed by the synthesis of Cu_2O @biochar nanocomposites. The modified biochar, enriched with oxygen-containing functional groups, acts as an efficient sorbent for Cu(II) ions released during leaching, enabling a simultaneous leaching-sorption process in a mild aqueous system[1]. Captured copper species are strongly bound within the porous carbon matrix through complexation and ion-exchange interactions. The Cu- loaded biochar is subsequently converted into Cu_2O -decorated biochar via chemical reduction, producing a stable nanocomposite. Structural and morphological analyses using XRD, SEM, and EDS confirm the formation and uniform dispersion of crystalline Cu_2O nanoparticles on the biochar surface[2]. The developed strategy demonstrates a closed-loop and environmentally benign route that combines biomass valorization with urban mining, offering a scalable platform for copper recovery and the generation of value-added functional nanomaterials for catalytic and electrochemical applications.

Keywords: Electronic waste (e-waste), Biochar, Leaching–sorption process, Electrochemical energy conversion

References:

1. Kobayashi, H.; Kaiki, H.; Shrotri, A.; Techikawara, K.; Fukuoka, Chem. Sci. 2016, 7 (1), 692–696.
2. Mathaiyan, R.; Nechikott, A. A.; Babu M. K., S.; Nayak, P. K.; Kancharla, S.. J. Mater. Chem. A Mater. 2024, 12 (41), 28107–28118.

AFM-101

MXene Nanocomposite for Ultrasensitive Two-terminal Artificial Synaptic Devices

Shraboni Ray[1,2], Pranab Kumar Sarkar[2*]

[1]*Department of Physics, Assam University, Silchar 788011, India.*

[2*]*Department of Applied Science and Humanities, Assam University, Silchar 788011, India*

***Corresponding Author email:** pranab.sarkar83@gmail.com

ABSTRACT

Brain-inspired parallel computing based on an MXene nanocomposite memory device has attracted significant interest due to its simple fabrication process, scalable neuromorphic computing capabilities, and affordability. Two-dimensional transition metal carbides, nitrides, or carbonitrides, known as MXenes, have attracted significant interest for a wide range of energy and environmental applications due to their excellent electrical conductivity, high mechanical strength, large surface area, rapid charge transport, good thermal properties, and tunable surface properties.[1] Herein, we fabricated an MXene nanocomposite device to improve the stability and electrical conductivity. Specifically, we synthesised and characterised Ti_3CNT_x MXene. The analogue memory effect and replicated different synaptic learning functions utilising the Ag/Ti_3CNT_x/PMMA/ITO-PET memristor. This device mimics several bio-synaptic characteristics, including excitatory postsynaptic current (EPSC), paired-pulse facilitation (PPF), and long-term potentiation/depression. The findings indicated that the MXene Nanocomposite perform as a promising nanomaterial for applications in brain-inspired computing.

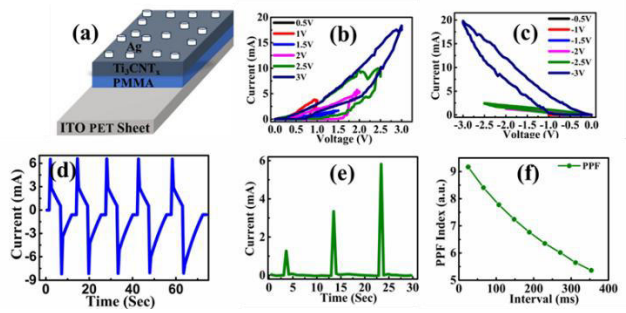


Fig. 1(a) Schematic representation of Ag/Ti_3CNT_x/PMMA/ITO-PET memristive device. (b,c) Analogue I-V curves under different positive and negative voltage dual sweeps. Synaptic behaviours of the device by applying (d) EPSC, (e) Pair-pulse facilitation, (f) The PPF index as a function of the pulse interval.

Keywords: MXene, Neuromorphic computing, Two-dimension, EPSC, PPF index.

References:

1. Hussain, T., Chandio, I., Ali, A., Hyder, A., Memon, A. A., Yang, J., & Thebo, K. H., Nanos., 16 (2024) 17723-17760.

AFM-102

Defect-Engineered Metal–Organic Framework/Layered Double Hydroxide Photoelectrodes for Enhanced Photoelectrochemical watersplitting.

Priyanka Venkatesh[1], Kiruthika Murugesan[1] Jayakaushalya Manogaran[1], Nihil Vishwa Ravi[1], Maheswaran Ratinam[1*]

Department of Physics and Nanotechnology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur, Tamilnadu, 603 203, India

***Corresponding author e-mail address:** maheswar@srmist.edu.in

ABSTRACT

For the past few decades, the rapid increase in global energy demand has intensified the development of cost-efficient and sustainable energy conversion technologies. For this, the earth-abundant electrocatalysts have been employed to derive hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) in alkaline media, which demonstrate scalable and sustainable green hydrogen production by their strong catalytic activity and operational durability. More specifically, the Layered Double Hydroxides (LDHs) are leading candidates in this field due to their groundbreaking potential, such as structural and compositional viability, large specific surface area, and abundant active sites. However, their limited intrinsic conductivity and charge-transfer efficiency reduce the overall catalytic activity, thereby decreasing their practical performance. To overcome the limitation, numerous research efforts have devoted to the compositional engineering of Metal–Organic Frameworks (MOFs) with Layered Double Hydroxides (LDHs). This strategy increases the density of available active sites and suppresses the charge recombination rate, thereby significantly improving the catalyst activity and overall electrochemical performance. Accordingly, in this work, we have successfully synthesised LDH directly on top of a defective MOF scaffold, forming a Z-scheme heterojunction that facilitates enhanced photocatalytic activity through improved charge separation. For that, we followed a two-step synthesis approach to demonstrate the expected composition. The phase purity and structural confirmation of all compositions were established through XRD peak analysis. Additionally, defect site identification and configuration analysis were carried out using TGA, FTIR, and SEM, which are discussed in detail. Overall, this work highlights the role of heterostructure formation and defect engineering in improving high-performance catalyst design.

References:

1. Dou, Y.; Zhou, J.; Yang, F.; Zhao, M.-J.; Nie, Z.; Li, J.-R. Hierarchically structured layered-double-hydroxide@zeolitic-imidazolate-framework derivatives for high-performance electrochemical energy storage. J. Mater. Chem. A 2016, 4, 12526–12535.
2. Vandichel, M.; Hajek, J.; Vermoortele, F.; Waroquier, M.; De Vos, D. E.; Van Speybroeck, V. Active site engineering in UiO-66 type metal–organic frameworks by intentional creation of defects: a theoretical rationalization. CrystEngComm 2015, 17, 395–406
3. Sk, S.; Islam, H.; Abraham, B. M.; Mondal, I.; Pal, U. Defects in MOFs for Photocatalytic Water Reduction to Hydrogen Generation: From Fundamental Understanding to State-of-Art Materials. Small Methods 2025, 9, 2401689

AFM-103

Cu Metal Organic Framework for Adsorption based Reversible Hydrogen Storage

Vijay Vel Rajankumar [a], Ajaijawahar Kaliyaperumal [a, b], Karthigeyan Annamalai [a, b], Siva Chidambaram [a] *

[a] *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu 603203, Tamil Nadu, India.*

[b] *Hydrogen Storage Materials and Nanosensors Laboratory, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu-603203, Tamil Nadu, India.*

***Corresponding author e-mail:** sivac@srmist.edu.in

ABSTRACT

Hydrogen storage remains a critical challenge for the advancement of hydrogen-based energy systems. In this study, Cu Imidazole based metal organic framework (MOF) was synthesized one-pot coprecipitation route using water as a solvent to ensure scalability. It was then investigated for its physisorption-based hydrogen storage capability using thermogravimetric analysis under controlled hydrogenation conditions. The MOF was exposed to varying hydrogenation pressures (5 bar, 10 bar) at a constant temperature of 150 °C to evaluate the effect of pressure on hydrogen uptake and release behaviour. The reversible nature of physisorption was confirmed through multiple hydrogen adsorption–desorption cycles. Consistent with conventional physisorption mechanisms, the results emphasized that higher pressure and temperature substantially enhance the adsorption efficiency. Further the post application characterizations revealed that the structure of MOF remains intact without any phase or functional degradation. To gain mechanistic insights and to identify the preferential adsorption sites, density functional theory computations were performed. The interaction between hydrogen molecule and the framework was quantified by Bader charge analysis.

References

1. Zhang C., Liu X., Wu K., Wu T., Zhang S., Wu X., *J. Water Process. Eng.*, 79 (2025) 108937.
2. Hoang T.K.A., Antonelli D.M., *Adv. Mater.*, 21 (2009) 1787–1800.
3. O'Brien M.C.M., Chancey C.C., *Am. J. Phys.*, 61 (1993) 688–697.
4. Nguyen T.T., Tran H.V., Nguyen L.H., Nguyen H.M., Phan T.B., Nguyen-The T., et al., *RSC Adv.*, 14 (2024) 26611–26624.

Dielectric–Magnetic PVDF Composites for Electromagnetic Interference Shielding (EMI) Applications

Shubha A, Payel Bandyopadhyay*

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203

***Corresponding author e-mail**: payelb@srmist.edu.in

ABSTRACT

The increasing use of electronic and wireless devices has led to a significant rise in electromagnetic interference (EMI), which can disturb the performance and reliability of electronic systems. Developing lightweight and flexible EMI shielding materials has therefore become an important. Polymer-based composites are considered promising candidates because of their low density, easy processing, and good mechanical stability. Among them, Polyvinylidene fluoride (PVDF) has gained considerable attention due to its excellent chemical resistance, good dielectric properties, and mechanical strength. In this study, PVDF-based composites containing Barium titanate ($BaTiO_3$) and Nickel ferrite ($NiFe_2O_4$) nanoparticles are explored for EMI shielding applications. $BaTiO_3$ is a high dielectric constant material that can enhance dielectric polarization within the composite, while $NiFe_2O_4$ is a magnetic ferrite that contributes to magnetic loss and electromagnetic wave absorption. The combination of dielectric and magnetic fillers within the PVDF matrix is expected to improve the attenuation of electromagnetic waves through multiple mechanisms, including reflection, absorption, and interfacial polarisation. The composites are prepared using a solution casting method to obtain uniform films with well-dispersed nanoparticles. Structural and morphological characterisation confirms the successful incorporation of $BaTiO_3$ and $NiFe_2O_4$ within the PVDF matrix. The presence of both dielectric and magnetic components will improve the composite's overall shielding performance.

References:

1. Priteesh et al., ACS Appl. Electron. Mater. 2025, 7, 24, 10984–10997.
2. Yishen et al., Composites Science and Technology, 2026,278, 0266-3538
3. Pingping et al., J. Mater. Chem. C, 2025,13, 12242-12253
4. Saubhagya et al., ChemistrySelect, 2025,Volume 10, Issue 35, e02498

AFM-105

Sustainable Energy Harvesting by Molecular Ferroelectrics Based on Cu(II) Complexes

Rajashi Haldar, Maheswaran Shanmugam*
Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra, India 400076
***Corresponding author e-mail:** eswar@chem.iitb.ac.in

ABSTRACT

To tackle the growing global energy demand and the rapid exhaustion of nonrenewable fossil fuels, it is crucial to develop sustainable alternatives. One promising strategy involves harvesting abundant but otherwise wasted environmental energies—such as mechanical vibrations, pressure, heat, sunlight, and tidal motion—and converting them into usable electricity through self-powered nanogenerators (SPNGs). A wide range of materials have been explored for this purpose, including inorganic oxides (e.g., perovskites and ceramics), polymers, organic molecules, peptides, and organic–inorganic hybrids. Among these, oxide systems exhibit strong piezoelectric and ferroelectric properties, making them highly effective for energy harvesting. However, they suffer from key limitations: high-cost, high-temperature synthesis, brittleness, limited tunability, and toxicity due to heavy metals. In contrast, polymers and peptides offer mechanical flexibility but often struggle to maintain stable polar states (e.g., the β-phase of PVDF) necessary for ferroelectric functionality. Hybrid organic–inorganic perovskites present a middle ground, combining low-temperature processability with excellent output performance, but are hampered by poor environmental stability and the presence of toxic components such as lead-based halides.

Through strategic molecular engineering and controlled design, we have addressed many of these challenges by developing biocompatible, discrete molecular complexes. These materials are lightweight, mechanically flexible, and readily polarizable under external electric fields, making them ideal for SPNG integration. Our synthesized Cu(II)-based molecular complexes exhibit high piezoelectric coefficients (d_{33} = 10–25 pm/V), comparable to $LiNbO_3$, ZnO, and polymers such as PVDF and PVDF-TrFE, along with substantial spontaneous polarization that enables efficient energy conversion in both single-crystal and composite forms. In a flexible composite device fabricated by embedding a ferroelectric complex into a nonpolar polyvinyl alcohol (PVA) matrix, we achieved a peak-to-peak output voltage of 4.94 V and an acoustoelectric response of 40 mV from a 60 Hz sound wave.[1,2] By combining the low-frequency sensitivity of the acoustoelectric nanogenerator (AcNG) with a machine-learning approach, voice signals were distinguished with 95% accuracy. Compared to conventional oxide single crystals, these molecular complexes are simpler to synthesize and exhibit desirable anisotropic properties, offering strong potential for directional sensors, ultrasound transducers, and acoustic devices where minimizing multidirectional mechanical and thermal noise is essential. This work highlights the versatility of molecular materials for next-generation, soft, and sustainable energy technologies.

References:

1. Haldar, R.; Naskar, S.; Mondal, B.; Iqbal, A.; Thapa, R.; Mandal, D.; Shanmugam, M., *Advanced Materials*, **2025**, 25040868.
2. Haldar, R.; Sarkar, U.; Kumar, A.; Mandal, D.; Shanmugam, M. Inducing Polar Phase in Poly(Vinylidene Fluoride) with a Molecular Ferroelectric Copper(II) Complex for Piezoelectric Energy Harvesting. *Adv. Funct. Mater.* **2024**, 34, 2407611.
3. Haldar, R.; Kumar, A.; Mallick, B.; Ganguly, S.; Mandal, D.; Shanmugam M. *Angew Chem. Int. Ed.* **2023**, 62 (9), 202216680.

TF-001

Experimental and Simulation Study on Magnetic Abrasive Finishing Process of Inconel 625 and Inconel 718

Vritika Sree K P[1], Anbu C[1], Varshana G[1], Narmatha V[1]*

[1]*Kongu Engineering College, Perundurai, Tamilnadu, India, 638060*

***Corresponding author e-mail:** vritikasreekp.22mts@kongu.edu

ABSTRACT

The Nickel-based superalloys, such as Inconel 625 and Inconel 718, find wide application in aerospace, marine, and power generation industries due to their excellent strength, corrosion resistance, and heat resistance. These properties extend their use in very demanding applications, they make the alloys extremely difficult to machine. Most of the traditional methods of finishing result in poor surface quality, rapid tool wear, and higher processing costs. To solve these problems, Magnetic Abrasive Finishing has emerged as a promising alternative. In MAF, a controlled magnetic field retains a mixture of ferromagnetic particles and abrasive grains, which forms a flexible magnetic brush. This brush, upon interaction with the workpiece, removes minute surface irregularities and thereby gives a smooth finish. The process is gentle, generates very little heat, and avoids tool wear, thus being especially suitable for finishing hard to machine superalloys.

This project examines, both experimentally and through simulation, the MAF process for Inconel 625 and Inconel 718. The experimental work covers how the variation in the magnetic field strength, abrasive size, finishing time, and rotational speed influences surface roughness and material removal rate. Simulations examine the behavior of particles, stress distribution, and material removal mechanisms. These approaches go together to optimize the MAF process for an improved surface finish with controlled material removal for these advanced materials.





References:

1. Amit Chaurasia, Vijay Wankhede, International Research Journal of Engineering and Technology, 5 (2018) 1165–1168.
2. T. C. Kanish, S. Narayanan, P. Kuppan, S. D. Ashok, Materials Today: Proceedings, 5 (2018) 12734–12743.
3. T. C. Kanish, S. Narayanan, P. Kuppan, S. Denis Ashok, Procedia Manufacturing, 30 (2019) 276–283.
4. M. Yousuf Khan, P. Srinivasa Rao, B. S. Pabla, Advances in Materials and Processing Technologies, 8 (2022) 2204–2230.
5. Hyoung Jin Kim, Ling Heng, Sung Dae Mun, Metals, 14 (2024) 242.

TF-002

Impact of Growth and Thermal Annealing in Oxygen and Nitrogen Atmospheres on the Properties of Terbium Oxide Thin Films for Advanced Semiconductor Applications

Abubakar A[1]. Sifawa[1]*

[1]*Department of Physics, Sokoto State University, Sokoto 852101, SSU, Sokoto, Nigeria*

***Corresponding author e-mail:** aasifawa13@gmail.com

ABSTRACT

This study investigates the impact of post-deposition annealing in oxygen (O_2) and nitrogen (N_2) environments on the structural and surface properties of RF-sputtered Tb_4O_7 thin films on silicon (Si). Samples were annealed at 500 °C and compared with an unannealed (standard) sample. GIXRD results show that annealing enhances crystallinity and grain growth while retaining the cubic Tb_4O_7 phase, with crystallite sizes increasing from 10.97 nm (standard) to 17.26 nm (O_2-annealed) and 25.86 nm (N_2-annealed). FESEM images confirm substantial grain growth, especially in the N_2-annealed film, which displays the largest and most uniform grains with a smooth, void-free surface. AFM measurements further support this trend, showing RMS roughness decreasing from 1.91 nm (standard) to 1.58 nm (N_2) and 0.98 nm (O_2). EDX analysis verifies the presence of Tb, O, and Si, with the N_2-annealed film having the highest oxygen concentration (22.87 at%), while the O_2-annealed film shows a lower value (15.79 at%) due to oxygen diffusion toward the interface. Overall, N_2 annealing yields the most uniform, defect-free Tb_4O_7 films, making it the most promising route for high-quality Si-based semiconductor applications.

Keywords: Tb_4O_7 films; GIXRD pattern; AFM roughness; post-deposition annealing; surface properties; uniform grain.

References:

1. S. M. Abed, S. M. Mohammad, Z. Hassan, M. R. Shahrier, and A. S. Abubakar, AIP Conf. Proc. 3310 (2025) 070004.
2. X. M. Bai, A. F. Voter, R. G. Hoagland, M. Nastasi, and B. P. Uberuaga, Science 327 (2010) 1631–1634.
3. S. V. Belaya, V. V. Bakovets, I. P. Asanov, I. V. Korolkov, and V. S. Sulyaeva, Chem. Vap. Deposition 21 (2015) 150–155.

RF- Magnetron Sputtered, Electrochromic NiO-based Ion Storage Electrodes for Flexible Smart Window Applications

S. Aravinthan[1], P. Kavitha[1], M. Sridharan[2], K. Mahalakshmi[3], K. Jeyadheepan[1]*

[1]*Multifunctional Materials and Devices Lab, Anusandhan Kendra – II, School of EEE, SASTRA Deemed University, Thanjavur – 613401*

[2]*Functional nanomaterials & Devices Lab, Centre for Nanotechnology & Advanced Biomaterials and School of Arts, Sciences, Humanities & Education, SASTRA Deemed University, Thanjavur–613 401*

[3]*Department of Physics, Providence College for Women, Coonoor, The Nilgiris – 643104*

***Corresponding author e-mail:** jeyadheepan@eee.sastra.edu

ABSTRACT

Electrochromic devices rely on materials that can reversibly change their optical transmittance when an electrical stimulus is applied, and nickel oxide has gained considerable attention as an effective ion storage layer because of its strong optical contrast, high colouration efficiency, and good chemical stability, making it suitable for use in next generation flexible electrochromic systems [1-2]. In this work, flexible nickel oxide thin films were deposited on ITO/PET substrates using RF-reactive magnetron sputtering, a deposition method that offers precise control over composition, surface uniformity, and adhesion, all of which are crucial for reliable integration into flexible device architectures [3]. The study involved a systematic optimisation of sputtering parameters, particularly the applied reactive power and deposition duration, to produce films with desirable structural, mechanical strength, and electrochemical responsiveness. Films fabricated under optimised conditions maintained excellent adhesion and structural integrity during repeated bending tests, showing no visible cracking or delamination, which confirm their suitability for flexible applications. Structural analysis indicated that the films predominantly possess an amorphous structure, an attribute that facilitates ion transport by providing abundant diffusion pathways during electrochromic cycling. SEM analysis revealed that the films exhibit a uniformly nanostructured and continuous surface with minimal defects, indicating that controlled sputtering conditions support the formation of smooth and uniform films. Optical transmittance measurements were carried out to evaluate the optical properties of the films, and the results show that the optical band gap increases with increasing sputtering power, indicating that deposition energy plays a significant role in tuning the electronic structure of nickel oxide. Electrochemical studies evaluating charge transfer and cycling stability confirmed that the films exhibit stable ion insertion behaviour and a reliable long-term response. These findings emphasise the significance of optimising sputtering conditions to produce nickel oxide films that are mechanically robust, electrochemically stable, and optically adjustable for high performance flexible electrochromic applications.

References:

1. Nuroldayeva, Gulzat, and Mannix P. Balanay. Polymers 15 (2023): 2924.
2. Pehlivan, Esat, Claes G. Granqvist, and Gunnar A. Niklasson. Solar Energy Materials and Solar Cells 269 (2024): 112795.
3. Lin, Han, et al. Materials Science and Engineering: B 270 (2021): 115196.

TF-004

Effect of Cu, Sn, and Ti Doping on the Structural, Morphological, Surface, Electrical and Optical Properties of ZnO Nanorods grown on FTO Substrates

Nageswara Rao Muddapati[1], Naveen Kumar Reddy Bussi Reddy[1]*

[1]*Vignan Foundation for Science, technology and Research Vadlamudi, Guntur Andhra Pradesh-522213.*

***Corresponding author e-mail:** bnkr_sh@vignan.ac.in, bussireddynaveen@gmail.com

ABSTRACT

Undoped and Cu, Sn, and Ti-doped ZnO nanorods were synthesized on FTO glass substrates using the hydrothermal method, and their structural, morphological, and optical properties were investigated. XRD analysis confirmed a hexagonal wurtzite structure with strong (002) preferential orientation, indicating vertical alignment along the c-axis. The diffraction peak position remained unchanged for undoped and Cu-doped ZnO nanorods, while a slight shift toward lower angles was observed for Sn- and Ti-doped samples. FESEM studies revealed that the nanorod length and diameter increased from undoped to Sn-doped ZnO nanorods and decreased for Ti-doped ZnO nanorods. Energy-dispersive X-ray spectroscopy (EDX) analysis confirmed the presence of only zinc (Zn), oxygen (O), copper (Cu), tin (Sn), and titanium (Ti) without detectable impurities. Additionally, the surface characteristics of un-doped and doped ZnO nanorods were studied by using X-ray photoelectron spectroscopy (XPS). UV–Visible analysis showed a slight reduction in the optical band gap for Cu-doped ZnO nanorods, followed by an increase for Sn- and Ti-doped ZnO nanorods. The emission peak is slightly shifted towards a higher wavelength in the range of 500-550 nm. This shift indicates a reduction in oxygen vacancy-related defects from un-doped to titanium-doped ZnO nanorods.

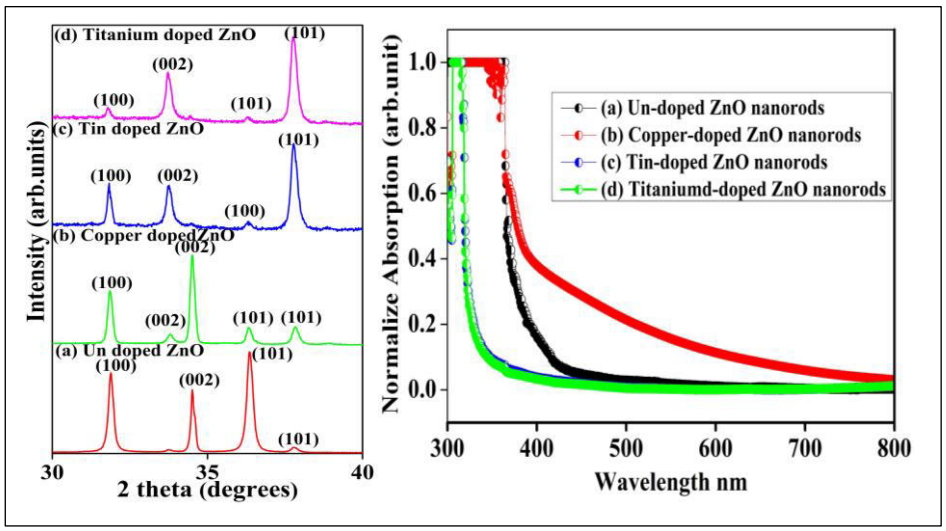


Fig. Represents the XRD and UV-Visible spectrum of doped and un-doped ZnO nanorods

Keywords: ZnO nanorods, FESEM, XPS, UV-Visible, Energy Bandgap, EDX, Photoluminescence

Reference:

1. K.H. Kim, Z Jin, and Y. Abe, Superlattices Microstruct., 75 (2014), 455-460.
2. M. Babikier, D. Wang, and J. Wang., Nanoscale Res. Lett., 9 (2014), 199.

TF-005

Structural, Optical, and Photoluminescence Studies of $BiFeO_3$ Thin Films Prepared by Sol–Gel Dip Coating

G Viswarupahari[1] and Ramanjaneyulu Mannam [1]*

[1]*Department of Physics, Vignan's Foundation for Science Technology and Research - 600036, Guntur, India.*

***Corresponding author e-mail:** ramu.nov9@gmail.com

ABSTRACT

Nanocrystalline bismuth ferrite ($BiFeO_3$) thin films were successfully deposited on glass substrates using the sol–gel dip-coating technique. In this study, the annealing temperature was fixed at 550 °C, while the growth duration was varied from 30 to 120 minutes to explore its influence on the structural and optical properties of the films. X-ray diffraction (XRD) analysis confirmed the formation of single-phase, polycrystalline $BiFeO_3$ with lattice constants a = 5.575 Å and c = 6.912 Å. The results indicate that extended growth durations enhance crystallinity and phase purity. Optical characterization revealed a systematic decrease in the optical bandgap from 2.2 eV to 1.8 eV as the growth time increased, attributed to improved film density and reduced defect states. UV–Vis transmittance measurements showed high transparency (~70%) in the visible range, which also improved with growth duration. Fourier-transform infrared (FTIR) spectroscopy confirmed the presence of strong Fe–O stretching vibrations, indicating the stability of the perovskite structure. Photoluminescence (PL) spectra exhibited a prominent emission peak at around 2.0 eV, emphasizing the films' optical activity. These findings demonstrate that growth time is a key parameter in tuning the optical bandgap and structural quality of BiFeO3 thin films for potential applications in multifunctional optoelectronic and photovoltaic & Photocatalytic Applications.

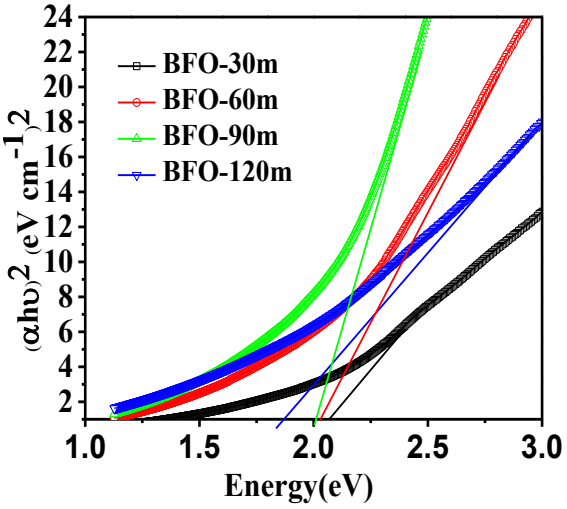


Fig: Optical bandgap of BFO films with growth on Dip coating time

Keywords: sol-gel , Dip-coating, and photoluminescence

Reference:

1. Byung-Geon Park et al. matlet.285(2020) 129006,
2. Katja Andrina Kravanja et al. Materials & Design 217 (2022) 110653
3. B.S. Soram et al. Thin Solid Films 524 (2012) 57–61

TF-006

Microstructure-Driven Oxidation of Sputtered Tungsten Films

Gomathi Natarajan*, Ramanathaswamy Pandian, Arun K Prasad and R. Ramaseshan

Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamilnadu

***Corresponding author e-mail:** gomathinatarajan@igcar.gov.in

ABSTRACT

We report a precursor-controlled oxidation study of sputtered tungsten thin films subjected to post-deposition annealing in air between 350 and 400 °C. Tungsten films deposited at room temperature and at 400 °C form precursors with distinctly different microstructures, phase compositions, and defect densities, which directly govern oxygen incorporation and oxide phase evolution during annealing. Raman spectroscopy and X-ray diffraction show that oxidation proceeds through an oxygen-deficient WO_x intermediate, but the stability of this intermediate and its transformation to crystalline WO_3 are strongly controlled by the initial metallic precursor.

Room-temperature deposited films exhibit a highly disordered, β-W rich microstructure. Upon air annealing up to 400 °C, these films oxidize slowly and remain dominated by defective WO_x phases, as indicated by a broad Raman band in the 650–720 cm^{-1} range and only weak development of the ~805 cm^{-1} band associated with crystalline WO_3. XRD confirms that the metallic structure remains largely unchanged, indicating oxidation confined to a thin, poorly ordered surface layer.

In contrast, films deposited at 400 °C are dominated by relaxed α-W with sharper diffraction peaks. These precursors undergo a clear $WO_x \rightarrow WO_3$ transformation between 375 and 400 °C. Raman spectra reveal the emergence of a sharp ~805 cm^{-1} mode characteristic of monoclinic WO_3, accompanied by suppression of WO_x-related features [1, 2]. The results demonstrate that precursor engineering during sputtering provides a direct route to control tungsten oxide phase formation at low temperatures, relevant for gas sensors, electrochromic coatings, and resistive switching devices.

References:

1. Siciliano, T. et al., WO_3 gas sensors prepared by thermal oxidization of tungsten, Sensors and Actuators B: Chemical, 130 (2008) 88–94.
2. Escalante, G. et al. Correlation between Raman spectra and color of tungsten oxide thin films, AIP Advances, 11 (2021) 055103

Impact of Deposition Parameters on Resistive Switching Behaviour of HZO ($Hf_{0.5}Zr_{0.5}O_2$) Thin Films.

Tanya Dasila[1], Kajal Jindal[2], Arijit Chowdhuri[3], Monika Tomar[4], Anjali Sharma[1]*

[1]*Department of Physics and Astrophysics, University of Delhi, Delhi-110007*

[2]*Department of Physics, Kirori Mal College, University of Delhi, Delhi -110007*

[3]*Department of Physics, Acharya Narendra Dev College, University of Delhi, Delhi -110019*

[4]*Department of Physics, Miranda House, University of Delhi, Delhi -110007*

***Corresponding author e-mail:** asharma@physics.du.ac.in

ABSTRACT

Resistive switching (RS) devices serve as the foundation for artificial neural networks which is inspired by the biological synapse combining memory and processing. In traditional computing architecture, memory and processing units are separated, thus the information has to be moved back and forth which leads to high power consumption, poor scalability and delay in real time cognitive tasks. RS devices work on the principle that there is a change in resistance with an applied voltage. When an external voltage is applied, the device switches between high resistive state (HRS) or OFF state and low resistive state (LRS) or ON state. In RS devices, a thin insulator or semiconductor layer is sandwiched between two metal electrodes. In recent years, doped hafnium oxide based thin films are extensively explored for memory applications. In the past decade, various dopant like Al, Zr, Gd, Y, Si and so on are incorporated in hafnium oxide to enable applications such as ferroelectric memories, resistive switching and high-k dielectrics. Among other dopants, zirconium has proven to be the most suitable dopant for memory storage application. Furthermore, $Hf_{1-x}Zr_xO_2$ for x = 0.5 is an emerging candidate for resistive switching because of its scalable thickness, ferroelectric behaviour and CMOS compatibility.

In the present work, HZO ($Hf_{0.5}Zr_{0.5}O_2$) thin films are deposited via RF magnetron sputtering using commercially procured HZO target at different deposition pressures (3 mTorr, 5 mTorr, 7.5 mTorr and 10 mTorr) with a substrate temperature of 400 ˚C. The device was prepared using metal-insulator-metal (MIM) configuration where indium tin oxide (ITO) is used as bottom electrode and tungsten (W) is utilized as top electrode. It is observed that the ON - OFF ratio (RHRS/RLRS) increases with decrease in sputtering deposition pressure. RHRS/RLRS for the film deposited at 7.5 mTorr is of the order of 10 which increases to 102 for the film deposited at 5 mTorr. Structural, morphological and optical studies show that deposited thin films are of high quality. The prepared HZO thin films are highly suitable for resistive switching applications.

References:

1. Cervo Sulzbach, M., Tan, H., & Fontcuberta, J. ACS Applied Electronic Materials, 3(8) (2021), 3657–3666.

TF-008

Activation Energy Calculation for Li Doped SnO_2 Thin Films via the Arrhenius Method

Soumya Shukla[1], Rajnish Kurchania*[1], Ramarajan Ramanathan[1]*

[1] *Department of Physics, Maulana Azad National Institute of Technology, Bhopal, 462003.*

***Corresponding author e-mail:** rkurchania@gmail.com, ramarajan@manit.ac.in

ABSTRACT

Understanding activation energy in metal oxide-based semiconductors is essential for advancing optoelectronic and energy technologies, as it governs charge transport and directly influences device performance (1,2). With increasing temperature, activation energy reveals a transition from electronic to ionic conduction, underscoring its critical role in functional optimization (3,4). In this work, Lanthanum (Li)-doped SnO2 thin films were deposited on glass substrates with varying Li concentrations and systematically optimized. The structural properties of the films were analysed using X-ray diffraction (XRD), while surface morphology was examined through optical microscopy. Optical transmittance and band gap values were determined via UV–Visible spectroscopy, providing insights into the film's optoelectronic behaviour. Furthermore, temperature-dependent electrical conductivity measurements, carried out using the four-probe technique across 300 K to 680 K, enabled precise calculation of activation energy (Figure G). The results reveal significant variations in activation energy with Li doping, highlighting its importance in tailoring the electronic and ionic transport properties of SnO2 thin films for advanced applications.

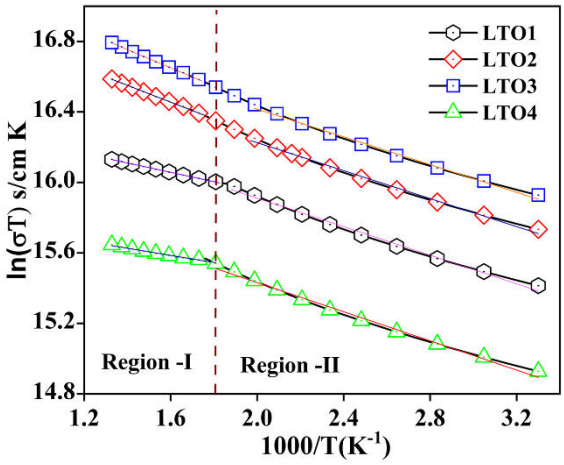


Fig. Temperature-dependent electrical conductivity of Li-doped SnO2 thin film as a function of film thickness.

References:

1. A. R. Babar, S. S. Shinde, A. V. Moholkar, C. H. Bhosale, J. H. Kim, and K. Y. Rajpure, J. Alloy. Compd., 505 (2010) 416–422.
2. R. Ramarajan, M. Kovendhan, K. Thangaraju, D. P. Joseph, and R. R. Babu, Appl. Surf. Sci., 487 (2019) 1385–1393.
3. Y. Qiang, Y. Xie, Y. Qi, P. Wei, H. Shi, C. Geng, and H. Liu, Sol. Energy, 201 (2020) 523–529.
4. C. R. Osterwald, T. J. McMahon, and J. A. del Cueto, Sol. Energy Mater. Sol. Cells, 79 (2002).

TF-009

Exploring the Dual Functionality of a Vacancy-Ordered Layered Double Perovskite ($Cs_4MnBi_2Cl_{12}$) as an Efficient Red Phosphor and UV Photodetector

Nalini Ravi, Prakash Kanapathi, Tamilselvan Appadurai*

LEEP Device Research Group, Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India - 603 203.

***Corresponding author e-mail**: tamilsea3@srmist.edu.in

ABSTRACT

Recent advancements in optoelectronic devices have driven intensive research into stable, lead-free semiconductors to replace highly toxic lead-based perovskites in high-performance LEDs, photodetectors, and displays, prioritising the urgent demand for sustainable technologies. In this context, lead-free halide perovskites, particularly layered double perovskites, have emerged as promising semiconductors owing to their superior photoelectric properties, such as high absorption coefficient, long carrier diffusion length, environmental friendliness, etc. Among the various lead-free HP systems, $Cs_4MnBi_2Cl_{12}$, a vacancy-ordered layered double perovskite, remains largely unexplored for optoelectronic applications despite its wide bandgap and efficient Mn^{2+} based red emission. In this work, we systematically investigate the photophysical and photodetection properties of the low-temperature hydrothermally prepared solid solution of $Cs_4MnBi_2Cl_{12}$ (HP). Primarily, structural analysis showcased the formation of the trigonal structure with $R\bar{3}m$ space group, accompanied by predominant absorption in the UV region and strong red photoluminescence. Notably, photoelectric studies including I-V characteristics exhibit a Schottky diode behaviour in a symmetric device configuration of FTO/HP/FTO. Furthermore, other photodetection studies, including photodetectivity, photoresponsivity, and sensitivity, will be studied in detail, highlighting the dual functionality of $Cs_4MnBi_2Cl_{12}$ as a red phosphor and UV photodetector for environmentally benign optoelectronic devices.

Keywords: Layered perovskite, UV photodetector, Red phosphor, Mn^{2+} emission

References:

1. Y. Ma, L. Zhang, Y. Tang, S. Wu, M. L. Tong, K. Wang, B. Zou, and M. R. Li, ACS Appl Energy Mater 4, 7513 (2021).
2. D. Y. Guo, C. X. Shan, S. N. Qu, and D. Z. Shen, Sci Rep 4, 1 (2014).

TF-010

Ultrafast Chemical Bath Deposited FeOOH Nanostructures on Nickel Foam for Efficient Alkaline Water Splitting

Elumalai Dhandapani, Gowdhaman Arumugam, Navaneethan Mani*

Nanotechnology Research Centre, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India – 603203

***Corresponding author e-mail:** m.navaneethan@gmail.com

ABSTRACT

The rational design of efficient and low-cost electrocatalysts through controlled thin-film deposition is crucial for advancing sustainable hydrogen production via alkaline water splitting. In this work, ultrafast chemical bath deposition (CBD) was employed to synthesize iron oxyhydroxide (FeOOH) nanostructured thin films directly on three-dimensional nickel foam substrates with deposition times of 2, 5, 10, and 15 s. The influence of deposition duration on surface morphology, porosity evolution, and electrocatalytic oxygen evolution reaction (OER) performance was systematically investigated. Morphological analysis revealed the formation of a sponge-like porous FeOOH network at shorter deposition times, with progressively increased pore density up to 15 s. Prolonged deposition beyond the optimal duration resulted in pore coalescence and partial structural collapse, leading to reduced electrochemically active surface area. Electrochemical measurements in alkaline media demonstrated a strong correlation between surface architecture and catalytic activity. The FeOOH film deposited for 15 s exhibited superior OER performance, delivering a low overpotential of 260 mV at a current density of 60 mA cm-2, indicating highly efficient catalytic kinetics. Furthermore, a full alkaline water-splitting device assembled using FeOOH as the anode achieved a cell voltage of 1.6 V at 10 mA cm-2, confirming excellent bifunctional performance and device-level applicability. The enhanced activity is attributed to the optimized porous, thin-film morphology, improved electrolyte accessibility, and efficient charge transfer at the FeOOH/Ni foam interface. This study highlights ultrafast CBD as a scalable and energy-efficient strategy for fabricating high-performance FeOOH thin films and underscores the importance of deposition-time-controlled surface engineering for advanced electrocatalytic applications.

References:

1. Smith J. et al., J. Mater. Chem. A, 5 (2017) 21012–21020.
2. Wang L. et al., Applied Catalysis B: Environmental, 247 (2019) 200–209.
3. Zhang Y. et al., Journal of Colloid and Interface Science, 654 (2024) 112–121.

TF-011

Microstructural Heterogeneity and Mechanical Behaviour of Inconel 690: A Nickel-Based Superalloy

N. Yogeshwaran[1], T. Dharini[1]*

[1]*Sathyabama Institute of Science and Technology, Chennai, Tamil Nadu, India, 600119.*

***Corresponding author e-mail:** dharini2110@gmail.com

ABSTRACT

In this research, the microstructure and mechanical deformation of Inconel 690 (INC690) – a nickel-based superalloy is investigated by a series of nanoindentation experiments. The macroscopic mechanical behaviour of the alloy is governed by the microstructural heterogeneities and precipitates at the grain level. Therefore, instrumented indentation at various indentation depths was performed to evaluate the nano hardness of the alloy such as hardness, reduced modulus, indentation size effect, strain tolerance, elastic recovery and resistance to plastic deformation. The load-displacement curves show a discrete pop-in event at lower indentation depths, indicating that the plastic deformation of the alloy initiates through dislocation nucleation. Analysis based on the Oliver-Pharr method indicates that prolonged aging and higher particle-volume fraction increase the nano hardness and creep resistance, simultaneously decreasing the indentation affected zone of INC690. Field Emission Scanning Electron Microscope analysis shows pile-up behaviour associated with localized plastic deformation. Overall, the combined mechanical and microstructural analysis provide a quantitative understanding of early damage initiation and the reliability of components made of INC690, especially in aerospace and nuclear industries. This study also helps in mechanical modelling and microstructural engineering of this alloy, particularly for high-temperature environments.

Keywords: Inconel 690; mechanical behaviour; nanoindentation; hardness.

References:

1. Mozafari, Amirhosein., Fu Bolin., Chalapathi Darshan., Abdolvand Hamidreza., Mat & Des. 257 (2025)1.
2. Oleksandr Pshyk, Olesya Nakonechna and Emerson Coy. ACS Appl. Mater. Interfaces 17 (2025) 36300.
3. Abo Znemah, R., Voyiadjis, G. Z., Wood, P., and Akbari, E. ASME. J. Eng. Mater. Technol. 144 (1) (2022) 011010.

TF-012

Bio-Chelating Assisted Spray Pyrolysis of Fe-Doped CeO_2 Thin Films: Structural, Optical, Magnetic, and Photocatalytic Studies

A. Joselin Akila, L. Ganesh, M. Beaula Ruby Kamalam S. Stephen Rajkumar Inbanathan*

PG & Research Department of Physics, The American college, Madurai, Tamilnadu

***Corresponding author e-mail:** stephenrajkumarinbanathan@americancollege.edu.in

ABSTRACT

Iron-doped cerium oxide (Fe–CeO_2) thin films with 2 wt% and 4 wt% Fe were successfully fabricated using a bio-chelating assisted spray pyrolysis technique for photocatalytic applications. X-ray diffraction analysis confirmed the formation of a single-phase cubic fluorite CeO_2 structure, with Fe ions effectively incorporated into the lattice at both doping levels, without secondary phase formation. Scanning electron microscopy and atomic force microscopy revealed dense, uniform, and crack-free films with controlled surface roughness and consistent thickness. Fourier transform infrared spectroscopy confirmed the presence of characteristic metal–oxygen bonding, indicating successful film formation. Optical studies using UV–Visible spectroscopy showed a gradual reduction in band gap with increasing Fe content, while photoluminescence measurements indicated suppressed electron–hole recombination due to the dopant, suggesting improved charge carrier dynamics. Magnetic properties measured by vibrating sample magnetometry revealed weak ferromagnetic behavior at room temperature, which increased with higher Fe doping, reflecting defect-mediated magnetic interactions. The photocatalytic activity of the Fe–CeO_2 thin films was evaluated through the degradation of methylene blue dye under light irradiation, and both doping levels exhibited significantly enhanced activity compared to undoped CeO_2. The observed improvements in photocatalytic and magnetic properties are attributed to Fe incorporation, defect-induced charge separation, and the favorable microstructural, optical, and morphological characteristics achieved through bio-chelating assisted spray pyrolysis. This study demonstrates that this simple and eco-friendly approach is effective for producing multifunctional Fe–CeO_2 thin films with potential applications in environmental remediation and spintronic devices.

Keywords: Fe-doped CeO2 thin films; Spray pyrolysis; Photocatalytic degradation; UV-Vis Spectroscopy; Magnetic properties; Environmental remediation

References:

1. S. Kumar, F. A. Alharthi, F. Ahmed, N. Ahmad, K. H. Chae, and K. Kumari, Ceram. Int., 47 (2021) 4012–4019.
2. L. E. L. Gana, J. Zimou, M. Addou, N. Lotfi, K. Nouneh, M. Fahoume, and M. M. Hafid, Ceram. Int., 51 (2025) 4206–4216.

TF-013

Dual-Functional MnO_2-V_2O_5 based Heterostructure Film Prepared by Pulsed Laser Deposition for Enhanced Electrochromic Supercapacitor Display

Vilya K[1], Shaik kaleemulla[2]*

[1]*Department of Physics, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamilnadu, India, 632 014*

[2]*Thin Films Laboratory, Centre for Functional Materials, Vellore Institute of Technology, Vellore, Tamilnadu, India, 632 014*

***Corresponding author e-mail:** skaleemulla@gmail.com

ABSTRACT

Inorganic oxide materials have attracted extensive research interest for their visible electrochromic behavior, making them promising candidates for use in display technologies, sensing devices, and advanced electronic systems. Nevertheless, individual inorganic electrochromic materials generally demonstrate a single-color transition, thereby constraining their spectral modulation capability in display applications. In this study, a broad-spectrum electrochromic device was developed by integrating V_2O_5 and MnO_2 heterostructure layers, fabricated through thermal and pulsed laser deposition techniques, to achieve improved color modulation efficiency and reduced energy consumption. The XRD, Raman and XPS analyses confirm the structural purity and oxidation states of the material. Cyclic voltammetry demonstrates its electrochromic capability and ion intercalation governed by diffusion-driven processes. The rod-like V_2O_5 morphology provides an enlarged active surface area, and its MnO_2 coating deposited via pulsed laser deposition significantly improves structural and electrochemical stability, sustaining performance over 5000 switching cycles. The films show improved optical modulation with faster response times and moderate efficiency, also functioning as energy-storage electrodes via redox activity.



Fig. Electrochromic switching of MnO_2 chromic layer due to redox reaction.

Keywords: Electrochromic, Manganese Oxide, Vanadium pentoxide, Heterostructure, Thin films.

References:

1. C. Zhang, S. Li, R. Wu, S. Wu, X. Wang, H. Xie, D. Yan, Y. Liu, W. Ye, C. Wang, S. Cong, Z. Wang, and Z. Zhao, Nano Lett., 24 (2024) 16360.
2. D. Ma, A. Lee-Sie Eh, S. Cao, P. S. Lee, and J. Wang, ACS Appl. Mater. Interfaces, 14 (2022) 1443.

TF-014

The Optoelectronic Performance of a Cu_2SnS_3 Photodetector at Key Wavelengths for Medical Diagnostics and Fiber Optic Communication Applications

Hosuru Satishkumar Reddy[1], Putha Kishore[1]*, D. Amaranatha Reddy[1] and M. Padmavathi[2]

[1]*Department of Sciences, Indian Institute of Information Technology Design and Manufacturing, Kurnool, AP, India-518007.*

[2]*Department of Physics, KVR GDCW Kurnool, Cluster University Kurnool, AP, India-518002.*

***Corresponding author e-mail:** kishore.photonics@iiitk.ac.in

ABSTRACT

In this work, copper–tin sulfide (CTS) nanostructures were synthesized via a solvothermal method and subsequently employed in the fabrication of metal–semiconductor–metal (MSM) photodetectors. Polyvinyl alcohol (PVA) was utilized as a surfactant, and the CTS material was dispersed and coated onto glass substrates using the drop-casting technique. Silver electrodes were deposited by thermal vapor deposition to complete the device structure. The fabricated photodetectors were characterized through current–voltage (I–V) measurements under illumination at various wavelengths. The devices exhibited responsivities of 0.08 A/W at 940 nm and 0.09 A/W at 1050 nm, with corresponding specific detectivities of 0.25 × 10^{11} Jones for boIn this work, copper–tin sulfide (CTS) nanostructures were synthesized via a solvothermal method and subsequently employed in the fabrication of metal–semiconductor–metal (MSM) photodetectors. Polyvinyl alcohol (PVA) was utilized as a surfactant, and the CTS material was dispersed and coated onto glass substrates using the drop-casting technique. Silver electrodes were deposited by thermal vapor deposition to complete the device structure. The fabricated photodetectors were characterized through current–voltage (I–V) measurements under illumination at various wavelengths. The devices exhibited responsivities of 0.08 A/W at 940 nm and 0.09 A/W at 1050 nm, with corresponding specific detectivities of 0.25 × 10^{11} Jones for both wavelengths. These results highlight the potential of CTS-based MSM photodetectors as cost-effective candidates for applications in medical diagnostics and fiber-optic communication technologies.th wavelengths. These results highlight the potential of CTS-based MSM photodetectors as cost-effective candidates for applications in medical diagnostics and fiber-optic communication technologies.

Keywords: nanostructure, solvothermal method, metal-semiconductor-metal

References:

1. Dias, S., & Krupanidhi, S. B. Materials Research Express, 3(10), 105006 (2016).

2. Yadav, S. M., & Pandey, A, IEEE Transactions on Electron Devices, 66(8), 3417-3424. (2019).

Ultrathin Hexagonal Boron Carbon Nitride Films as Universal SERS Substrate

N. Hassan[1], S. Kumar[1], R. Beeram[2], V. R. Soma[2], J. Lahiri[1],*

[1]*Department of Physics, Banaras Hindu University, Varanasi, Uttar Pradesh, India 221005*

[2]*School of Physics and DIA-CoE, University of Hyderabad, Hyderabad, Telangana, India 500046,*

***Corresponding author e-mail:** jl.physics@bhu.ac.in

ABSTRACT

Surface-enhanced Raman spectroscopy (SERS) is a powerful analytical technique for the detection of trace analytes. In this study, we demonstrate that ultra-thin, highly crystalline hexagonal Boron Carbon Nitride (hBCN) films can be used as a robust SERS substrate. These hBCN films were synthesized on Cu foil using atmospheric pressure chemical vapor deposition (APCVD). Four model dyes, Methylene Blue (MB), Crystal Violet (CV), Nile Blue (NB), and Rhodamine 6G (R6G), were used to systematically investigate the performance of the hBCN substrate on Raman scattering enhancement. We observed the highest enhancement for R6G with an analytical enhancement factor of 8.9 × 105, at least one order higher than the other dyes. We could detect very low concentrations of R6G dye molecules till 10-8 M. We conducted tests to check the uniformity, reproducibility, and recyclability of the hBCN substrates. Reproducibility tests conducted on 5 different samples from different batches showed minimum variation in Raman signals. The hBCN substrates could be recycled up to 5 times with only 10 % loss in intensity, beyond that there was a reduction of Raman signals by 50 %. The films retained the SERS performance after heating at 450 ◦ C and exhibited negligible degradation even after 180 days of ambient exposure, outperforming graphene and metallic SERS substrates in long-term and high-temperature stability. We demonstrate a synergistic enhancement when silver nanoparticles prepared using femtosecond laser pulses were used in conjunction with these substrates1.

References:

1. N. Hassan et al., Sens. Actuators A: Phys., 397 (2026) 117237.

Effect of Post-Deposition Annealing on the Structural, Morphological, Optical, and Electrical Properties of $Cd_{1-x}Mn_xS$ Thin Films

Himanshu Sharma Pathok[1]*, Padma Pani Shahu[1], Prasanta Kumar Saikia[1]

[1]Thin film laboratory, Department of Physics, Dibrugarh University, Dibrugarh-786004, Assam, India

***Corresponding author e-mail:** hspathok@gmail.com

ABSTRACT

Ternary $Cd_{1-x}Mn_xS$ thin films were fabricated using a cost-effective chemical bath deposition technique, and the influence of post-deposition annealing at 150°C, 200°C, and 250°C on their structural, morphological, optical, and electrical characteristics was systematically examined. X-ray diffraction analysis confirmed the polycrystalline nature of both as-deposited and annealed films, revealing a cubic zinc blende phase with a pronounced enhancement in crystallinity at elevated annealing temperatures. Field-emission scanning electron microscopy demonstrated uniform, crack-free, and well-adherent films consisting of nearly spherical nanograins, with a progressive reduction in porosity upon annealing. Optical studies using UV–Vis spectroscopy revealed high transmittance in the visible region, accompanied by an increase in absorbance and a gradual narrowing of the optical band gap from 2.932 ± 0.002 eV to 2.736 ± 0.003 eV with increasing annealing temperature. Electrical characterization under both dark and illuminated conditions revealed a marked decrease in resistance and resistivity, confirming the semiconducting and photoconductive nature of the films. The observed enhancement in electrical conductivity with annealing temperature underscores the pivotal role of post-deposition annealing in tailoring the physicochemical properties of $Cd_{1-x}Mn_xS$ thin films for advanced optoelectronic applications

Keywords: Thin film, Cd_{1-x} Mn_xS, chemical bath deposition, absorbance, optical band gap

Tunable Photoresponse of Solution-Processed Cd-doped CuI/Si Self-Powered Photodetectors

Naga Lakshmi Kappala, Rajesh Kumar Thanneeru, I. Tejaswi1, Murtaza Bohra,

Anil Annadi*

Department of Physics, Ecole´ Centrale School of Engineering, Mahindra University.

Bahadurpally, Jeedimetla, Hyderabad, Telangana 500043, India.

***Corresponding author e-mail:** anilannadi@gmail.com

ABSTRACT

Herein, solution-processed earth-abundant CuI films are employed for low-cost photodetectors and variations in the elemental composition are highly relevant to photo detector properties. Cadmium-doped copper iodide (Cd: CuI) thin films were successfully fabricated using a dip-coating technique, which offers a simple, low-cost, and scalable fabrication route. Structural and optical studies confirm the formation of Cd-incorporated CuI films with good uniformity. The fabricated films were employed to realize a p-Cd: CuI/n-Si heterojunction, and their ultraviolet (UV) photodetection performance was systematically investigated under illumination at 365 nm and 254 nm wavelengths. Devices exhibit a pronounced photo response with a clear distinction between dark and illuminated states. Notably, the device with 5% Cd doping into CuI exhibits the best performance in terms of ON/OFF current ratio, nearly four orders of magnitude under zero-bias conditions, and good responsivity of 70 mA/W at light intensity of 13 mW/cm2 (365 nm) demonstrating self-powered operation. The enhanced UV photo response is attributed to efficient charge separation at the heterojunction interface and improved film quality resulting from cadmium doping. These results highlight the potential of dip-coated Cd: CuI thin films as promising candidates for low-power, self-powered UV photodetector applications.

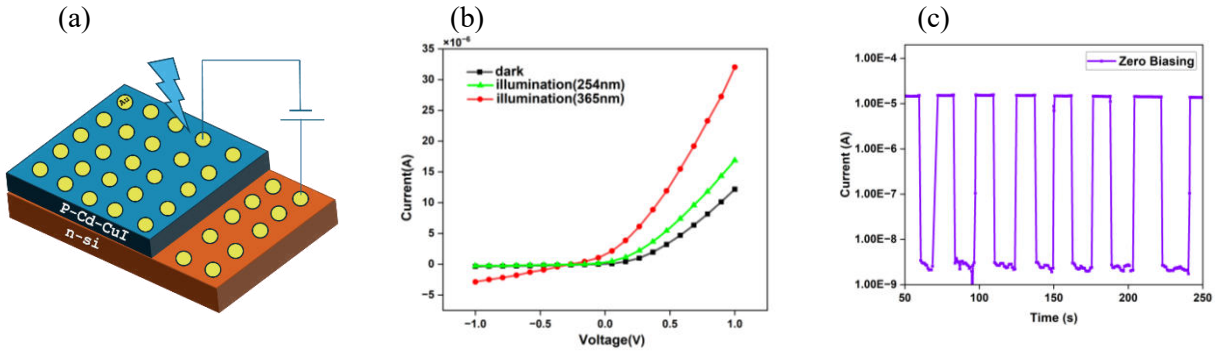


Fig. (a) p-n junction diode constructed with p-Cd:CuI/n-Si thin films (b)I-V curves of the heterojunction diode measured in the dark and under illumination (c) Photo response at zero biasing under illumination of 365 nm.

TF-018

A Review of Ice-Resistant Coatings Enabled by Carbon Nanotube Composites

Monika Tarnowska[1], Artur P. Terzyk[2], Joanna Kujawa[3], Sławomir Boncel[1]*

[1]*Silesian University of Technology, Faculty of Chemistry, Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, NanoCarbon Group, Gliwice, Poland, 44-100*

[2]*Nicolaus Copernicus University in Torun, Department of Chemistry, Physicochemistry of Carbon Materials Research Group, Torun, Poland, 87-100*

[3]*Nicolaus Copernicus University in Torun, Chair of Physical Chemistry and Physiochemistry of Polymers, Torun, Poland 87-100*

***Corresponding author e-mail:** slawomir.boncel@polsl.pl

ABSTRACT

Ice accumulation remains a critical challenge for infrastructure systems, including aviation, power transmission, wind power plants, and telecommunications. Recent advances in nanomaterials have positioned carbon nanotubes (CNTs) as key enablers in the development of high-performance anti-icing and de-icing coatings. Owing to their outstanding thermal, electrical, and surface properties, CNTs support both passive icephobic strategies and active deicing.[1]

Here, we critically analyze the incorporation of pristine and chemically modified CNTs into functional coating systems, focusing on synthesis routes, surface engineering strategies, performance metrics, and underlying ice-mitigation mechanisms reported between 2016 and 2025.[2] Among superhydrophobic, photothermal, and electrothermal strategies, the most effective are hybrid approaches combining photothermal and superhydrophobic properties, which can achieve even 250 times longer droplet freezing time.[3] Particular attention is given to the relationship between coating efficiency and the physicochemical characteristics of CNT surfaces. These interactions are interpreted using the Hansen Solubility Parameters (HSP) framework as a predictive tool for assessing CNT–matrix compatibility and icephobic performance.

This work provides insight into the rational design of scalable, durable, and climate-resilient CNT-based anti-icing and de-icing coatings, highlighting future directions for advanced ice-mitigation technologies.

References:

1. Yizhou Shen, Xinghua Wu, Jie Tao, Chungling Zhu, Yuekun Lai, Zhong Chen, Prog. Mater. Sci. 103 (2019) 509-557.
2. Monika Tarnowska, Artur P. Terzyk, Joanna Kujawa, Sławomir Boncel, Mater. Horiz., Advance Article (2026)
3. Wen Sun, Yutong Wei, Yanhui Feng, Fuqiang Chu, Energy, 286 (2024) 129656.

Performance Study of Two Terminal Solution Processed Al Doped ZnO Thin Films for UV Sensing.

I. Tejaswi [1], Rajesh Kumar Thaneeru[1], Naga Lakshmi. K[1], Souradyuti Ghosh[2,3], Murtaza Bohra[1], Anil Annadi[1,3]*

[1]*Department of Physics, Ecole Centrale School of Engineering, Mahindra University, Hyderabad 500043, Telangana, India*

[2]*Centre for Life Sciences, Mahindra University, Hyderabad 500043, Telangana, India.*

[3]*Interdisciplinary Center for Nanosensors and Nanomedicines, Mahindra University, Hyderabad 500043, Telangana, India*

***Corresponding author e-mail:** anil.annadi@mahindrauniversity.edu.in

ABSTRACT

Thin film sensing technology has been extensively researched so as to make miniaturized smart sensors for various applications. Sol-gel dip coating method was used to deposit ZnO thin films with various Al doping concentrations. By controlling the molar concentration, dip speed, and choice of stabilizers (DEA, MEA), thin films as thin as 40 nm were achieved with excellent electrical properties. Surface morphology was analyzed with FE-SEM, which reveals that the particle size decreases with Al doping, consistent with the XRD data. Thin films with 1% and 2% Al doping have shown excellent sensitivity to UV sensing at 365nm and 254nm wavelengths with tunable Responsivity and good current ON/OFF ratio.

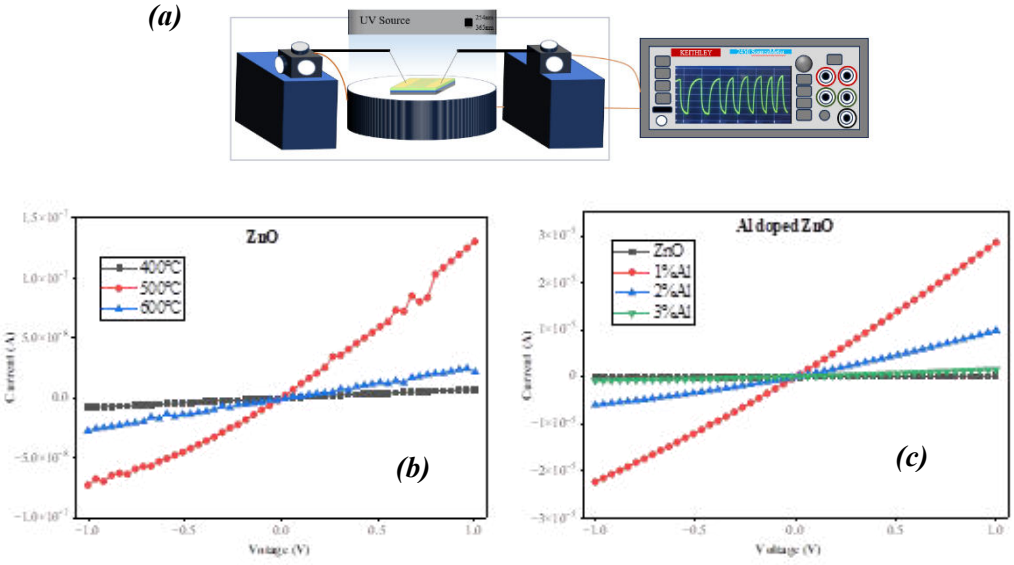


Fig. 1 (a) Schematic of the sensing station. All the current vs voltage and current vs time are measured using Keithley 2450 source meter. I vs V under 365nm wavelength (b) ZnO at different annealing temperatures (c) Al doped ZnO at 500°C

Keywords: DEA, Sol Gel, Al Doped ZnO.

References:

1. Shivank Sahu, Mitradip Bhattacharjee.,Sensors and Actuators A: Physical.,383(2025)
2. Nowak E, Chłopocka E, Szybowicz M, Stachowiak A, Koczorowski W, Piechowiak D, Miklaszewski A., Gels. 8(8):512 (2022)

Opto-Electrical Optimization of Semi-Transparent Perovskite Tandems Using Advanced Interconnecting Layers via SETFOS

Anurag Chandrakar*, Ayush Khare

Thin Film Research Laboratory, Department of Physics, National Institute of Technology Raipur, GE Road, Raipur - 492010, India.

***Corresponding author e-mail:** anuragchandrakar1997@gmail.com

ABSTRACT

In recent years, tandem solar cells have garnered intense research interest as they exceed the Shockley-Queisser limit of single-junction devices through monolithic integration of a wide-bandgap top cell and a narrow-bandgap bottom cell, leveraging complementary bandgap energies to broaden light absorption and boost power conversion efficiency (PCE). Current lead-based perovskite solar cells face critical challenges from lead toxicity and environmental hazards, prompting the search for sustainable alternatives. Lead-free $Cs_2AgBiBr_6$ addresses these issues by replacing lead, offering a 2.05 eV wide bandgap for strong visible light absorption, superior structural stability, and reduced ecological impact, making it ideal as the top-cell absorber paired with a Si bottom cell in a novel two-terminal all-inorganic tandem.

Interconnecting layers (ICLs) play a crucial role in monolithic tandem solar cells by enabling current matching, efficient tunnel junction formation, and optical transparency across subcells. This study systematically evaluates ICL variants, including ITO, FTO, IZO, and AZO to optimize top-subcell semitransparency and overall optoelectronic performance. Numerical simulations using Semiconducting Thin Film Optics Simulation (SETFOS) model the CABB-based top subcell (with SnO_2 ETL and Spiro-OMeTAD HTL) paired with a Si bottom subcell, leveraging complementary bandgaps to enhance light absorption and power conversion efficiency while probing ICL impacts on device physics. Computations encompass electrical metrics such as J-V characteristics, photovoltaic parameters, charge carrier densities, electric fields, and recombination rates, alongside optical analyses including EQE/IQE, absorption/reflectance/transmittance spectra, and SIER/SIA values. The analysis also quantifies parasitic losses, providing actionable insights to enhance efficiency and stability in tandems for scalable photovoltaic applications.

References:

1. M. R. Fitzsimmons, B. Roose, Y. Han, T. Kang, Y. Chiang, C. Huang, Y. Lu, T. C. Yang, C. Chosy, S. Guan, and M. Anaya, ACS Energy Lett. 10 (2025) 713.
2. J. Jhou, A. Gaurav, H. Lin, and C. Lin, ACS Appl. Energy Mater. 6(2023) 9434.

Enhanced Magnetic Anisotropy and Dual Magnetoresistance in LSMO Thin Films Induced by Interface Effects on (001) Si Substrates

Sandip Kumar Padhi[1], Santosh Kumar Sahu[1], Rasmi Ranjan Mohapatra[1], Umesh Kumar Sinha[1], and Prahallad Padhan[1]

[1]*Department of Physics, Nanoscale Physics Laboratory, Indian Institute of Technology Madras, Chennai 600036, India*

***Corresponding author e-mail:** ph21d053@smail.iitm.ac.in

ABSTRACT

Magnetic oxide thin films with strong anisotropy and tunable magnetotransport properties are crucial for next-generation spintronic devices. One effective strategy for manipulating these properties is through the use of interfaces in correlated oxide systems. The interface is created by growing a series of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) films on (001) oriented silicon substrates using pulsed plasma deposition techniques. The LSMO thin films with varying thicknesses ($\leq$ 20 nm) demonstrate a strong magnetic anisotropy on the order of 106 erg/cm3, surpassing many reported heterostructures and comparable to state-of-the-art oxide thin films and metal/oxide interfaces. Analysis using the Stoner-Wohlfarth model and density functional theory (DFT) reveals that the observed anisotropy predominantly arises from shape effects and interfacial spin reordering, modulated by charge transfer at the Si–O–Mn interface, which induces non-collinear antiferromagnetic ordering of Mn ions. These highly oriented, LSMO films exhibit both positive and negative magnetoresistance (MR) in contrast to the typical colossal negative MR found in bulk LSMO. Low-field, in-plane positive MR reaches a maximum of ~7% for 12.4 nm films and ~12% for 20.0 nm films, while out-of-plane MR variation is limited to ±0.8%. Electronic structure calculations further demonstrate the absence of half-metallicity at the Si–LSMO interface due to interfacial charge transfer, the expansion of Mn–O–Mn bond angles, and a tunable Curie temperature driven by substrate-induced strain and electronic reconstruction. The unique dual sign MR, strong tunability, and anisotropic switching behaviour observed in these Si/LSMO films reveal new opportunities for the design of advanced magnetic sensors and memory devices compatible with silicon technology.

References:

1. Umesh Kumar Sinha, Antarjami Sahoo, Prahallad Padhan, J. of Alloys Compd., 952 (2023) 170035.

TF-022

White-Light Emission and Improved Electrical Performance in Graphene Oxide Modified Al-ZnO Thin Films

Veena Shivadas Kindalkar[1]*, Felcy Jyothi Serrao[2] and S. M. Dharmaprakash[3]

[1]*Department of Physics, KLS Gogte Institute of Technology, Udyambag, Belagavi, Karnataka, 590008, India*

[2]*Department of Physics, Sahyadri College of Engineering and Management, Mangaluru, Karnataka, 575007, India*

[3]*Department of Physics, Mangalore University, Mangalagangothri, Mangaluru, Karnataka, 574199, India*

***Corresponding author. e-mail:** vskindalkar@git.edu

ABSTRACT

White-light emitting transparent conducting thin films based on Al-doped ZnO (Al-ZnO) modified with graphene oxide (GO) were fabricated by a spin-coating technique, and the influence of GO concentration (15% and 25%) on their structural, optical, photoluminescence, morphological, colorimetric, and electrical properties was systematically investigated. X-ray diffraction analysis revealed that all films possess a polycrystalline hexagonal wurtzite structure with a preferred c-axis (002) orientation, while the incorporation of GO resulted in reduced crystallinity, decreased grain size, and increased lattice strain. Ultraviolet–visible spectroscopy showed high optical transparency (>85%) in the visible region, accompanied by a redshift in the absorption edge and band gap narrowing from 3.24 eV (Al-ZnO) to 3.07 eV (25%GO:Al-ZnO). Photoluminescence studies demonstrated enhanced defect-related visible emission and an increased IVIS/IUV ratio with GO addition, indicating efficient modulation of radiative recombination pathways. The chromaticity coordinates derived from CIE 1931 analysis shifted toward the white-light region with decreasing color purity, confirming a white-light emission tendency in GO-incorporated films. Field-emission scanning electron microscopy revealed uniform, crack-free surfaces with reduced particle size upon GO incorporation. Electrical measurements exhibited ohmic behavior, a significant reduction in sheet resistance, enhanced carrier concentration, and an improved figure of merit, with the 25%GO:Al-ZnO film showing the highest electrical conductivity of 1.49 S m^{-1}. The combined optical and electrical enhancements demonstrate that GO-modified Al-ZnO thin films are promising candidates for white-light optoelectronic and transparent conducting applications.

References:

1. Nath, D., Mandal, S. K., Deb, D., Rakshit, J. K., Dey, P., & Roy, J. N., J. Appl. Phys. 123, (2018) 95115.
2. Wang, X., Zhi, L. & Müllen, K., Nano Lett. 8, (2008), 323–327.
3. Paul, R., Gayen, R. N., Biswas, S., Bhat, S. V. & Bhunia, R., RSC Adv. 6, (2016), 61661–61672.

AI-Driven Structural Analysis of Native Defects in Atomically-Thin $Mo_{1-x}W_xS_2$

S Pooja[1], Senthil Kumar Eswaran [1*]

[1]*2D Materials and Devices Laboratory (2DML), Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST),*

Kattankulathur- 603 203, India

***Corresponding author e-mail:** senthile2@srmist.edu.in

ABSTRACT

Defect Engineering is a crucial degree of freedom for manipulating the optical and electrical properties of atomically-thin transition metal dichalcogenides (TMDs). However, native defects, including sulfur vacancies, antisites, line defects, and grain boundaries, are inherently unavoidable and are often unintentionally introduced during synthesis. Their formation is governed by relatively low formation energy and favorable chemical potentials, including temperature, metal/chalcogen ratio, precursor flow dynamics, growth substrates, and substrate effects. In this study, we thoroughly explore the nature of native defects in metal-organic chemical vapor (MOCVD) deposited pristine MoS_2 and $Mo_{1-x}W_xS_2$ monolayers utilizing High-Resolution Transmission Electron Microscopy (HRTEM). We further demonstrate that the obtained structural and statistical data can be readily passed on to computational and analytical tools.Comprehensive structural analysis uncovers significant insights into the relationship between local strain distribution and the emergence of native defects, enhancing the comprehension of defect-strain coupling mechanisms in two-dimensional TMD materials.

Keywords: 2D materials, metal-organic chemical vapor deposition, transition metal dichalcogenides, molybdenum disulfide, defects.

References:

1. Murugan, Vijaykumar, and Senthil Kumar Eswaran, et al. *ACS Applied Nano Materials* 8.14: 6849-6856(2025).
2. Lin, Zhong, et al. 2D Materials 3.2: 022002(2016).
3. Sitek, Jakub, et al. *Scientific Reports* 15.1: 28517(2025).

Tailored MoO_3-V_2O_5 Composite Thin Films for Functional Devices

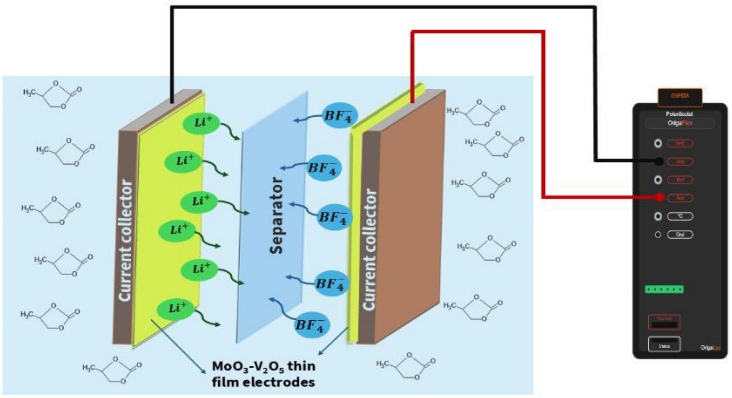
Revansiddappa, Gokul R, Anuragh B, Mahesha M.G*

Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, 576104, India

*** Corresponding author e-mail:** mahesha.mg@manipal.edu

ABSTRACT

Transition metal oxide electrodes offer high theoretical capacitance for electrochemical energy storage, yet their practical application is fundamentally constrained by chemical instability in aqueous electrolytes, where high valence metal centers undergo rapid hydrolytic dissolution. Here, we prepared MoO_3-V_2O_5 heterostructured thin films across the full compositional range to elucidate the coupled roles of lattice chemistry, interfacial structure, and electrolyte environment in governing pseudocapacitive performance. Structural characterization reveals a composition dependent evolution from well ordered orthorhombic phases in the pure oxides to highly strained heterostructures at intermediate compositions, where lattice mismatch between Mo-O and V-O polyhedra generates defect rich Mo-O-V interfacial bonding. We employ an aprotic organic electrolyte ($LiBF_4$ in propylene carbonate), which suppresses hydrolytic degradation pathways and enables stable operation over an expanded electrochemical window. Under these conditions, V-rich heterostructures exhibit pronounced pseudocapacitive behavior, with the M20 composition delivering the highest capacitance, fast charge-discharge kinetics, and long term cycling stability exceeding 5000 cycles in a symmetric device configuration. These results demonstrate that electrolyte selection is as critical as materials design in oxide based supercapacitors and establish a stable, high performance pseudocapacitive energy storage system.



References:

1. M. Krichen, Y. Basheer, S. M. Qaisar, A. Waqar, Energies 16 (2023) 2271.
2. J. Mitali, S. Dhinakaran, A. A. Mohamad, Energy Storage 5 (2022) 100073.

Ion Beam Induced Modulation of $ZnTiO_3$ Thin Films for Next Generation Optoelectronics

Priya Mittal[1], Ashish Yadav[1], Kamlendra Awasthi[1], Vaibhav Kandwal[2], Govind Gupta[2], M. Durga Ganesh[3], Pamu Dobbidi[3], Srinivasa Rao Nelamarri[1*]

[1] *Department of Physics, Malaviya National Institute of Technology Jaipur, J.L.N. Marg, Jaipur, 302017, Rajasthan, India*

[2] *CSIR-National Physical Laboratory, K.S. Krishnan Marg, New Delhi, 110012, India*

[3] *Department of Physics, Indian Institute of Technology Guwahati, Guwahati 781039, Assam, India*

***Corresponding author e-mail:** srnelamarri.phy@mnit.ac.in

ABSTRACT

Ion implantation is a powerful technique for tailoring the properties of oxide thin films for advanced optoelectronic applications. In this talk, we present a systematic investigation of the effect of 100 keV Ni ion implantation on the structural, morphological, and optical properties of $ZnTiO_3$ thin films, implanted at three fluences: 1×10^{14}, 1×10^{15}, 1×10^{16} ions/cm^2. Ni ion incorporation plays a key role in tailoring the lattice structure and band gap of $ZnTiO_3$ films by modifying their electronic structure and defect states. Structural analysis done using X-ray diffraction (XRD) reveals a significant, gradual decrease in crystallinity, with pronounced amorphization observed at 1×10^{16} ions/cm^2, due to defect-induced lattice distortion and the incorporation of Ni ions into the matrix. Atomic force microscopy (AFM) shows an increase in surface roughness from 5.51 nm (pristine) to 5.78 nm at 1×10^{15} ions/cm^2 due to enhanced adatom mobility and ion-induced sputtering, followed by a decrease at 1×10^{16} ions/cm^2. Optical measurements indicate a continuous decrease in transmittance and a red shift of the absorption edge with increasing ion fluence, leading to bandgap narrowing from 4.02 eV (pristine) to 3.47 eV (1×10^{16} ions/cm^2). The observed optical change is attributed to implantation-induced lattice damage, defect generation, and increased Urbach energy, signifying enhanced structural disorder and band-tail state formation. Photoluminescence (PL) spectra exhibit a strong peak ~380 nm emission with a weak shoulder around 307 nm, corresponding to defect-related states and band to band transition, respectively. The increasing PL intensity with ion fluence indicates enhanced oxygen-vacancy concentration arising from lattice disorder. The ability to control the bandgap and defect states via Ni ion implantation makes $ZnTiO_3$ a promising candidate for UV optoelectronic devices.

TF-026

Silk Fibroin–PVA Bio-Composite Films as a Platform for Algal Immobilization in Wastewater Treatment and Biosensing Application

Bhakti Jagdale, Komal Jain, Shravani Pagare*, Parth Bakal*

MIT World Peace University, Pune, Maharashtra, India, 411038

***Corresponding author e-mail:** shravani.pagare@mitwpu.edu.in, parth.bakal@mitwpu.edu.in

ABSTRACT

This research explores the development of a novel bio-composite film designed for the removal of heavy metal contaminants from aqueous environments. The matrix was synthesized by extracting silk fibroin (SF) from *Bombyx mori* cocoons through a $NaHCO_3$ degumming process. This regenerated silk solution was then blended with Polyvinyl Alcohol (PVA) at concentrations of 2% to 7% to optimize the mechanical flexibility and stability of the resulting films.

By immobilizing algae cells within the SF/PVA blend, a bioactive film was fabricated. The structural characteristics of these composite films were evaluated using Scanning Electron Microscopy (SEM). SEM analysis provided critical insights into the surface topography and the distribution of algae within the polymer matrix. The integration of PVA served to bridge the inherently brittle fibroin chains, creating a robust, biodegradable scaffold that maintains the viability of the algae. These findings suggest that the SF/PVA/Algae films are a highly effective and sustainable platform for immobilization of algae cells. Such bio-composite systems show significant potential for applications in wastewater treatment and the development of whole-cell biosensors.

References:

1. Y. Liu, H. Shao, X. Liu, and J. Hu, J. Hazard. Mater., 424 (2022) 127–135.
2. K. Wang, S. Hazra, M. Basu, and J. Kundu, Int. J. Biol. Macromol., 151 (2020) 879–889.
3. M. Han, Y. Wang, L. Xu, and Q. Jin, Water Res., 215 (2022) 118257.
4. S. Kundu, S. C. Kundu, and J. Kundu, Biosens. Bioelectron., 165 (2020) 112345.

TF-027

Development of an Electron Beam–Pumped, Localized Surface Plasmon–Enhanced Nanoscale Light Source for Electron-Beam–Assisted Optical Microscopy

Atsushi Nakamura*, Shunpei Shiba, Kei Hosomi, Atsushi Ono, Yoshimasa Kawata, and Wataru Inami

Research Institute of Electronics, Shizuoka University, 3-5-1 Johoku, Hamamatsu, 432-8011 Shizuoka, Japan,

***Corresponding author e-mail:** nakamura.atsushi@shizuoka.ac.jp

ABSTRACT

We demonstrated LSP-enhanced cathodoluminescence (CL) from an ALD-grown $Al_2O_3/ZnO/Al_2O_3$ heterostructure incorporating Ag nanoparticles, aiming to develop a bright nanoscale light source for an EXA optical microscope. The observed luminescence enhancement is attributed to LSP–exciton coupling and the refractive-index gradient of the heterostructure, which improves light-extraction efficiency.

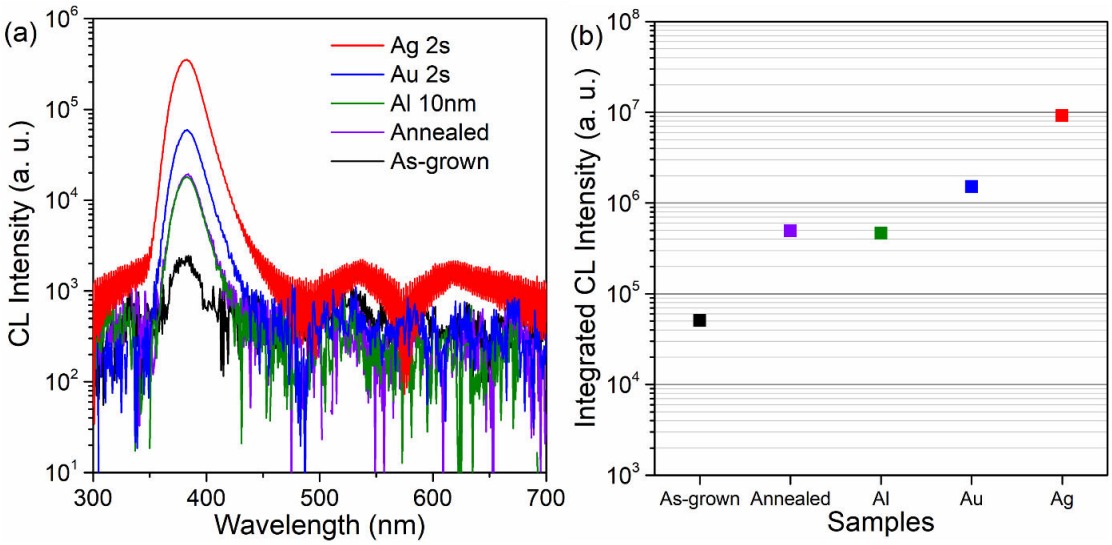


Fig. 1 (a) Comparison of CL spectra for $Al_2O_3/ZnO/Al_2O_3$ heterostructures at different stages of growth/annealing/encapsulation of metals. (b) Comparison of integrated CL intensity for $Al_2O_3/ZnO/Al_2O_3$ heterostructures at different stages of growth/annealing/encapsulation of metals. For the CL measurement, the acceleration voltage was 30 kV and the beam current was 300 nA.

Keywords: Localized surface plasmon; Cathodoluminescence; Atomic layer deposition

References:

1. Nakamura, S. Shiba, K. Hosomi, A. Ono, Y. Kawata, and W. Inami, Microscopy, 74 (2025) 71–77.

TF-028

Hybridizing SnS and G-C_3N_4 for Self-Powering Ultrafast UV-NIR Photodetectors for Environmental Monitoring

Bhavasree Sreedhar[1], Nivin Thulasibai Sasidharan[2], Arbacheena Bora[3], Karthigeyan Annamalai[2], Yuvaraj Sivalingam[3], Elangovan Elamurugu*[1]

[1]*iDARE Laboratory, Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603 203, Tamil Nadu, India*

[2]*Hydrogen Storage Materials and Nanosensors Laboratory, Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603 203, Tamil Nadu, India*

[3]*Laboratory of Sensors, Energy and Electronic Devices (Lab SEED), Department of Physics and Nanotechnology, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603 203, Tamil Nadu, India*

***Corresponding author e-mail:** elangove@srmist.edu.in, eevan2003@yahoo.co.in

ABSTRACT

Fabrication of ultrafast responsive broadband photodetectors is challenging since they are mutually exclusive. This challenge is tackled by hybridizing tin sulfide (SnS) and graphitic carbon nitride (g-C_3N_4). When Vis-NIR sensitive SnS and UV-Vis sensitive g-C_3N_4 are hybridized, the photodetection window is extended across UV-Vis-NIR region with ultrafast responsivity. The hybrids are prepared using various concentrations of g-C_3N_4 (0.5 - 15 wt.%) through ultrasonication and coated on p-Si substrates to device photodetectors. Among which 1 wt.% g-C_3N_4 doped SnS sample (named SG-1) exhibited a strong photocurrent (-2.24 μA) even at zero bias, indicating the self-powering nature. SG-1 showed a detectivity of 1.9×10^9 Jones (~9× of SnS) and a responsivity of 2.8 mA W^{-1}. It also showed ultrafast rise and decay times of 0.48 ms and 0.47 ms, respectively, at 500 Hz. Enhancement of photocurrent is confirmed using scanning Kelvin probe measurements. The achieved performance evidence that SnS/g-C_3N_4 hybrids are promising for next-generation self-powered broadband photodetectors.

References:

1. P. Sreekala A, B. Krishnan, F. C. Pelaes R, D. A. Avellaneda, J. A. Aguilar-Martínez, and S. Shaji, Appl. Surf. Sci., 609 (2023) 155277.
2. Z. Lv, S. Yan, W. Mu, Y. Liu, Q. Xin, Y. Liu, Z. Jia, and X. Tao, Adv. Mater. Interfaces, 10 (2023) 2202130.
3. H. Yu, Y. Xie, J. Wei, P. Zhan, and Z. Cui, Adv. Mater. Interfaces, 9 (2022) 2200896.

TF-029

TF Investigations on Structural and Magnetic Properties of Fe-Ga Thin Films Grown in Presence of External Magnetic Field

K. Sai Maneesh[1,2*], Himalay Basumatary[2], M. Manivel Raja[2], Radhika Chada[1],

[1]*Department of Mechanical Engineering, Kakatiya University, Warangal, India.*

[2] *Advanced Magnetics Group, Defence Metallurgical Research Laboratory, Hyd. India.*

***Corresponding author e-mail:** maneeshkundhojjala@kakatiya.ac.in

ABSTRACT

Magnetostrictive Fe-Ga thin films gained attention of researchers due to their large spectrum of applications in actuators, MEMS, energy harvesting devices and sensors [1,2]. Major advantages of Fe-Ga films include superior magnetic properties combined with features like corrosion resistance, magnetostriction, machinability and mechanical properties. [3-5]. Fe-Ga thin films were widely studied under different deposition conditions. However, understanding the film densification, magnetic behaviour is important especially when magnetic Fe-Ga films with non-magnetic underlayers were deposited in presence of external magnetic field. The present study investigates the magnetic and structural properties of Fe–Ga thin films deposited on Si substrates under an external magnetic field, with and without non-magnetic buffer layers (Cu and Ta) and varying film thickness. X-ray diffraction revealed crystallization in the BCC A2 phase across all films. At low thickness, buffer-layered films exhibited preferred (110) orientation, while modified Williamson–Hall analysis indicated tensile residual stress. X-ray reflectivity provided estimates of layer density and roughness, showing that low-thickness films on Si had high density, whereas Ta-buffered films were rougher. At higher thickness, Ta-buffered films exhibited increased density, while direct Si-deposited films showed elevated roughness. Magnetic characterization revealed that saturation magnetization correlated positively with film density and inversely with oxide layer thickness. At low thickness, films on Si exhibited higher saturation magnetization, while at higher thickness Ta-buffered films dominated. Coercivity varied inversely with tensile residual stress and systematically with film roughness. These findings highlight the interplay of buffer layers, thickness, and structural features in tailoring the magnetic behaviour of Fe–Ga thin films.

References:

1. L. Shu, G. Wu, D. Chen, and M. J. Dapino, Smart Mater. Struct., 25 (2016) 035046.
2. Y. Kim and Y. Y. Kim, Sens. Actuators A Phys., 133 (2007) 447–456.
3. M. Niu, B. Yang, Y. Yang, and G. Meng, Precis. Eng., 66 (2020) 255–268.
4. L. Shu, J. Yang, B. Li, Z. Deng, and M. J. Dapino, Syst. Signal Process., 139 (2020) 106418.
5. Y. Torii, H. Wakiwaka, T. Kiyomiya, Y. Matsuo, Y. Yamada, and M. Makimura, J. Magn. Magn. Mater., 290–291 (2005) 861–864.

TF-030

Preparation of garnet-type sacrificial layer for free-standing single-crystalline thin film of solid electrolyte LLZTO

Akito Machino[1*], Naonori Sakamoto[1], Naoki Wakiya[1], and Takahiko Kawaguchi[1]

[1]*Department of Engineering, Graduate School of Integrated Science and Technology, Shizuoka Univ.,3-5-1 Johoku, Chuo-ku, Hamamatsu, 432-8561, Japan*

***Corresponding author e-mail:** takahiko.kawaguchi@shizuoka.ac.jp

ABSTRACT

Garnet-type $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$(LLZTO), which exhibits high ionic conductivity (10^{-4} to 10^{-3} S/cm), has attracted significant attention as a solid electrolyte for oxide-based all-solid-state lithium-ion batteries. To enhance battery power and suppress internal short-circuits, the fabrication of free-standing solid electrolyte single-crystalline membranes is highly desirable. In this study, we focused on $Ca_3Sn_2TiFe_2O_{12}$(CTTIG) as a candidate for a garnet-type sacrificial layer that is soluble in acid and possesses a small lattice mismatch with LLZTO. CTTIG thin films were deposited on $Gd_3Ga_5O_{12}$ (GGG) (001) substrates using dynamic aurora pulsed laser deposition (PLD). Subsequently, LLZTO thin films were grown on the CTTIG layer using the LiOH flux liquid phase epitaxy (LPE) method. X-ray diffraction (XRD) analysis revealed that both CTTIG and LLZTO layers were epitaxially grown on the GGG substrate, with the {224} pole figure exhibiting fourfold symmetry. Furthermore, cross-sectional SEM images confirmed that the LLZTO thin film formed a continuous layer with a nearly flat interface. These results indicate that by dissolving the CTTIG layer, a submicrometer-thick LLZTO single-crystalline membrane with high ionic conductivity can potentially be obtained.

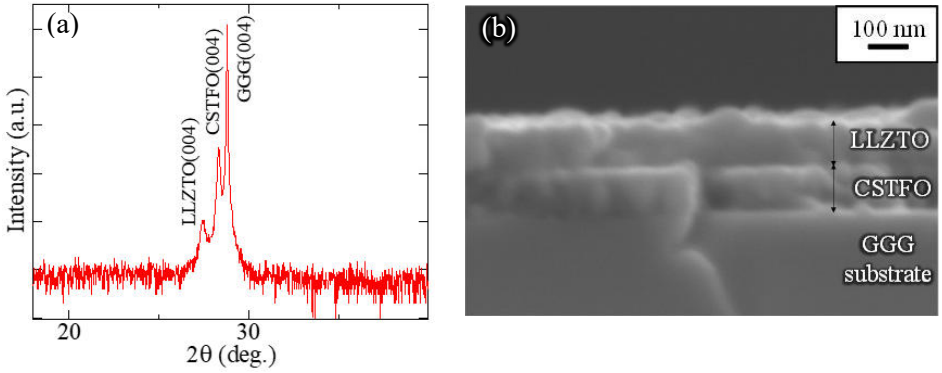


Fig. 1 (a) XRD pattern of LLZTO/CTTIG thin film grown on GGG (001) substrate, (b) Cross-sectional SEM image of LLZTO/CTTIG thin film grown on GGG (001) substrate.

Keywords: LLZTO, sacrificial layer, epitaxial thin film, PLD, garnet structure

References:

1. M. Moriya *et al., J. Ceram. Soc. Jpn.,* **133**, 343-348 (2025). (2025).
2. B. Cartie *et al.*, *J. Mater. Sci. Lett.*, **11,** 1163-1164 (1992).

TF-031

Influence of Lattice Volume on the Electrical Conductivity of Spinel-Type Transparent Oxide Thin Films Fabricated via Pulsed Laser Deposition

T Ragavi[1], Akifumi Wada[1], K Gunasekaran[2], Praveenkumar P[1], Takahiko Kawaguchi[1], Naonori Sakamoto[1,2,3], S Harish[4], M Krishna Mohan[5], Naoki Wakiya*[1,2,3]

[1]*Graduate School of Science and Technology, Shizuoka University*

3-5-1 Johoku, Naka-ku, Hamamatsu, 432-8011 Japan

[2]*Research Institute of Electronics, Shizuoka University,*

3-5-1 Johoku, Naka-ku, Hamamatsu 432-8561, Japan

[3]*Graduate School of Integrated Science and Technology, Department of Engineering, Shizuoka University,*

3-5-1 Johoku, Naka-ku, Hamamatsu 432-8561, Japan

[4]*Nanotechnology Research Center, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India*

[5]*Center of Excellence in Materials and Advanced Technologies (CeMAT), SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India*

***Corresponding author e-mail:** wakiya.naoki@shizuoka.ac.jp

ABSTRACT

Transparent conductors have been extensively investigated to combine electrical conductivity with optical transparency in thin metal oxide layers. Spinel structured oxides (AB_2O_4) especially wide bandgap spinel structured semiconductors have emerged as promising candidates for transparent and conductive oxide systems. Among these, ZnO and SnO_2 based compounds are particularly attractive due to their low cost and natural abundance. Zn_2SnO_4, a spinel type transparent conducting oxide, has demonstrated electrical conductivities on the order of 100 Scm^{-1}. Epitaxial growth, in which the film crystallographic orientation is aligned with that of the substrate, offers a pathway to enhance structural quality and functional properties. In this work, we investigate the relationship between electrical conductivity and lattice volume in Zn_2SnO_4 spinel thin films deposited without rare metals by pulsed laser deposition. By optimizing deposition conditions, we clarify how structural variations, particularly changes in lattice volume, influence the electrical performance of Zn_2SnO_4 transparent conductive films.

Keywords: Spinel structure, transparent conducting oxide, lattice volume, epitaxial growth, thin film

References:

1. G. Socol, M. Socol, N. Stefan, E. Axente, G. Popescu-Pelin, D. Craciun, L. Duta, C.N. Mihailescu, I.N. Mihailescu, A. Stanculescu, D. Visan, V. Sava, A.C. Galca, C.R. Luculescu, V. Craciun, *Applied surface science* **260** (2012).

TF-032

Matrix-Composition-Dependent Tunnel Magnetoresistance in Co–(Ta_2O_5–Al_2O_3) Nanogranular Thin Films by Sputtering with Pressed Powder Target

Yu-Ting Chen[1], Cheng Wang[1], Nobukiyo Kobayashi[2], Shigehiro Ohnuma[2,1], and Hiroshi Masumoto*[1]

[1]*TOHOKU University, Aoba-ku district, Sendai, Japan, 980-8579*

[2]*Research Institute for Electromagnetic Materials (DENJIKEN), Tomiya, Miyagi, Japan 981-3341*

***Corresponding author e-mail:** hiromasu@fris.tohoku.ac.jp

ABSTRACT

Nanogranular thin films, consisting of ferromagnetic metal nanogranules dispersed in an insulating matrix, exhibit spin-dependent tunneling phenomena such as tunnel magnetoresistance (TMR)[1]. TMR describes the modulation of electrical resistivity (ρ) by an applied magnetic field. TMR has been widely utilized in magnetoresistive random access memories (MRAM) and magnetic sensors. Recent studies have suggested that TMR performance depends not only on the nanogranule concentration but also on the design of the insulating matrix[2]. In particular, mixed-oxide matrices have been reported to enhance TMR compared to single-oxide systems[3]. However, their compositional effects have not been systematically clarified. In this study, TMR properties of Co nanogranular thin films embedded in mixed-oxide matrices of $(Ta_2O_5)_{100-y}(Al_2O_3)_y$ were investigated. Prior to sputtering, pressed powder targets were prepared by mixing reagent-grade Ta_2O_5 and Al_2O_3 powders with y varied from 0 to 100 at.%. Using these targets together with a Co target, Co_x–$[(Ta_2O_5)_{100-y}(Al_2O_3)_y]_{100-x}$ thin films were prepared on quartz and Si(100) substrates by tandem sputtering method. After deposition, their compositions, nanostructures, ρ, magnetization, and TMR ratios were evaluated. The Co concentration x of the films was varied from 0 to 60 at.%. Transmission electron microscopy (TEM) has revealed nanogranular structures consisting of Co granules with diameters of 3–5 nm embedded in mixed-oxide matrices. ρ decreased exponentially with increasing x. All films exhibited superparamagnetic behavior, indicating the presence of nanoscale magnetic particles. The TMR ratio was strongly influenced by both x and y, and enhanced TMR of 7.6 % was observed at x = 50 at.% and y = 50 at.%.

These results demonstrate that both metallic nanogranule concentration (x) and mixed-oxide matrix composition (y) play critical roles in controlling TMR in nanogranular thin films, providing guidelines for materials design in spin-dependent tunneling systems.

References:

1. H. Fujimori *et al.*, *J. Magn. Mag. Mater.*, **304** (2006) 32-35.
2. Y. Cao *et al.*, *Acc. Mater. Res.* **6** (2025), 979-990
3. M. Yonemura *et al.*, *Jpn. J. Appl. Phys.*, **40** (2001) pp.740-745.

Curcumin-Loaded Ag-MOF@Carbon Dot Blended Agarose/PVA Nano thin film as a Synergistic Anticancer Drug Delivery Platform

Sutharsan Karunanithi [1], Kalaivizhi Rajappan [1*]

[1]*Department of Chemistry, Faculty of Engineering and Technology,*

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu-603203, India

ABSTRACT

The effective delivery of hydrophobic anticancer agents remains a major challenge in cancer therapy. In this work, curcumin-loaded Ag-MOF@carbon dot (Ag-MOF@CD)–blended agarose/poly (vinyl alcohol) (PVA) nanocomposite nanofibers were developed as a synergistic anticancer drug delivery platform. The nanofibers were fabricated via electrospinning, where PVA served as the primary spinnable matrix and low-concentration agarose enhanced bioactivity and drug retention. Ag-MOF@CDs were homogeneously distributed within the fibrous network, providing structural stability, fluorescence traceability, and reactive oxygen species (ROS) mediated cytotoxicity. Curcumin was successfully encapsulated, exhibiting sustained and controlled release behaviour. In vitro cytotoxicity studies demonstrated enhanced anticancer efficacy of the nanocomposite nanofibers compared to free curcumin, attributed to the combined effects of controlled drug release and Ag-MOF@CD-induced ROS generation, while maintaining acceptable biocompatibility toward normal cells. These findings highlight the potential of Ag-MOF@CD integrated agarose/PVA nanofibers for advanced anticancer drug delivery applications.

Keywords: nanofibers, biocompatibility, fluorescence traceability, drug release

TF-034

Impact of Interfacial Dielectric Engineering on the Performance and Reliability of HfO_2-Based NC-GAA Nanosheet FETs at the 10-nm Node for Low-Power and High-Speed Logic Applications

Chandrashekar Murthy B N[1], Prasad M[2] , U B Mahadevaswamy[1],*

[1]*Department of Electronics and Communication Engineering, JSS Science and Technology University ,Sri Jayachamarajendra College of Engineering, Mysuru, Karnataka, India - 570006*

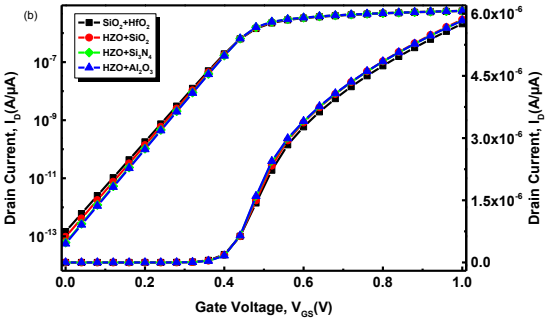
2 Department of Electronics and Communication Engineering, Nitte Meenakshi Institute of Technology, Bengaluru, Karntaka, India 56064

***Corresponding author e-mail:** mahadevaswamy@sjce.ac.in

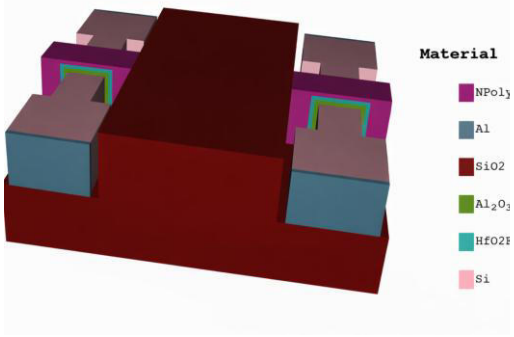
ABSTRACT

Gate symmetric -all-around nanosheet (GAA NS) field-effect transistors (FETs) and their negative capacitance (NC) counterparts were investigated at a 10 nm gate length, alongside a baseline HfO_2 + SiO_2 GAA NS FET tested at 30 nm. At V_{DS}= 0.7 V, the 10 nm conventional device exhibited a subthreshold swing (SS) of 65.24 mV/dec, drain-induced barrier lowering (DIBL) of 16 mV/V, and an on/off current ratio of 10^7. To enhance performance, a metal–ferroelectric–insulator–semiconductor (MFIS) NC-GAA NS design employing ferroelectric HfO_2 (HZO) with various interfacial dielectrics was evaluated. Among these, the HZO + Al_2O_3 configuration achieved an SS of 60 mV/dec, DIBL of 9 mV/V, and an on/off current ratio exceeding 10^8 at V_{DS}= 0.7 V, along with improved intrinsic gain, reduced gate capacitance, and higher cutoff frequency. Device stability was assessed under temperature variations from 300 K to 400 K and work function tuning between 4.6 eV and 4.8 eV. A CMOS inverter simulated at 300 K and 4.7 eV demonstrated switching, sharp transfer characteristics, and favourable transient response. These findings highlight HZO + Al_2O_3 NC-GAA NS FETs as promising candidates for low-power, high-speed nanoscale logic applications.

Keywords: Gate-All-Around (GAA), Nanosheet Field-Effect Transistor (FET), Negative Capacitance, Ferroelectric, Subthreshold Swing (SS), Drain-Induced Barrier Lowering (DIBL).



The I_D-V_{GS} characteristics with various dielectric and HZO stack (a) V_{DS}=0.1 V (b) V_{DS}=0.7 V



The Negative Capactiatnce-Gate All around NanoSheet FET CMOS inverter

TF-035

A Review of Solution-Processing Strategies for Chalcogenide Ink Formation

Deepthi G[1], P. Malar[1*]

[1]*Thin Film Photovoltaics Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203*

***Corresponding author e-mail:** *malarp@srmist.edu.in*

ABSTRACT

A vital segment of materials science is the development of solution-processed chalcogenide thin films, which aim to lower costs and enhance throughput for optoelectronic applications like Sb_2 (S, Se)$_3$ based photovoltaics. The inherent insolubility of bulk metal chalcogenides, which results from their strong covalent bonding is a significant hurdle in obtaining miscible inks. Three primary synthetic routes for generating processable inks addressed in this review.

First, "alkahest" solvent systems consisting of binary mixtures of 1,2-ethanedithiol and 1,2-ethylenediamine have demonstrated efficient dissolving of nine distinct V_2VI_3 bulk semiconductors, including Sb_2Se_3 and Sb_2S_3 at room temperature. Second, the solubility of Sb or Se metals are achieved through nucleophiles formation enabled by thiol-amine solutions. Lastly, salt precursors (such as chloride salts) are used in processes like spray pyrolysis, where they are thermally broken down in conjunction with a chalcogen source such as thiourea. By dissecting extended frameworks into distinct molecular anions, methods like "dimensional reduction" further improve solubility. Together, these techniques allow for the formation of molecular inks that is useful in the preparation of device quality crystalline thin films with very little organic residue.

Keywords: Solution-processing, chalcogenide, Ethanedithiol, Ethylenediamine.

References:

1. Webber, David H.; Brutchey, Richard L Journal of the American Chemical Society, (2013) 135(42), 15722–15725
2. McCarthy, Carrie L. Chem. Commun., (2017) 53(36), 4888–4902.
3. Zhou, Ying; Leng, Meiying; Xia, Zhe; Zhong, Jie; Song, Huaibing; Liu, Xinsheng; Yang, Bo; Zhang, Junpei; Chen, Jie; Zhou, Kunhao; Han, Junbo; Cheng, Yibing; Tang, Jiang. Advanced Energy Materials, (2014)
4. Kondrotas, Rokas; Chen, Chao; Tang, Jiang. Joule, (2018).
5. Pakdel, Amir; Guo, Quansheng; Nicolosi, Valeria; Mori, Journal of Materials Chemistry A, (2018). 6(43), 21341–21349.

TF-036

Sulfonated Cr-MIL-101 Anchored SPSEBS/PEG Polymer Blend as High-Performance Proton Exchange Membranes for Fuel Cells.

Preethi Dayalan[1], Ragasudha Sudhakaran[1] ,Paradesi Deivanayagam[1]*

[1]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur 603203, Chengalpattu District, Tamil Nadu, India*.

***Corresponding Author E-mail:** paradesd@srmist.edu.in

ABSTRACT

Modern society is highly dependent on electrical energy to satisfy the increasing demands of portable electronic devices and electric vehicles. This rapid growth in energy consumption has resulted in significant environmental pollution and escalating energy requirements. Therefore, the development of clean, sustainable, and alternative energy technologies has become imperative to address the critical challenges of environmental degradation and depletion of conventional energy resources. Proton Exchange Membrane Fuel Cells (PEMFCs) have considerable attention as one of the most promising alternative energy technologies due to their high power density, rapid response to varying load conditions, low operating temperature, and environmentally benign nature. Sulfonated polystyrene-block poly (ethylene-ran-butylene)-block-polystyrene (SPSEBS) and Polyethylene glycol (PEG) blend membranes have potential uses in proton exchange fuel cells. In this study, chlorosulfonic acid was used as a sulfonating agent to sulfonate PSEBS. [1] Sulfonated chromium MOF (Cr-MIL-101-SO_3H) was developed by the solvothermal method. Using the solvent casting approach, composite membranes was prepared by incorporating an appropriate quantity of Cr-MIL-101-SO_3H into the SPSEBS/PEG blend polymer solution. [2] The incorporation of these additives can endow the composite membranes with more attractive advantages, encompassing improved proton conductivity and water retention at high temperature, higher thermal and chemical stability, etc. The incorporation of Cr-MIL-101-SO_3H to the S-PSEBS/PEG blend membrane is confirmed by the FT-IR and XRD results. Water uptake, swelling ratio, ion exchange capacity, and proton conductivity were among the physicochemical and electrochemical characteristics that were used to assess the composite membranes and establish their possible suitability for fuel cell applications.

Keywords: Proton exchange membrane fuel cells, SPSEBS, Cr-MIL-101-SO_3H, Ionic conductivity.

References:

1. Berlina Maria Mahimai, et al. *ACS Applied Nano Materials* 2023 *6* (19), 18139-18149

2. Niknam, Esmaeil, et al. *ACS omega* 3.12 (2018): 17135-17144.

Tin Selenide Thin Films Grown on Surface-Textured Glass Substrates with Periodic Microstructures for Improved Optical Absorption

Jegatheesan G[1], Monica Arputharaj[1], Malar Piraviperumal[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, 603203, Tamilnadu, India*

***Corresponding author e-mail:** malarp@srmist.edu.in

ABSTRACT

Surface texturing is an effective method to modulate the optical performance of thin-film materials. In this work, micro-structured glass substrates were prepared using cross-linked SU-8 2000.5 photoresist through an optical photolithography process. Periodically arranged cylindrical microstructures with a diameter of 40 µm and spacing of 40 µm (40/40 µm) and a height of about 500 nm were patterned over a 20 mm × 20 mm area. Tin selenide (SnSe) was deposited on both plain and textured glass substrates via thermal evaporation at a substrate temperature of 200 °C. Surface morphology and conformal growth of the films were examined using optical microscopy and scanning electron microscopy, wherein preservation of micro cylindrical patterns was observed. Structural properties analyzed using X-ray diffraction indicated single phase polycrystalline nature, while optical absorption study of plain and textured SnSe films showed enhanced optical absorption in films grown on textured substrates due to improved light scattering and trapping effects. To support the observations, COMSOL simulation studies have been carried out.

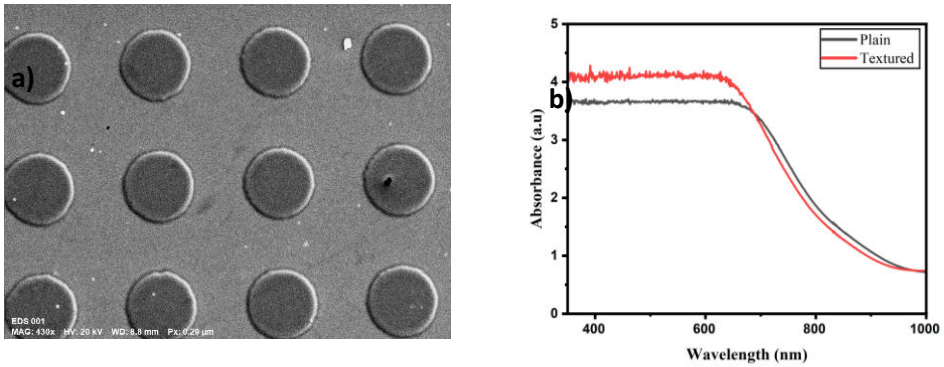


Fig.1 a) SEM images of textured substrate & b) UV-Vis spectra of plain and textured substrates

References:

4. Rajendran, Jagadish, et al. *Solar Energy* 211 (2020): 977-987.
5. Vashishtha, Pargam, et al. *Materials Science and Engineering: B* 297 (2023): 116808.

TF-038

Optimization of growth conditions of Thermally Evaporated SnSe Thin Films

Monica Arputharaj[1], Srinivasan Moosi Govindharajulu[1], Malar Piraviperumal[1]*

[1]*SRM institute of Science and Technology, Kattankulathur, 603203, Tamilnadu, India*

***Corresponding author e-mail:** *malarp@srmist.edu.in*

ABSTRACT

Tin selenide (SnSe) thin films were grown via thermal evaporation method using ball-milled SnSe powder on glass substrates held at room temperature, 100°C, 200°C, 250°C and 300°C. The as-deposited films were subsequently annealed at 450°C for 30 minutes to enhance crystallinity and optoelectronic properties. Structural characterization via X-ray diffraction analysis revealed polycrystalline orthorhombic phase with enhanced crystallinity at higher deposition temperature and annealing. Surface morphology, examined by scanning electron microscopy, showed improved grain size and uniformity in as-grown and annealed films. Raman spectroscopy of thin films showed sharp peaks due to Raman modes of SnSe confirming absence of any secondary phases. Optical properties, assessed through UV-Vis spectroscopy, indicated a that optimal bandgap of 1.2 eV was obtained for films grown at 200°C (both as-grown and annealed) Electrical performance, evaluated by current-voltage (I-V) and current-time (I-T) measurements under dark and illumination conditions demonstrated showed photoresponsivity in films grown at higher deposition temperatures. Among the samples, the SnSe glass substrate grown at 200°C delivered the fair characteristics, making it suitable for heterojunction photodetector applications.

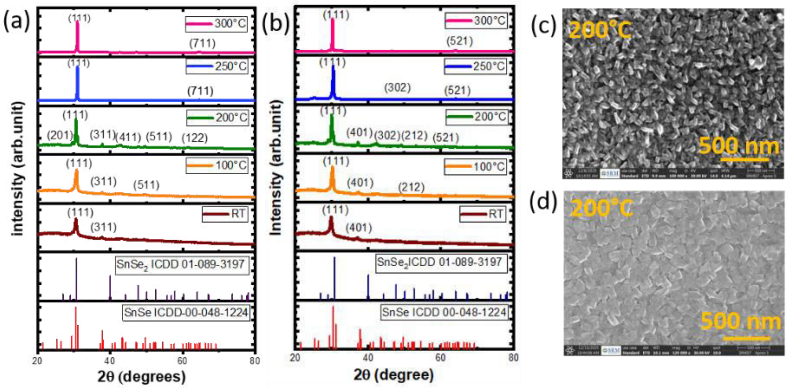


Figure (a),(b) XRD and (c), (d) SEM images of as-grown and annealed thin films

References:

1. Devarajan A, et.al, Fabrication of SnSe nanostructures visible light photodetectors, Inorganic Chemistry. Communications, 2024, 113276.
2. Vashishtha P, et al, Highly efficient, self-powered, and air-stable broadband photodetector based on SnSe thin film, 2023, 116808.

TF-039

Optical and Vibrational Properties of MOCVD grown monolayer $Mo_{1-x}Nb_xS_2$ ternary alloys

Vijaykumar Murugan[1], Abhishek Singh Sindhu[1] and Senthil Kumar Eswaran[1*]

[1] *2D Materials and Devices Laboratory (2DML), Sir C. V. Raman Research Park, Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, Chennai, India*

***Corresponding author e-mail:** senthile2@srmist.edu.in

ABSTRACT

Band gap engineering of monolayer transition metal dichalcogenides is indispensable to tailoring the functionalities, manipulate the emission properties and create countless combinations of heterostructures with different band offsets for potential use in solar cells, photodetectors, phototransistors and valley spintronics. Here, we present a detailed study on the controlled synthesis of $Mo_{1-x}Nb_xS_2$ monolayer alloys, with compositions ranging from x = 0 to 0.67 using metal organic (MOCVD) chemical vapor deposition. The formation of ternary $Mo_{1-x}Nb_xS_2$ alloys and the associated strain resulting from alloying were demonstrated through a combination of optical spectroscopy and XPS characterization techniques. Our finding suggest that defects like dimers, vacancies, and metal dopant substantially induced FWHM and induce a larger red shift in the alloy films, as confirmed by Raman spectroscopy. A lattice tensile strain (~0.58 %) and compressive strain (~1.25 %) was estimated when the Nb atom substituted in the MoS_2 lattice calculated utilizing Raman spectroscopy. Furthermore, we investigate the impact of alloying mediated strain on optical absorption and emission behavior, particularly trions and impurity-bound excitons in monolayer $Mo_{1-x}Nb_xS_2$ ternary alloys.

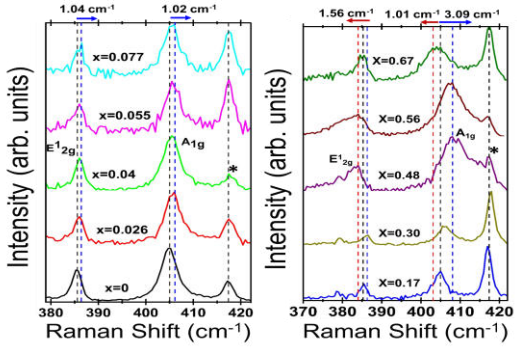


Figure 1. Raman spectra of $Mo_{1-x}Nb_xS_2$ monolayer alloy with different Nb concentrations.

References:

1. Schulpen JJ et al. ACS Applied Nano Materials. 2024 Apr 1;7(7):7395-407
2. Song B et al. ACS Applied Electronic Materials. 2021 May 26;3(6):2564-72

TF-040

Elastic Moduli as Determinants of Lattice Thermal Conductivity in Layered MoS_2

Sanju Shree Ramar[1] Senthil Kumar Eswaran[1*]

[1]*2D Materials and Devices Laboratory (2DML), Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, India*

***Corresponding author e-mail:** senthile2@srmist.edu.in

ABSTRACT

Thermal conductivity plays a vital role in understanding lattice heat transport and energy dissipation in materials, especially in two-dimensional transition metal dichalcogenides (TMDs) such as MoS_2 etc. In this present study, thermal conductivity is quantitatively evaluated using Young's modulus obtained through the acoustic force atomic microscopy (AFAM) technique. The Lattice thermal conductivity is estimated with the aid of the Slack model, which is primarily governed by Debye temperature and Debye sound velocity. Our results reveal a strong layer dependence of thermal conductivity, exhibiting a monotonic decrease with increasing layer number. The monolayer MoS_2 exhibited a higher thermal conductivity of 56.69 $Wm^{-1}K^{-1}$ compared to that of thick MoS_2 layer (~20 layers) ~ 12.94 $Wm^{-1}K^{-1}$. This reduction in thermal conductivity arises due to the phonon boundary scattering, surface disorders, and thickness-induced anharmonicity, which inhibits the thermal transport potential of flexural acoustic phonons. These findings highlight that the Young's modulus solely plays a crucial role in determining the layer-dependent thermal conductivity of MoS_2.

Keywords: Thermal conductivity, MoS_2, Young's modulus, Debye temperature.

References:

1. Peng, Bo, et al. "Thermal conductivity of monolayer MoS2, MoSe2, and WS2: interplay of mass effect, interatomic bonding and anharmonicity." *RSC advances* 6.7 (2016): 5767-5773.
2. Jo, Insun, et al. "Basal-plane thermal conductivity of few-layer molybdenum disulfide." *Applied Physics Letters* 104.20 (2014).
3. Bae, Jung Jun, et al. "Thickness-dependent in-plane thermal conductivity of suspended MoS2 grown by chemical vapor deposition." *Nanoscale* 9.7 (2017): 2541-2547.

TF-041

Synthesis and Development of MXene Composites for Wearable Thermoelectric Applications

S.T. Venkata Sai Varma[1,4], G.S. Nikhil Reddy[4], K Washiyama [4], V. Pandiyarasan[2], K. Ikeda[3], H. Hamasaki[4], H. Ikeda*[1,4]

[1] *Graduate School of Science and Technology, Shizuoka University, Japan*

[2] *Indian Institute of Information Technology, Design and Manufacturing, (IIITDM)Kancheepuram, India*

[3] *Nara Institute of Science and Technology, Japan*

[4] *Research Institute of Electronics, Shizuoka University, Japan*

***Corresponding author e-mail:** ikeda.hiroya@shizuoka.ac.jp

ABSTRACT

Flexible wearable thermoelectric generators (FWTEGs) have been developed as an effective solution for capturing waste heat and converting it into electrical energy, providing a self-sustaining power source for advanced wearable electronics. Despite substantial improvements in device architecture, traditional thermoelectric materials such as Bi_2Te_3 and Bi_2Se_3 [1] present toxicity risks and manufacturing constraints. We propose MXene-based wearable thermoelectric generators to address this issue. MXenes offer a safer, solution-processable alternative that maintains functional performance. MXenes are an emerging category of two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides that have lately attracted interest as versatile possibilities for flexible thermoelectric applications. Their excellent electrical conductivity, tunable characteristics, remarkable mechanical compliance, and chemically reactive surfaces make them especially suitable for incorporation into fabric-based thermoelectric devices [2]. This study includes the synthesis of Ti_3C_2Tx MXene from Ti_3AlC_2 MAX thereafter undergoing controlled etching at temperatures of 30°C, 40°C, and 50°C under systematically varied gas-phase conditions. This thermal and atmospheric manipulation was designed to improve interlayer spacing and surface termination, yielding MXene layers with thicknesses ranging from 0.7 to 3.0 nm [*Fig1*]. The generated structures were evaluated for their compatibility in fabric-integrated thermoelectric devices.

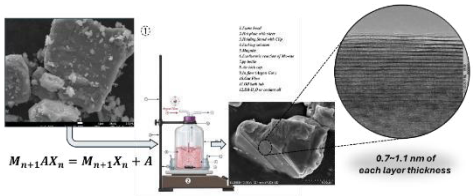


***Fig. 1** MAX phase to Mx-ene phase transformation during etching processes.*

Keywords: Flexible wearable thermoelectric generators; 2D materials; MXene

References:

1. Liang Miao, Shan Zhu, Cheng Liu, *Nat. Commun.*, 15 (2024) 1–12.
2. *Yan Xu, Bin Wu, Chao Hou, Flexible Mater., (2024) flm2.28.*

IA-001

Hydrogen Reduction of Iron Scale for Sustainable Steelmaking

Wondayehu Yeshewas Alemu, Ping-Hsuan Lee, Jhewn-Kuang Chen*

Institute of Materials Science and Engineering, National Taipei University of Technology,

No. 1, Sec. 3, Zhong-Xiao E. Rd., Taipei 106344, Taiwan

***Corresponding author e-mail:** jkchen@ntut.edu.tw

ABSTRACT

Iron scale generated during steel manufacturing constitutes a significant industrial waste stream while also representing a valuable secondary iron resource. Addressing this industrial challenge, the present study applies academic materials science methodologies to investigate hydrogen-based reduction of untreated and thermally pretreated iron scale toward sustainable steelmaking and circular resource utilization. Reduction behavior, kinetics, and microstructural evolution were examined under H_2-N_2 atmospheres using thermogravimetric analysis (TGA), X-ray diffraction (XRD), and scanning electron microscopy (SEM). The as-received iron scale, composed mainly of FeO, Fe_3O_4, and Fe_2O_3, exhibited a dense morphology that restricted hydrogen diffusion and resulted in incomplete reduction. Thermal oxidation pretreatment at 700-800 °C transformed FeO and Fe_3O_4 into porous Fe_2O_3, significantly enhancing hydrogen accessibility and reducibility by improving gas-solid contact. Under optimized conditions (800 °C, 80% H_2), the pretreated scale achieved over 90% reduction, compared with ~83% for untreated material. Kinetic analysis based on the Avrami-Erofeev model revealed a multistage reduction mechanism transitioning from nucleation-controlled growth to diffusion-controlled processes, with low apparent activation energies of 19-26 kJ mol^{-1}, indicating reduced reaction barriers relative to conventional iron oxides. Microstructural observations confirmed the evolution from dense oxide layers to a porous metallic iron network, facilitating efficient oxygen removal and iron recovery. Overall, the findings demonstrate the potential of hydrogen-assisted thermochemical processing as a scalable and low-carbon solution for valorizing steelmaking waste, providing a scientific foundation for industry-academia collaboration aimed at advancing green steel production.

Keywords: Hydrogen reduction; iron scale; sustainable steelmaking; reaction kinetics; industry-academia collaboration

Effect of Heat treatment on Corrosion Behaviour of F55 Duplex Stainless Steel

Ratnesh Kumar Gupta[1]*

[1]*National Institute of Advanced Manufacturing Technology, Ranchi, 834003*

***Corresponding author e-mail:** ratneshg@niamat.ac.in

ABSTRACT

Super Duplex Stainless Steels (SDSSs) are being widely used these days, because of their unique combination of properties and is widely used by the industries. Their applications and markets are growing continuously, and without any doubt, there is a great potential for further volume increase. In recent years, intensive research has been performed on lean SDSSs improving mechanical properties. In the present work, we will focus on F55-UNS S32760 Duplex stainless steel, their microstructural investigation and different thermal treatments. Firstly, the investigated specimens have been undergone a thermal treatment solution, and then, an annealing treatment with different holding times, to compare the microstructures of various heat treatment processes and as in received condition. Electron Backscatter Diffraction (EBSD) was also performed to justify the austenitic and ferritic phases. Moreover, EDS (Energy Dispersive X-ray Spectroscopy) experiments were performed to study the segregation and distribution of alloying elements in the microstructure from which we can calculate the pitting resistance equivalent number which gives the idea of corrosion resistance. X-ray Diffraction was also conducted to examine whether it is consistent with the Phase fraction of EBSD and the determination of undesirable phases. Potentiodynamic polarization corrosion tests were conducted on the received sample and various heat-treated samples to compare the corrosion resistance.

References:

1. R. N. Gunn, Duplex Stainless Steels: Microstructure, Properties and Applications, Woodhead Publishing, Cambridge (1997).
2. J. O. Nilsson, Mater. Sci. Technol., 8 (1992) 685–700.
3. J. Charles, Proc. Duplex Stainless Steels Conf., Beaune, France (2007).
4. C.-O. A. Olsson and D. Landolt, Electrochim. Acta, 48 (2003) 1093–1104.
5. P. Bala Srinivasan et al., Corros. Sci., 48 (2006) 93–109.

CloudCover AI: ML-powered real-time data masking in cloud storage for GDPR/DPDP compliance

Jyothishree Rajkumar, Karthikeyan V2 Hema M*

Easwari Engineering College, Ramapuram, Chennai, Tamilnadu, India, 600087

***Corresponding author e-mail:** hema.m@eec.srmrmp.edu.in

ABSTRACT

Due to the fast implementation of digital systems based on the clouds in the industry, the method organizations process and keep huge amounts of sensitive information is being disrupted especially in the controlled industries like healthcare, finance and governance. Such industrial transformation has heightened anxieties of data privacy, security and compliance concerns. Traditional methods of managing Personally Identifiable Information (PII) and Protected Health Information (PHI) such as post-storage masking and third-party anonymization are prone to exposing raw data at intermediate processing levels, which subjects compliance risk and operational reliance to risk. To respond to these issues, this paper introduces CloudCover AI, which is a cloud-native AI-driven system that offers real-time privacy-preserving data processing in the enterprise. The suggested system combines machine learning and Natural Language Processing (NLP) models at the very top of the data ingestion tier, which allows realizing on-fly the detection of sensitive entities and their anonymization prior to cloud storage. Such architecture avoids exposures of raw data and requires a smooth integration with the current industrial cloud architecture. With the General Data Protection Regulation (GDPR) and the Digital Personal Data Protection Act (DPDP), the system has automated auditor and compliance validation controls that ensure the constant compliance with regulations. Experimental analysis shows that masking is very accurate, processing latency is low and that there is consistent obedience to structured, semi-structured and unstructured datasets. CloudCover AI provides an effective and secure data management model in the contemporary enterprise operations by reconciling research with industry implementation.

References:

1. Mollashaik A. S., Int. J. Sci. Res. Arch. 8 (2023) 1053–1070.
2. Sandhu R., Sharma M., Gupta V., J. Cloud Comput. 12 (2023) 511–530.
3. Mishra K., Pagare H., Sharma K., Sci. Rep. 15 (2025) 1–14.

Carbon Nanotube Morphology–Tribology Relationships

Sz. Ruczka[1,2,3], A. Marek[1,4], M. Skrzypek[5], Ł. Wojciechowski[5], S. Boncel[1,2,3]*

[1] *NanoCarbon Group, Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Silesian University of Technology, Bolesława Krzywoustego 4, 44-100 Gliwice, Poland*

[2] *Centre for Organic and Nanohybrid Electronics (CONE), Silesian University of Technology, Stanisława Konarskiego 22B, 44-100 Gliwice, Poland*

[3] *NanoCarbonGroup.com Co. Ltd., Ks. Marcina Strzody 7, 44-100 Gliwice, Poland*

[4] *Department of Chemical Organic Technology and Petrochemistry, Silesian University of Technology, Bolesława Krzywoustego 4, 44-100 Gliwice, Poland*

[5] *Institute of Construction Machines and Automotive Vehicles, Poznań University of Technology, Piotrowo 3, 60-959 Poznań*

***Corresponding author e-mail:** slawomir.boncel@polsl.pl

ABSTRACT

Carbon nanotubes (CNTs) are studied as additives to various lubricants such as polyalphaolefins or ionic liquids. The introduction of CNTs can improve properties of the so-formed (io)nanofluids (INFs) or nanogreases such as reduction in wear and friction thus improving rheological properties [1]. The final efficiency depends on the morphology of the CNT structure for example aspect ratio, metallic residue, no. of walls, and overall carbon purity. Within those parameters, one can tailor CNTs for targeted applications. The existing literature shows significant differences between CNTs in the case of tribological properties [2]. In this work, we focus on describing the morphology influence of CNTs on their impact on the tribological and rheological properties of INFs. Analysis of rheological and tribological parameters of in-house synthesized high-purity multi-walled CNTs (MWCNTs) can lead to a more reliable description of such systems. As was proven in the latest work, even a small addition of CNTs can lead to drastic changes in the rheological parameters of INFs [3]. To parametrize CNTs, we apply thermogravimetric analysis (TGA), scanning and transmission electron microscopy with energy-dispersive X-ray spectroscopy (TEM, SEM/EDX), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS). At the same time, to quantify functional characteristics of INFs, we implement rheological (viscosity, shear rate and shear stress) and tribological measurements in the polymer-steel (UHMWPE/steel AISI 4130) tribo-pairs.

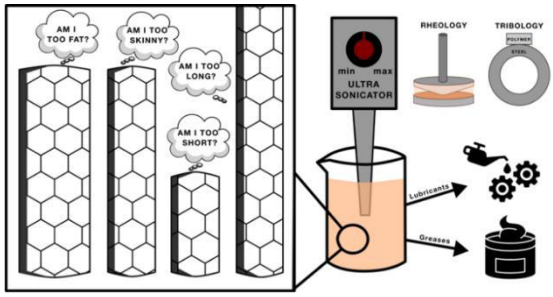


Fig. 1. Various morphology of carbon nanotubes in tribological application

References:

1. N. Nyholm, N. Espallargas, Carbon, 201, 1200-1228, (2023)
2. Ł. Wojciechowski et al., Tribol. Int 191, 109203 (2024).
3. S. Boncel et al., J. Mol. Liq. 391, 1-10 (2023).

IA-005

Design and Standardization of Near Infra-Red (NIR) Spectral Sensor for Rapid Detection of Microplastics in Wastewater

Mullaimalar A[1], Saraswathi A[1], Krishnakumar M[1], Krishnaveni M[1], Vijayakumar P[2]*, Jeyalakshmi R[1]*

[1]*Department of Chemistry, College of Engineering and Technology, SRM Institute of Science and Technology, Kattangulathur, Tamil Nadu, India, 603203*

[2]*Professor, Department of Electronics and Communications and Engineering, SRM Institute of Science and Technology, Kattangulathur, Tamil Nadu, India, 603203*

***Corresponding author e-mail:** vijayakp@srmist.edu.in, jeyalakr@srmist.edu.in

ABSTRACT

Microplastic pollution in wastewater creates a critical environmental challenge due to its small size (< 5µm), and its impacts on different environment including human, wildlife, marine system etc has already been described. Further, the standard methodologies for detection, classification, and quantification are complicated and associated with expensive instrumentation techniques, stationary sampling, and high cost. Though the conventional spectroscopic methods like fluorescence spectroscopy, Infrared spectroscopy, Raman spectroscopy, and hyperspectral imaging offer high specificity but are hindered by high costs, complexity, and limited field usability. In view of the above, this study program attempts to design the near-infrared (NIR) spectral sensor (200–900 nm) for detection of various microplastics in the simulated waste water. This study program collects the NIR spectral signatures of common polymers include Polyethylene, Polystyrene, and Poly Methyl Methacrylate, from different channels provided in different frequency ranges. The analysis of data was performed by varying the concentration of the MP's, interfering ions in the water, and the e pH alteration of the medium to validate the captured data. Repeatability and reproducibility have been established for the verification of methodology. The test results are cross-verified by spectrochemical data. The test results showed that the sensor leverages the distinct spectral signatures that are comparable with the chemometric method of analysis. This portable NIR sensor enables scalable, on-site monitoring, advancing microplastic remediation strategies.

Keywords Microplastics, Sensors, NIR, Polymers, Detection

Development of 316L Stainless Steel Robot Assisted Additive Manufactured Sample for Energy and Space Applications

Senapathi Yaswanth[1], Kavya R[2], Akash Vincent, N. Harshavardhana*

SRM Institute of Science and Technology, Kattankulathur, Tamilnadu, India, 603203

***Corresponding author e-mail:** harshavn@srmist.edu.in

ABSTRACT

316L stainless steel is a corrosion-resistant austenitic alloy extensively used in energy and space applications due to its superior mechanical properties and structural reliability. This study presents the development and evaluation of robot-assisted additively manufactured 316L stainless steel components fabricated using Wire Arc Additive Manufacturing (WAAM) and Directed Energy Deposition (DED) powder-based techniques. The work emphasizes robotic integration, process parameter control, and the influence of deposition strategy and geometry on material quality and dimensional accuracy. Fabricated samples were subjected to comprehensive mechanical and microstructural characterization, including tensile testing, hardness measurement, optical microscopy, scanning electron microscopy (SEM), and X-ray diffraction (XRD). A systematic correlation between processing conditions, microstructural evolution, and mechanical performance was established, along with identification of potential defects associated with arc-based and powder-based deposition processes. The results demonstrate the feasibility and reliability of robot-assisted additive manufacturing for producing high-performance 316L stainless steel components with enhanced scalability and structural integrity, contributing to advanced manufacturing solutions for energy and space engineering applications.

Keywords: Wire Arc Additive Manufacturing, Directed Energy Deposition, 316L Stainless Steel, Robot-Assisted Manufacturing, Microstructure Property Relationship, Mechanical Characterization.

Government-Supervised Community Delivery Model for Strengthening the Public Distribution System (PDS)

Kathir Kamesh K[1], Rithika S*[2], Santhosh R[3], Tejas M U[4]

***Corresponding author e-mail:** rithikasenthilkumar16@gmail.com

ABSTRACT

The Public Distribution System (PDS) plays a vital role in ensuring food security for economically weaker sections of society. However, traditional ration distribution methods often face challenges such as overcrowding, lack of transparency, delivery delays, and risk of diversion or fraud. This paper proposes a Government-Supervised Community Delivery Model supported by a digital mobile application to improve efficiency, accountability, and last-mile delivery of essential commodities. The proposed system restricts delivery personnel eligibility to verified and trusted individuals such as current postmen, retired postmen, Anganwadi workers, women Self-Help Group (SHG) members, and verified rural youth. By leveraging locally known and government-affiliated personnel, the model ensures enhanced trust, reduced fraud risk, and improved service reliability compared to open gig-based delivery systems.

The mobile application integrates secure registration, Aadhaar-based verification, OTP-based delivery confirmation, geo-tagged proof of delivery, GPS tracking, and an administrative monitoring dashboard. Government officers can assign deliveries, monitor real-time status, track performance metrics, and generate reports for transparency and accountability. This model not only strengthens the PDS distribution mechanism but also generates structured rural employment opportunities under a semi-official supervised framework. The system is scalable at district and state levels and can significantly enhance transparency, operational efficiency, and beneficiary satisfaction in public welfare delivery systems.

Keywords: Public Distribution System, Last-Mile Delivery, Government Supervision, Digital Monitoring, Rural Employment, OTP Verification, Geo-Tagging.

SPONSORS

OUR SPONSORS

Anusandhan National Research Foundation

CSIR
भारत का नवाचार इंजन
The Innovation Engine of India

DRDO
DEFENCE R&D ORGANISATION
MINISTRY OF DEFENCE

INTERNATIONAL SOCIETY OF ELECTROCHEMISTRY
ISE

IOP
Institute of Physics

Netweb
TECHNOLOGIES
Tyrone
A Netweb Brand

SYINCO
SYSTEMS · INSTRUMENTS · COMPONENTS

ADVANCE RIKO

RENISHAW
apply innovation™

LABINDIA
INSTRUMENTS
AIMING FOR THE BEST

Greatify

GMS
Driven by Excellence

SISCON
SOUTHERN INDIA
SCIENTIFIC CORPORATION

NANO TEC

CODETANTRA

SOLARIS

IR TECH

DELTA

NETZSCH
Proven Excellence.

JEOL

PRINTOGRAPHY
SYSTEMS (INDIA) PRIVATE LIMITED

Firstline infotech

SWANS ENTERPRISES
Empowering Renewables...

VTPL
VACUUM TECHNOLOGIES PVT. LT

ICON
Analytical

BRINGING YOU THE BEST IN ADVANCED TECHNOLOGIES

SYINCO
SYSTEMS · INSTRUMENTS · COMPONENTS

METALLURGY

THERMAL

THERMOELECTRIC

VACUUM

ANALYTICAL

MEDICAL

WE SECURE

SERVICE • EFFICIENCY • QUALITY • RELIABILITY

URL: https://syinco.in/ | Whatsapp: +91- 7382 292929 | Phone: +91-40-2414 2929 | Email : syincoindia@gmail.com

Syinco Technologies is a global services company well acquainted with various advanced technologies. We, Syinco is dedicated to Manufacturer, Sales and Services of Advanced, Customized and Specialized Systems, Instruments and Components for Metallurgy, Thermal, Thermoelectric, Vacuum, Analytical and Medical application.

ADVANCE RIKO CHINO EDWARDS FUJI-SPS Pioneer of SPS Technology

PROCDUCT LIST

+ Thermal analysis evaluation systems
+ Thermal property measuring systems
+ Thermoelectric evaluation systems
+ Seebeck coefficient measuring systems
+ Electric resistance measuring systems
+ Thermal conductivity measurement systems
+ Power efficiency, Heat flow measuring systems
+ Rapid heating Infrared gold image (IR) furnaces
+ RTA / RTP systems various atm. controlled.
+ Iron & Steel, Steel sheet evaluation systems
+ High temperature observation systems
+ Arc plasma deposition (APD) systems
+ Spark plasma sintering (SPS) systems
+ Nano particle deposition systems
+ Gas analysis systems
+ Handy arc and Spot welder for thin wires

+ Vacuum pumps, gauges, components and fittings
+ Helium leak detectors
+ Residual gas analysers and Systems
+ Vacuum coating systems
+ Helium leak checking systems
+ Closed water Circulation systems (Chillers)
+ We offer filed services of Vacuum components, Instruments and Systems supplied by us.
+ We stocking of Pure materials, Alloys, Spares, Overhau kits, Vacuum oils, Greases, Vacuum fittings.
+ We stocking consumables like Thermocouples, Crucibles, Pure Metals, Alloys and Chemicals for R&D application.

ADVANCE RIKO

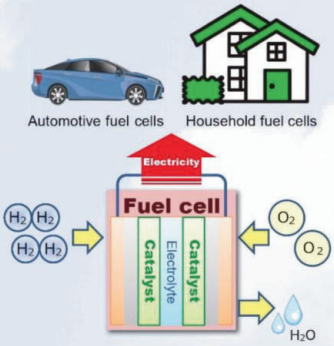
Aiding the realization of a hydrogen society by arc-plasma film deposition technology

Arc-plasma nano-particle deposition system

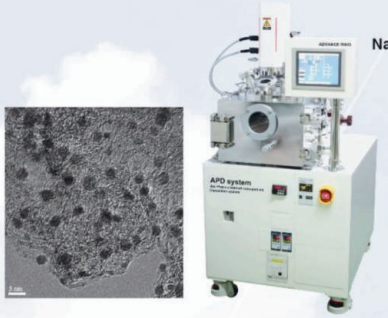
APD series

Fuel-cell catalysts

Support of activated nanoparticles on electrode materials for fuel cells



Exploration of catalytic nanoparticles

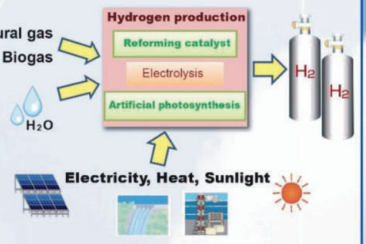


TEM image of Pt nanoparticles supported on carbon powder

Uniformly vapor-deposited onto rough carbon surface.

Hydrogen-producing catalysts

Formation of hydrogen-producing catalyst from nanoparticles



Catalyst for use with organic hydrides

Size-controlled nanoparticles using ionic liquid

Photocatalysts

Improve the performance of photo catalyst which manufactures hydrogen



Creation of materials having new properties

Creation of substances having new functions by simultaneously vapor-depositing different metals from multiple sources

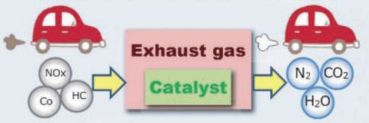
Arc-plasma source APS-1



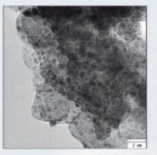
Exhaust gas catalysts

High catalytic activity of nanoparticles reduces usage of expensive noble metals

Control of greenhouse gas emissions



Support of Pt nanoparticles on alumina powder



Molded lens molds Industrial cutting tools

Hard thin film
Ultrananocrystalline diamond (UNCD)

ADVANCE RIKO, Inc.

http://advance-riko.com

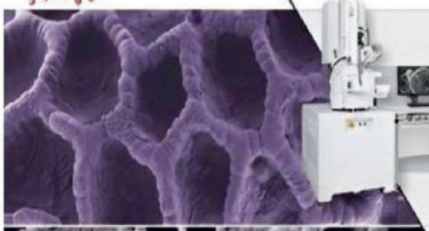
syincoindia@gmail.com

JEOL

Product Lineup

SMART • FLEXIBLE • POWERFUL



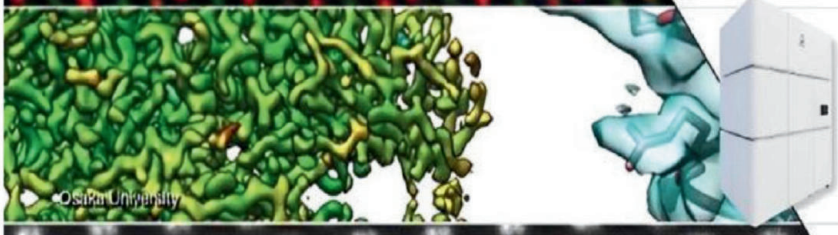


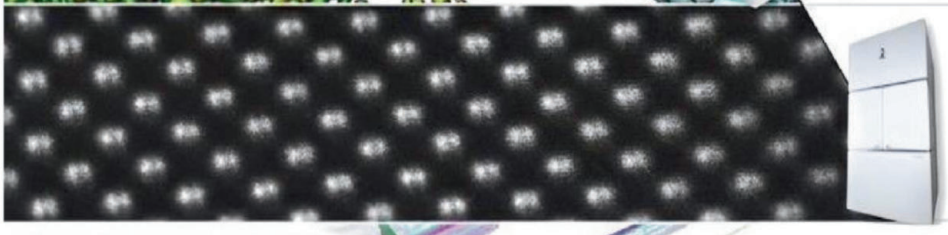
STEP INTO THE WORLD OF JEOL

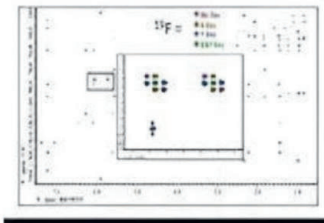


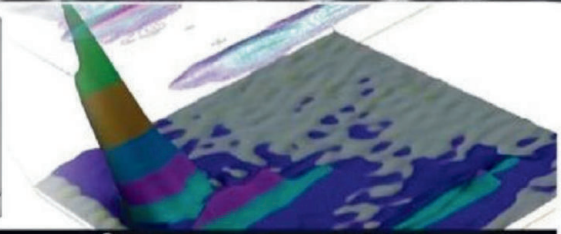
SEM
TEM
SAMPLE PREP
NMR
MASS SPEC
EPMA
LITHOGRAPHY













JEOL INDIA PVT LTD | https://www.jeol.com/in/
Email: info@jeolindia.com





LECO
EMPOWERING RESULTS


ONH 836


TGA801
Thermogravimetric/
Proximate Analyzer


844 Series C & S

Rigaku


Supermini200


ZSX Primus IV

ThermoFisher SCIENTIFIC

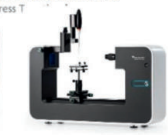

Scanning Electron
Microscope

EVIDENT
OLYMPUS


OLS5100 Confocal Laser
Scanning Microscope

Biolin Scientific
[Progress T


QSense Omni


Theta Flow

IR TECH

Rigaku


MiniFlex


SmartLab

MILESTONE
HELPING CHEMISTS


Microwave
Digestion System


Direct Mercury Analyzer


flexiwave


Synthwwave

I R Technology Services Pvt Ltd
EL-91, Electronic Zone, MIDC Industrial Area,
Mahape, Navi Mumbai, Maharashtra 400710

+918097595149 **info@irtech.in**

SWANS ENTERPRISES

Swans Enterprises is a renewable energy solutions provider specializing in the design, supply, and implementation of sustainable solar power systems. With strong technical expertise and industry experience, we deliver reliable and efficient solar solutions tailored to diverse energy needs across residential, commercial, institutional, and industrial sectors.

Our Core Expertise



Solar End to End Solutions



Solar Street Lights



Solar Pumps

Our Impact

20+ Locations	25+ Satisfied Clients	10+ MW Delivered	30+ Projects Implemented

+91 9445488110 /+91 9003252710 | info@swansenterprises.in | https://swansenterprises.in/

VTPL

VT VACUUM TECHNOLOGIES PVT. LTD.

www.vtvacuum.com

Connecting to the world's leading manufacturers

We are the representatives for the world's leading manufacturers of Vacuum and Cryogenic equipment and components in India

OUR PARTNERS:

mks Technology for Productivity **MKS Instruments, Inc.** 2 Tech Drive, Suite 201 Andover, MA 01810, USA www.mks.com	ARS **Advanced Research Systems, Inc.** 7476 Industrial Park Way Macungie, PA 18062, USA www.arscryo.com	BLUE FORS **BlueFors Oy** Arinatie 10, 00370 Helsinki FINLAND www.bluefors.com
Kurt J. Lesker Company **Kurt J. Lesker Company** 1925 Route 51 Jefferson Hills, PA 15025, USA www.lesker.com	MTI Corporation **MTI Corporation** 860 S. 19th Street Richmond, CA 94804-3809 www.mtixtl.com	GNB GROUP **GNB Corporation** 3200 Dwight Road, Suite 100 Elk Grove, California 95758 www.vacuumchamber.com
FerroTec **MeiVac (FerroTec)** 5830 Hellyer Avenue San Jose, CA 95138 www.meivac.ferrotec.com	UHV DESIGN **UHV DESIGN LTD** Judges House, Lewes Road Laughton, East Sussex England, BN8 6BN www.uhvdesign.com	Zurich Instruments **Zurich Instruments AG** Technoparkstrasse 1 8005 Zurich, Switzerland www.zhinst.com

NETZSCH

Proven Excellence.

The Analyzing & Testing business unit of the NETZSCH Group develops and manufactures a complete high precision instrument line for thermal analysis and thermophysical properties measurement, as well as offering world class commercial testing services in our laboratories. Our instrumentation is employed for research and quality control in the polymer sector, the chemical industry, the areas of inorganic and building materials, and environmental analysis. The Analyzing & Testing Business Unit portfolio includes Thermal analysis instruments such as Thermogravimetric analyzer (TGA), Differential scanning calorimeters (DSC) , Simultaneous Thermal Analyzer(STA), Thermomechanical Analyzer(TMA), Dilatometer, Dynamic Mechanical Analyzer(DMA), Thermal Conductivity by Laser Flash Method, Adiabatic Calorimeter, Heat Flow Meter and newly introduced Rheometers and Fire Testing devices.

Greatify

ExamX ● AI EMPOWERED

AI that creates, proctors & grades exams end-to-end.

From question authoring to result analytics, ExamX replaces your entire exam stack with one intelligent platform. Trusted by universities, governments, and enterprises in 50+ countries.

AI-Powered Question Authoring
Generate, tag, and manage question banks automatically with intelligent authoring tools.

Real-Time AI Proctoring
Behavioural analysis and anomaly detection maintaining academic integrity at scale.

AI-Powered Evaluation & Grading
Grades both typed and handwritten subjective answers automatically with human-level accuracy.

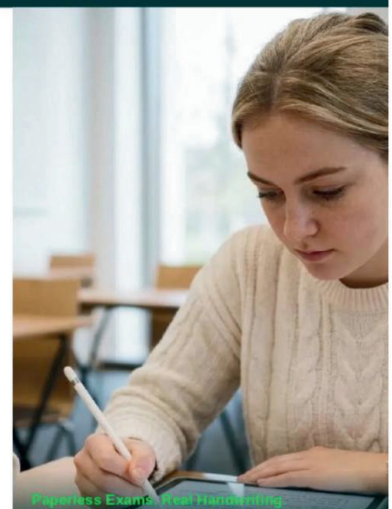
Device-Agnostic Platform
Runs on iPad, Android tablets, mobile, and web — zero compromise on security or experience.

Tablet & Stylus-Based Subjective Exams
Replicate the authentic pen-and-paper experience digitally. Students write naturally on tablets.

Enterprise-Grade Security
Biometric authentication, encrypted delivery, and tamper-proof exam environments.

Instant Result Analytics
Real-time dashboards with performance insights, question-level analysis, and exportable reports.

Multi-Language Support
Conduct exams in 50+ languages with on-device language conversion built in.



Paperless Exams, Real Handwriting.
Students write naturally on tablets with stylus — the authentic pen-and-paper experience, fully digital.

ABOUT THE FOUNDER

Dinesh Kumar
Founder & CEO, Greatify

Former AI & Systems Engineer at NVIDIA, USA — after a decade building GPU computing and AI infrastructure at one of the world's most innovative technology companies, Dinesh returned to India with one vision: to completely eliminate paper from the examination process and replace it with intelligent digital assessment.

www.greatify.ai/examx
+91 91648 11110

SOC 2 GDPR ISO 27001

LABINDIA®
INSTRUMENTS
AIMING FOR THE BEST

inVia™ Research grade confocal Raman Micrscope

InVia Key Features

1. HIGH optical efficiency, Spectral resolution & Spectral Stability.
2. Low wavenumber performance
3. Broad-range artefact-free spectra



RENISHAW
apply innovation™

Brands We Represent

Tescan	Park SYSTEMS	SENTECH Erfolg durch Leistung
Scanning Electron Microscopy	Atomic Force Microsopy	Spectroscopic & Laser Ellipsometer
HEIDELBERG INSTRUMENTS	KLA	nanoTherics
Lithography Solutions	Nano Indenter	Magnetic Hyperthermia Equipment

Corporate Office: Thane, Maharashtra | Branches: Kolkata, Bangalore, Chennai, Hyderabad, Gurugram | (022)-69086000 | +91 73049 85189 | enquiry@labindia.com | www.labindiainstruments.com

SISCON SOUTHERNINDIA SCIENTIFIC CORPORATION

No 5, 2nd Street, Thiruvengadam Nagar, Kandanchavadi, Chennai - 600096
E-Mail: thesiscon@gmail.com Web: www.siscon.in Ph: 9840023586, 7299076600, 7299076612

Products we deal:

- Lab -Chemicals
- Speciality Chemicals
- Bio Chemicals (Molecular Biology/Immunobioligicals, etc.)
- Bulk Chemicals & Solvents
- Bio-Kits
- All Laboratory Aids
- Lab consumables
- All Laboratory Instruments (Including Blood Bank instruments, Top Loading Balances, Analytical Balances, Bio safety cabinets, shakers & Biotechnology Instruments, etc.)

We are the authorized distributors for the major brands/principles such as:

SRL SISCO RESEARCH LABORATORIES PVT. LTD. — Research & Laboratory Chemicals, Animal culture, Nano Powders & Carbon Nano tubes, Dehydrated culture media, BioLIt (DNA & Protien tools & kits).

avantor delivered by VWR — Rankem Brand Chemicals, Glasswares, Syringe Filters, membrane filters, J.T Baker range of imported chemicals.

MERCK / SIGMA-ALDRICH — Merck & sigma aldrich Range of chemicals & antibodies (Indian & Imported) millipore membrane filters, Millex syringe filters, stericups and chromatography products.

ThermoFisher SCIENTIFIC — Acros, Alfa Aesar, liquid handling, & instruments (Indian & Imported)

FALCON — Corning technologies India Pvt. Ltd (Falcon range of plasticwares)

Spectrochem Pvt. Ltd (Speciality Chemicals)

GeNei™ — Genei Labs Pvt. Ltd (Bangalore Genei testings kits, Electroporosis apparatus)

SISCON SOUTHERNINDIA SCIENTIFIC CORPORATION

No 5, 2nd Street, Thiruvengadam Nagar, Kandanchavadi, Chennai - 600096
E-Mail: thesiscon@gmail.com Web: www.siscon.in Ph: 9840023586, 7299076600, 7299076612

MP Biomedicals — MP Biomedicals (Imported Chemicals)

Riviera — Riviera Glass Pvt. Ltd (Schott Duran glasswares, Riviera glasswares)

OLYMPUS — Olympus, Magnus range of Microscopes

LABOMED — Range of Microscopes & accessories

SHIMADZU Excellence in Science — Shimadzu range of electronic analytic balance

SYSTRONICS — FTIR, UV.VIS . Spectrophotometer

SSI SCIENTIFIC INSTRUMENTS — Range of scientific instruments like centrifuges, Magnetic stirrers, Analytical balances , vortex shakers, laminar airflow , Industrial furances, high temperature furances, Tubular and box furances, Humidity chambers, tray dryer, oven, incubator etc.

SSI PLASTICWARES — Lab consumables like microtips , petridish, centrifuge tubes etc.

LAMY RHEOLOGY INSTRUMENTS — Viscometers, Rheometers, accessories, texture analyzers etc.

LABTOP Quality Lab Equipment — Laboratory equipment's, Blood bank equipment's & Healthcare equipment's.

REMI — Range of Laboratory & Healthcare equipment's.



Intelligent Integerated InfraSuite
Self-Contained Edge Datacenter



Temp. & Humidity Sensor



Rack Mount UPS & Battery



Environment Monitoring System

iCool Rack

The ***iCool Rack*** leverages the latest advancements in data center technology to deliver cost-effective power and precision cooling, enabling the achievement of modular data center solutions and networking objectives.

Its plug-and-play functionality ensures easy deployment without the need for building a dedicated data center room. By addressing the challenges of networking infrastructure, this solution offers significant savings while effectively meeting your data center requirements.

Features

- Inbuilt UPS, precision cooling, real time monitoring of system performance
- Uninterrupted Power Supply, Rack Mount Cooling Unit, Enclosure for IT Component
- Inbuilt Temperature & Humidity Sensor with Safety and Security
- Inbuilt Aircon in 3.5kW & 7kW cooling capacity to maintain internal temperature.
- Dual Redundant Rack PDU to achieve high availability with suitable IEC C-13 & IEC C-19 sockets

---

Delta Group | Delta Power Solutions

www.deltaelectronicsindia.com
The power behind competitiveness

Contact our local consultant for knowing more on data center infrastructure total solutions.
Tel: +91 8802433666 E-mail: ups.india@deltaww.com

DELTA

NANO TEC

MADE IN INDIA

HIGH TEMPERATURE CVD SYSTEM

Chemical Vapor Deposition Equipment for Advanced Materials



Key Features



Digital Controller



Quartz Tube



Dual Heating Zones



Graphene Synthesis



Nanomaterials



Semiconductor Processing



NANOTEC
Chennai-India

+919445923469

sales@nanoteclab.com

SCAN ME

NAAC A++ | Category 1 with 12B Status | (2025) Ranked 11th University | (2026) World Ranking one among 54 Indian Universities | (2025) World Ranking one among 91 Indian Universities | (2025) World Ranking Ranked 8-9 in Indian Universities | (2025) World Ranking one among 18 Indian Universities | (2024) World Ranking one among 3 Indian Universities

SRM Institute of Science and Technology
(Deemed to be University under section 3 of UGC Act 1956)
SRM Nagar, Kattankulathur, Chengalpattu District
Chennai, Tamil Nadu, India – 603203.
Telephone: +91-44-27417000, +91-44-27417777
Website: https://www.srmist.edu.in/



For further detail, Contact
Conference Chair: AFMD-2026
Phone: +91-44-24717190
Mobile: +91 87544 20369

9 788198 799241