

एमआरएसआई की ३६वीं वार्षिक महासभा और ७वीं भारतीय
मटेरियल्स सम्मेलन एवं उभरते पदार्थों पर अंतर्राष्ट्रीय सम्मेलन २०२५

36th AGM of MRSI & 7th Indian Materials Conclave and International Conference on Emerging Materials 2025

MRSI-ICEM
2025

१७-२० दिसंबर २०२५

17-20 DECEMBER 2025



Organized By :
नाइजर भुबनेश्वर
NISER Bhubaneswar



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Abstract booklet

A Collection of abstracts from MRSI-ICEM 2025

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Symposia

MRSI - ICEM 2025

Symposium : A

Electronic and Photonic Materials

Topics:

- A-1: Wide bandgap semiconductors
- A-2: Device and materials design
- A-3: Semiconductor for photonics / photovoltaics
- A-4: Functional materials for optoelectronics
- A-5: Optical resonators / devices

Coordinators:

Dr. Shovon Pal
 - *NISER Bhubaneswar*
 Dr. Satyaprakash Sahoo
 - *IOP Bhubaneswar*
 Prof. Umapasanna Ojha
 - *IIT Bhubaneswar*

Symposium : B

Quantum Materials

Topics:

- B-1: Topological material and devices
- B-2: Magnetic and Superconducting materials and devices
- B-3: 2-D materials and devices
- B-4: Spintronics
- B-5: Skyrmions

Coordinators:

Prof. Subhankar Bedanta
 - *NISER Bhubaneswar*
 Dr. Anamitra Mukharjee
 - *NISER Bhubaneswar*
 Dr. Debakanta Samal
 - *IOP Bhubaneswar*

Symposium : C

Energy and Sustainable Materials

Topics:

- C-1: Self-powered devices
- C-2: Porous materials (MOFs, COFs, Cages and Zeolites)
- C-3: Perovskite materials
- C-4: Nuclear materials
- C-5: Piezo, Tribo, Pyro, Thermoelectric materials
- C-6: Sustainable materials for energy conversion and storage

Coordinators:

Dr. Satyaprasad P Senanayak
 - *NISER Bhubaneswar*
 Prof. Jogendra Nath Behera
 - *NISER Bhubaneswar*
 Dr. Dipak Samanta
 - *NISER Bhubaneswar*

Symposium : D

Applied Soft and Biomaterials

Topics:

- D-1: Bio-derived materials
- D-2: Materials for Bio/Medical applications
- D-3: Soft materials Technology
- D-4: Flexible and wearable materials

Coordinators:

Dr. Sumedha
 - *NISER Bhubaneswar*
 Dr. A V Anil Kumar
 - *NISER Bhubaneswar*
 Dr. Ramanujam Srinivasan
 - *NISER Bhubaneswar*

Symposium : E

Advanced Methods in Materials

Topics:

- E-1:** Advanced spectroscopic techniques
- E-2:** Advanced microscopic techniques
- E-3:** Advanced scattering and diffraction techniques
- E-4:** Advanced material characterisation techniques
- E-5:** Advanced device fabrication techniques

Coordinators:

Dr. Kartikeswar Senapati
- *NISER Bhubaneswar*
Prof. Himanshu Sekhar Biswal
- *NISER Bhubaneswar*
Dr. Chandra Shekhar Purohit
- *NISER Bhubaneswar*

Symposium : F

Alloys and Composites

Topics:

- F-1:** Metallurgical alloys
- F-2:** Soft alloys
- F-3:** Refractory composites
- F-4:** High entropy alloys
- F-5:** Polymer composites

Coordinators:

Dr. Ajaya K Nayak
- *NISER Bhubaneswar*
Dr. Mamata Mohapatra
- *IMMT Bhubaneswar*
Dr. Dinesh Topwal
- *IOP Bhubaneswar*

Symposium : G

Critical and Strategic Materials

Topics:

- G-1:** Ion/electron/photon interactions with materials
- G-2:** Materials for space and radiation hazards
- G-3:** Materials and techniques for national security
- G-4:** Materials from waste and strategic minerals

Coordinators:

Dr. Pratap K Sahoo
- *NISER Bhubaneswar*
Dr. Shyamal Chatterjee
- *IIT Bhubaneswar*
Prof. Tapobrata Som
- *IOP Bhubaneswar*

Symposium : H

Materials Modelling and Simulation

Topics:

- H-1:** DFT for new materials
- H-2:** First principle calculation
- H-3:** Search for emerging materials
- H-4:** Materials modeling methods beyond DFT

Coordinators:

Dr. Joydeep Bhattacharjee
- *NISER Bhubaneswar*
Dr. Prasanjit Samal
- *NISER Bhubaneswar*
Dr. Ashis K Nandy
- *NISER Bhubaneswar*

MRSI-ICEM 2025

Wednesday, December 17, 2025

Registration (Venue: Auditorium)

Inaugural Ceremony (Venue: Auditorium)

High Tea (Venue: Library foyer)

Morning session (Venue: Auditorium)

Session Chair :

International Medal: Prof. P M Ajayan, RICE University, USA (online presentation)

PT-01: Prof. Amar Mohanty, University of Guelph, CA

MRSI-ML-01: Prof. Narayan Chandra Das, IIT, Kharagpur, IN

Lunch (Venue -Library foyer)

	Parallel session - I	Parallel session - II	Parallel session - III	Parallel session - IV	Parallel session - V
	Symposium- A (Venue-LH4)	Symposium- C (Venue-LH5)	Symposium- D (Venue-LH3)	Symposium- G (Venue-LH2)	Symposium- H (Venue-LH 1)
8:00 AM - 9:30 AM	Session Chair	Session Chair	Session Chair	Session Chair	Session Chair
9:30 AM - 11:00 AM	IT-A01: Aswini Pradhan Hampton Uni, USA	IT-C01 Vijaya, Rangari Tuskegee Uni, USA	IT-D01 : Parikshit Moitra IISER-Berhampur, IN	IT-G01: Olivier Plantevin Paris-Saclay Uni, Orsay, FR	IT-H01 : Swapan Pati JNCASR, IN
11:00 AM - 11:30 AM	IT-A02: Siddhartha Ghosh SRM University, IN	IT-C02 : Manjusri Mishra University of Guelph, CA	IT-D02 : Manoj Nayak CSIR-CSIO, IN	IT-G02 Sanjeev Aggarwal Kurukshetra Uni, IN	IT-H02 : Bahadur Singh TIFR-Mumbai, IN,
11:30 AM - 12:15 PM	CT-A01: Anurup Das BARC, IN	CT-C01: Anu Bala Cardiff Catalysis Institute, UK	CT-D01: Prabhat Kumar Chaudhari AIIMS New Delhi, IN	CT-G01: Rumu Halder Banerjee BARC, IN	CT-H01: Anees P IGCAR Kalpakkam, IN
12:15 PM - 12:55 PM	CT-A02: Surajit Ghosh MNIT, Jaipur, IN	CT-C02: Ashish Kumar Kar ESPCI Paris, FR	CT-D02: Kunaal Dhingra AIIMS New Delhi, IN	CT-G02: Durgamadhab Mishra IIT Jodhpur, IN	
12:55 PM - 1:20 PM					
1:20 PM - 2:30 PM					
	Parallel session - I	Parallel session - II	Parallel session - III	Parallel session - IV	Parallel session - V
2:30 PM - 2:55 PM	Symposium- B (Venue-LH4)	Symposium- C (Venue-LH5)	Symposium- E (Venue-LH3)	Symposium- F (Venue-LH2)	Symposium- H (Venue-LH 1)
2:55 PM - 3:20 PM	Session Chair	Session Chair	Session Chair	Session Chair	Session Chair
3:20 PM - 3:32 PM	IT-B01: Atindra Nath Pal SNBNCBS, Kolkata, IN	IT-C03: Kaushik Parida IIT Roorkee, IN	IT-E01 : Deodatta Shinde BARC, Mumbai, IN	IT-F01 : Amit Ranjan RGIPT, IN	IT-H03 : Prasenjit Sen HRI, Allahabad, IN
3:32 PM - 3:45 PM	IT-B02: Abhishek Ranna, MPI-CPFS, DE	IT-C04: Trilochan Mishra NML Jamshedpur, IN	IT-E02: Bobby Joseph Elettra-Sincrotrone Trieste, IT	IT-F02 : Ujjwal Pal CSIR-IICT, Hyderabad, IN	IT-H04 : Rajan Kumar Pandey VIT, Vellore, IN
3:45 PM - 4:10 PM	CT-B01: Edward Prabu Amaldass IGCAR, IN	CT-C03: Pankaj Bhalla SRM University AP, IN		CT-F01: Archana Tiwari BHU, IN	CT-H02: Renjith S VSSC, ISRO, IN
	Parallel session - I	Parallel session - II	Parallel session - III	Parallel session - IV	Parallel session - V
4:10 PM - 4:35 PM					
4:35 PM - 5:00 PM					
5:00 PM - 5:12 PM					
5:15 PM - 6:30 PM					
6:30 PM- 7:30 PM					
7:30 PM- 9:30 PM					

Poster (P-01- P-100) + Tea (Venue: Library 3rd Floor)

Cultural Program (Venue-Auditorium)

Dinner

NOTES: PT: Plenary Talk (40 mins) ; ML- Medal Lecture (25mins); IT: Invited Talk (25 Mins) ; CT: Contributory Talk(12 Mins) ; P: Poster

MRSI-ICEM 2025

Thursday, December 18, 2025

Morning session I (Venue: Auditorium): Session Chair-

Distinguished Materials Scientist: Prof. S M Yusuf, BARC, Mumbai, IN

PT-02: Prof. Umesh V Waghmare, JNCASR, IN

PT-03: Prof. Ashok K Ganguli, IISER Berhampur, IN

Tea break (Venue - Library foyer)

Morning session II (Venue: Auditorium): Session Chair-

MRSI Annual prizes: Prof. Sujit Kumar Ghosh, IISER, Pune, IN

MRSI Annual prizes: Dr. R Vijay, ARCI, Hyderabad, IN

MRSI-ML-02: Dr. Parthasarathi Bera, CSIR-NAL, Bangalore, IN

MRSI-ML-03: Dr. Surya Prakash Singh, IICT, Hyderabad, IN

MRSI-ML-04: Dr. Parveen Saini, CSIR-NPL New Delhi, IN

Lunch (Venue - Library foyer)

Parallel session - I		Parallel session - II		Parallel session - III		Parallel session - IV		Parallel session - V	
Symposium- A (Venue-LH4)		Symposium- C (Venue-LH5)		Symposium- E (Venue-LH3)		Symposium- G (Venue-LH2)		Symposium- H (Venue-LH 1)	
Session Chair		Session Chair		Session Chair		Session Chair		Session Chair	
IT-A03: Jyoti Ranjan Mohanty, IIT-Hyderabad, IN		IT-C05: Sonil Nanda Dalhousie University, CA		IT-E03: Sajesh P Thomas IIT-Delhi, IN		IT-G03: Bibhudutta Rout University of North Texas, USA		IT-H05: Sridhar Sahu IIT(ISM)-Dhanbad, IN	
IT-A04: Tanuja Mohanty JNU, IN		IT-C06: Ashutosh Kumar Singh CeNS, IISc Bangalore, IN		IT-E04: Kailash Jena IIT Ropar, IN		IT-G04: Chandana Rath IIT BHU, IN		IT-H06: Debashis Bandyopadhyay BITS-Pilani, IN	
CT-A03: Shailesh Kumar Khamari RRCAI Indore, IN		CT-C04: Dibyendu Ghosh SNU, IN		CT-E01: Nirman Chakraborty Technische Universität Darmstadt, GE		CT-G03: Neha Shukla, IIT Mandi, IN		CT-H03: Kunchanapalli Ramya, SRM AP, IN	
CT-A04: Ravindra Naik Bukke IIT Mandi, IN						CT-G04: Dilruba Hasina IACS, IN		CT-H04: Nilakantha Tripathy, IIT Ropar, IN	
3:45 PM - 4:15 PM		Tea break (Venue - Library foyer)							

Parallel session - I		Parallel session - II		Parallel session - III		Parallel session - IV		Parallel session - V	
Symposium- B (Venue-LH4)		Symposium- C (Venue-LH5)		Symposium- D (Venue-LH3)		Symposium- F (Venue-LH2)		Symposium- H (Venue-LH 1)	
Session Chair		Session Chair		Session Chair		Session Chair		Session Chair	
IT-B03: Alok Kanjilal Shiv Nadar IE, Delhi, IN		IT-C07: Sanjay Kumar Srivastava Institute of Science, BHU, IN		IT-D03: Mrimov De IISc Bangalore, IN		IT-F03: Chandan Upadhyay IIT (BHU), IN		IT-H07: Abir De Sarkar INST, Mohali, IN	
IT-B04: Ram Shanker Patel, BITS-Pilani (Goa), IN		CT-C05: Anuradha M Ashok PSG-IAS, IN		IT-D04: Subinoy Rana, IISc Bangalore, IN		CT-F02: Ajay Tripathi Sikkim University, IN		IT-H08: Koushik Pal IIT-Kanpur, IN	
4:40 PM - 5:05 PM									

Poster (P-101- P-200) + Tea (Venue: Library 3rd floor)

MRSI-AGM + Award Session (Venue- Auditorium)

Banquet Dinner (Venue: SAC)

NOTES: PT: Plenary Talk (40 mins) ; ML- Medal Lecture (25mins); IT: Invited Talk (25 Mins) ; CT: Contributory Talk(12 Mins) ; P: Poster

MRSI-ICEM 2025

	Friday, December 19, 2025				
	Morning session I (Venue: Auditorium): Session Chair- CNR Rao prize lecture: Prof. V P S Awana, NPL, New Delhi, IN				
9:00 AM - 09:45 AM					
09:45 AM - 10:30 AM	Distinguished lectureship : Dr. B B Kale, Director Research and Development, Pimpri Chinchwad University Pune, IN				
10:30 AM - 11:10 AM	PT-04: Stephan Reitzenstein, Technische Universität, Berlin, DE				
11:10 AM - 11:30 AM	Tea break (Venue - Library foyer)				
11:30 AM - 11:55 AM					
11:55 AM - 12:20 PM	Morning session II (Venue: Auditorium): Session Chair- MRSI-ML-05: Prof. Tharamani C. Nagaiiah, IIT Ropar, IN				
12:20 PM - 12:45 PM	MRSI-ML-06: Dr. Venkata Krishnan, IIT Mandi, IN				
12:45 PM - 01:10 PM	MRSI-ML-07: Prof. Sasanka Deka, University of Delhi, IN				
01:10 PM - 01:35 PM	MRSI-ML-08: Prof. Ayan Datta, IACS, Kolkata, IN				
01:35 PM - 02:30 PM	MRSI-ML-09: Dr Sonu Gandhi, DBT-National Institute of Animal Biotechnology, Hyderabad, IN				
Lunch (Venue - Library foyer)					
	Parallel session - I	Parallel session - II	Parallel session - III	Parallel session - IV	
	Symposium- A (Venue-LH4)	Symposium- C (Venue-LH5)	Symposium- D (Venue-LH3)	Symposium- G (Venue-LH4) 2	
	Session Chair	Session Chair	Session Chair	Session Chair	
2:30 PM - 2:55 PM	IT-A05: Kaushik Mallik, University of Johannesburg, SA	IT-C09: Jatish Kumar Das SRM University, AP, IN	IT-D05: Deepa Ghosh INST, IN	IT-G05: Fouran Singh IUAC, IN	
2:55 PM - 3:20 PM	IT-A06: Kuntala Bhattacharjee, IIST, Trivendrum, IN	"CT-C06: Nisha T P St. Teresa's College Ernakulam, IN	CT-D03: Debendra Prasad Panda Uni. Naples Federico II, IT	IT-G06: Shiv Poojan Patel Delhi University, IN	
3:20 PM - 3:32 PM	CT-A05: Sreekanth G, MITS, Kochi, IN	CT-C07: Sreekanth M. S. VIT, Vellore	IT-D04: Aarti Jaiswal IIT Kanpur, IN	CT-G05: Gopinath Shit IGCAR, Kalpakkam, IN	
2:33 PM - 3:45 PM				CT-G06: A Chitharanjan Hegde NITK Surathkal, IN	
3:45 PM - 4:15 PM	Tea break (Venue - Library foyer)				
	Parallel session - I	Parallel session - II	Parallel session - III		
	Symposium- B (Venue-LH4)	Symposium- C (Venue-LH5)	GC Jain prize talk(Venue -LH3)		
	Session Chair	Session Chair	Session Chair		
4:15 PM - 4:40 PM	IT-B05 : Hari Srikanth University of South Florida, US	IT-C10: Ritesh Haldar TIFR-Hyderabad, IN	GCJP-01: Ashok Kumar, IIT Jodhpur (Online Presentation)		
4:40 PM - 5:05 PM	IT-B06: Ramesh Chandra Nath, IISER-Thiruvananthapuram, IN	IT-C11: Ashutosh Mohanty IITKGP, IN	GCJP-02: Neha Singh, IIT, Kanpur GCJP-03: Rishi Verma, Germany (online presentation)		
5:05 PM - 5:30 PM	IT-B07 : Tannoy Basu TCG-CREST, IN	CT-C08: Somnath Biswas LNMIIT, Jaipur, IN	GCJP-04: Hari Narayanan Vasavan, Sweden (online presentation)		
5:30 PM - 5:42 PM	CT-B03: Ashutosh Kumar CIT, Ranchi, IN	CT-C09: Y. Pushpalatha Devi BARC, Mumbai, IN	GCJP-05: Dalip Saini, IISER, Mohali (Online Presentation)		
5:42 PM - 5:54 PM	CT-B04: Subasa Chandra Sahoo Central University of Kerala, IN	CT-C10: Barnali Dasgupta Ghosh BIT Mesra, Ranchi, IN	SP-01: Raj Saha, KIIT, Bhubaneswar SP-02: Radhika Sandip Patil, Shivaji University, Kolhapur		
5:55 PM - 7:00 PM	Poster (201-311) + Tea (Venue-Library 3rd Floor)				
7:00 PM - 7:45 PM	Cultural Program (Venue-Auditorium)				
7:45 PM - 9:30 PM	Dinner				
NOTES: PT: Plenary Talk (40 mins) ; ML- Medal Lecture (25mins); IT: Invited Talk (25 Mins) ; CT: Contributory Talk(12 Mins) ; P: Poster					

MRSI-ICEM 2025				
Saturday, December 20, 2025				
Morning session I (Venue: Auditorium): Session Chair-				
9:00 AM - 09:25 AM	MRSI-ML-10: Prof. Suresh Kumar Kailasa, Sardar Vallabhai, NIT, Surat, IN			
09:25 AM - 09:50 AM	MRSI-ML-11: Dr. Debmalya Roy, DMSRDE, Kanpur, IN			
09:50 AM - 10:15 AM	MRSI-ML-12: Dr. Dillip K. Pradhan, NIT, Rourkela, IN			
10:15 AM - 10:40 AM	MRSI-ML-13: Prof. Ramesh L Gardas, IIT Madras, Chennai, IN			
10:40 AM - 11:20 AM	Tea break (Venue - Library foyer)			
Morning session II (Venue: Auditorium): Session Chair-				
11:20 AM - 11:45 AM	MRSI-ML-14: Dr. Arijit Sengupta, BARC, Mumbai, IN			
11:45 AM - 12:10 PM	MRSI-ML-15: Prof. Rupesh S Devan, IIT, Indore, IN			
12:10 PM - 12:35 PM	MRSI-ML-16: Dr. Sudip Chakraborty, HRI, Prayagraj, IN			
12:35 PM - 02:00 PM	Lunch (Venue - Library foyer)			
Parallel session - I		Parallel session - II		Parallel session - III
Symposium- A (Venue-LH4)		Symposium- C (Venue-LH5)		Symposium- D (Venue-LH3)
Session Chair		Session Chair		Session Chair
2:00 PM - 2:25 PM	IT-A07: Rajesh Kumar IIT-Indore, IN	IT-C12: Akshaya K. Palai CIPET, Bhubaneswar, IN	IT-D07: B Neppolian SRM University, IN	
2:25 PM - 2:50 PM	CT-A06: Mousm Charan Sahu UCM Madrid, SP CT-A07: Aparajita Mandal, IOP Bhubaneswar	CT-C12: Srabanti Ghosh, CSIR - CGCRI, IN CT-C13: Chandra Shekhar Pati Tripathi, BHU, IN	CT-D05: Manju S. SCTIMST, Trivandrum, IN CT-D06: Kumar Haunsbhavi Uni. of Free State, SA	
2:50 PM - 3:02 PM		CT-C14: Amanpreet Kaur Guru Nanak Dev University, IN	CT-D07: A. Sunil, SSSIHL, AP, IN	
3:05 PM - 3:30 PM	Tea break (Venue - Library foyer)			
Parallel session - I		Parallel session - II		
Symposium- A (Venue-LH4)		Symposium- C (Venue-LH5)		
Session Chair		Session Chair		
3:30 PM - 3:55 PM	IT-A08: Pramoda Kumar Nayak Jain University, IN	IT- C13: Manoranjan Kar IIT-Patna, IN		
3:55 PM - 4:07 PM	CT-A08: Koteswar Rao Peta Uni. of Delhi, South Campus , IN	CT-C15: Rakesh Kumar Behera SCS, NISER, IN		
4:07 PM - 4:19 PM	CT-A09: Ashutosh Thakur CSIR-NEIST, Jorhat, IN			
4:20 PM - 5:00 PM	Valedictory; Poster Awards, and Closing Ceremony			
7:00 PM - 9:00 PM	Dinner			
NOTES: PT: Plenary Talk (40 mins) ; ML - Medal Lecture (25mins); IT: Invited Talk (25 Mins) ; CT: Contributory Talk(12 Mins) ; P: Poster				

Contents

Patrons and Committees	iii
Symposia	MRSI - ICEM 2025 vii
MRSI Awardee Lectures	MRSI-ICEM 2025 1
2D and 3D Phases of Boron-Carbon-Nitrogen (<i>Pulickel M. Ajayan*</i>)	2
Exploring Emerging Magnetic Materials (<i>S M Yusuf</i>)	2
My encounter with superconducting materials (<i>V.P.S. Awana^{1,2*}</i>)	3
Layered organic molecules for energy generation and storage (<i>Dr. Bharat Kale</i>)	3
Critical Minerals Extraction by Functional Metal–Organic Frameworks (MOFs)+ (<i>Sujit K. Ghosh</i>)	4
Development of Advanced Materials and Technologies for Energy (<i>R. Vijay</i>)	5
Eco-friendly Recyclable and Reprocessable Advanced Polymer–Carbon Nanocomposites for Radiation Shielding: Addressing Environmental Pollution and Health Protection (<i>Narayan Chandra Das</i>)	6
Coatings for renewable energy applications (<i>Parthasarathi Bera</i>)	7
Development of Light-Harvesting Materials for Optoelectronic Devices (<i>Surya Prakash Singh</i>)	7
From Designing of Advance Materials to End-of -Life Management of Waste Streams: Holistic Approach for Technologies and Applications Development (<i>Parveen Saini*</i>)	8
Designing greener energy conversion system for a sustainable future (<i>Tharamani C. Nagaiah</i>)	9
Non-noble Metal based Materials as Sustainable Heterogeneous Catalysts for Plastic Waste Upcycling to Multiple Value Added Products (<i>Venkata Krishnan</i>)	10
Engineering Pt and Pd Single-Atom Catalysts on Semiconductors for Improved Photocatalytic Hydrogen Evolution and Oxygen Reduction Reactions (<i>Sasanka Deka</i>)	11
Buckling and Defects in Two - Dimensional Atomically Thin Monolayers (<i>Ayan Datta</i>)	12
Nanomaterials in Action: Translational Advances from Environmental Sensing to Biomedical Applications (<i>Sonu Gandhi</i>)	13
Surface modified nanostructured materials: Promising applications in analytical chemistry (<i>Suresh Kumar Kailasa</i>)	14
Stress-Induced Self-Organization of Nanostructures in Stretchable Matrices for Flexible Electronics (<i>Debmalya Roy</i>)	15
Structural Phase Transitions in Lead Free Ferroelectric Perovskite Oxides (<i>Dillip K. Pradhan</i>)	15
Ionic Liquids and Deep Eutectic Solvents for Sustainable Sorption and Extraction Processes (<i>*Ramesh L. Gardas</i>)	16
Ionic Liquid, Poly(Ionic Liquid) and Ionic Liquid Based Membranes: ‘Green’ Multi-Verse Materials For New Age Applications (<i>Arijit Sengupta</i>)	17
Atomic-layered 2D MXenes:Materials driving innovation in sustainable development and clean energy solutions. (<i>Rupesh S. Devan</i>)	18
Rashba and Excitonic Physics in Emerging Materials and Correlations with Light-Matter Interaction: A Computational Insight (<i>Dr. Sudip Chakraborty</i>)	19

Plenary Lectures	MRSI-ICEM 2025	21
Circular Bio-Economy Driven Sustainable Materials: Future is now in Mitigating the Climate Change (<i>Amar K Mohanty</i>)		22
New Vibrational Spectroscopies based on Quantum Geometry of Electrons (<i>Umesh V Waghmare</i>)		22
Frustrated Magnetism and Topological Electronic States in Noncentrosymmetric and Square-Net Rare-Earth Compounds (<i>Ashok K Ganguli</i>)		23
Single-Quantum-Dot Devices for Photonic Quantum Technologies: Design, Deterministic Nanofabrication, and Application Perspectives (<i>Stephan Reitzenstein*</i>)		24
Invited Talks	MRSI-ICEM 2025	27
Degenerate transparent wide Bandgap semiconductors for multiplication applications (<i>Aswini Pradhan</i>)		28
Aqueous Based Ultra-Small Magnetic Cr-doped CdSe Quantum Dots as a Potential Dual Imaging Probe in Biomedicine. (<i>Siddhartha Ghosh*</i> , <i>Nilja George</i> ¹ , <i>Shamili Bandaru</i> ² , <i>Sabyasachi Chakraborty</i> ²)		28
Emerging 2D borophene for photonics: Tunable nonlinear optical properties of iron oxide/borophene core shell nanostructure (<i>Tanuja Mohanty</i>)		29
Creation and manipulation of magnetic spin texture in ferrimagnetic thin film system for application (<i>Dr. Jyoti Ranjan Mohanty</i>)		30
Janus Sn on WS ₂ and Beyond (<i>Kuntala Bhattacharjee</i>)		30
Tailoring of functional materials for multidisciplinary research (<i>Kaushik Mallick</i>)		31
Multifunctional electrochromic materials and smart device (<i>Rajesh Kumar</i>)		31
Interlayer Excitons and Ultrafast Dynamics in Twisted van der Waals Heterostructures (<i>Pramoda K. Nayak</i> ^{1,2*})		32
Light-Matter Interactions, Contact Engineering and Single Defect Spectroscopy in Engineered 2D Heterostructures (<i>Atindra Nath Pal</i>)		32
Disorder as a Lens: Unconventional Superconductivity in Infinite-Layer Nickelates (<i>Abhishek Ranna</i> ¹ , <i>Romain Grasset</i> ² , <i>Martin Gonzalez</i> ^{3,4} , <i>Dongxin Zhang</i> ⁵ , <i>Wenjie Sun</i> ^{6,7} , <i>Kyuhoo Lee</i> ² , <i>Bai Yang Wang</i> ^{3,8} , <i>Edgar Abarca Morales</i> ³ , <i>Florian Theuss</i> ^{3,9} , <i>Zuzanna H. Filipiak</i> ^{3,9} , <i>Michal Moravec</i> ^{1,10} , <i>Marcin Konczykowski</i> ¹⁰ , <i>Manuel Bibes</i> ² , <i>Yuefeng Nie</i> ^{6,7,11} , <i>Lucia Iglesias</i> ⁵ , <i>Harold Y. Hwang</i> ^{3,9} , <i>Andrew P. Mackenzie</i> ^{1,10} , and <i>Berit H. Goodge</i> ¹)		33
Realization of ZnO@ β -SiC Composite for Neuromorphic Computing (<i>Aloke Kanjila</i>) . .		34
Anomalous temperature-dependent Raman spectrum of van der Waals ferromagnet Fe ₅ GeTe ₂ (<i>Sreelakshmi M. Nair</i> , <i>Aabhaas Vineet Mallik</i> , <i>R. S. Patel*</i>)		35
Anomalous Nernst and Hall Effects in Heuslers and Magnetic High-Entropy Alloys (<i>Hari Srikanth</i>)		35
Proximate spin-liquid behaviour in the double trillium lattice antiferromagnets (<i>Dr. Ramesh Chandra Nath</i>)		36
NV centers in diamond: Boosting quantum sensing through controlled implantation (<i>Tanmoy Basu</i>)		36
Fish scale-based Nano Hydroxyapatite Reinforced Polylactic Acid Composite Blown Film (<i>Vijaya Rangari*</i> , <i>Radhika Panickar</i>)		37
Biocarbon Economy for the 2050 Net Zero Target: Strategies to Reduce the global Carbon Foot print (<i>Manjusri Misra</i>)		37
Wearable Nanogenerators for Next-generation Electronics (<i>Kaushik Parida*</i>)		38
Harnessing the advantage of defects to improve photocatalytic water splitting of 2D tertiary heterojunctions (<i>Trilochan Mishra</i> ¹ , <i>Sudeshna Das Chakraborty</i>)		38
Efforts Toward Developing High-Performance Aqueous Rechargeable Zn-Ion Batteries (<i>Ashutosh K. Singh</i>)		39
Integrating Biorefinery and Waste Management for Environmental Sustainability, Decarbonization and Circular Economy (<i>Dr. Sonil Nanda</i>)		40
Eu ³⁺ -Doped Core-Shell Nanophosphor-Based Fluorescent Biosensor for Highly Selective and Sensitive Detection of Double-Stranded DNA (<i>S. K. Srivastava</i>)		40

Functionalized Spinel Ferrite Nanomaterials as a Unified Platform for Energy Conversion and Storage (<i>N. Kumar, Jatis Kumar Dash*</i>)	41
Manipulating molecular diffusion in nanoporous membrane (<i>Ritesh Halder</i>)	41
Structure, Dielectric Property and Cation Dynamics in $\text{MA}_{1-y}\text{FA}_y\text{PbX}_3$ Perovskites (<i>Dr. Ashutosh Mohanty</i>)	42
DIKETOPYRROLOPYRROLE (DPP) derivatives: Materials design, Optoelectronic and Energy Devices (<i>Akshaya Kumar Palai*</i>)	42
Conducting Filler Stimulated Polymer Nanocomposite-Based Smart Flexible Nanogenerator for Multiple Applications (<i>Manoranjan Kar*</i>)	43
Development of Novel Nanomaterials for Molecular Diagnosis of Certain Rare Genetic Disorders (<i>Parikshit Moitra*</i>)	43
Porous Hierarchical Functional Materials for Detection and Remediation of Food Toxins and Emerging Pollutants (<i>Manoj Kumar Nayak^{1,2*}</i>)	44
Selective Antibacterial Activity: Nanomaterials to Nano-assemblies (<i>Mrinmoy De</i>)	45
Salt-bridge mediated supramolecular systems with augmented catalysis (<i>Subinoy Rana</i>)	45
Biomaterials for tissue repair: Essential factors and engineering techniques (<i>Deepa Ghosh</i>)	46
Role of ultrasonication for material synthesis and environmental remediation (<i>B. Neppolian</i>)	46
Understanding Materials at Near-Atomic Spatial Resolution: An Atom Probe Tomography Perspective (<i>Deodatta Shinde</i>)	47
Ubiquitous isostructural phase transition in tin based alloys under compression (<i>Boby Joseph</i>)	48
Molecular Origin of Piezoelectricity and Flexoelectricity in Crystalline Materials from Micro-XRD and Quantum Crystallography (<i>Sajesh P. Thomas*</i>)	49
Exploring Molecules at Aqueous Interfaces Using Sum Frequency Generation Vibrational Spectroscopy (<i>Kailash C. Jena</i>)	49
Novel oxide semiconductor particles and their composites for adsorptive and photocatalytic removal of dyes and pollutants from liquid phase (<i>Amit Ranjan</i>)	50
From Electronic Band Design to Solar Hydrogen: A Materials-Driven Green Energy Vision (<i>Ujjwal Pal^{1,*}</i>)	50
Role of Chemical Pressure and Magnetic Disorders in Rare-earth Spin-Ices (<i>Chandan Upadhyay</i>)	51
Defect tolerance & defect engineering in hybrid perovskite materials (<i>O. Plantevin¹, S.K. Gautam¹, V.L.R. Jacques¹, M. Kim², B. Geffroy²</i>)	52
Engineering Functional Surfaces with Low-Energy Ion Beams: Role of Surface Composition and Processing Parameters (<i>Sanjeev Aggarwal</i>)	52
Radiation effects on Energetic Materials and Devices (<i>Bibhudutta Rout, Mritunjaya Parashar, Mohin Sharma, Darshpreet Kaur Saini, Soumya S. Sahoo, Todd A. Byers, and Gary A. Glass</i>)	53
Thickness Dependent Phase Transformation and Resistive Switching Performance of HfO_2 Thin Films (<i>Chandana Rath</i>)	53
Ion beams in Organic-inorganic hybrid heterojunction devices (<i>Fouran Singh*</i>)	54
Crystallization dynamics of Si and Ge in metal/semiconductor bilayer thin films under ion irradiation (<i>Shiv P. Patel</i>)	55
Computational Modeling of Materials for finding Glass-like Thermal Conductivity and Quantum Spin Liquid Candidates (<i>Swapan K Pati</i>)	55
Modeling Topology, Flat Bands, and High-Order van Hove Singularities in Quantum Materials (<i>Bahadur Singh</i>)	56
Accelerated Materials Design using Generative AI (<i>Prasenjit Sen</i>)	56
First principles modelling and materials engineering at the gate stack of nanoscale MOS devices (<i>Rajan Kumar Pandey</i>)	57
Functionalized Porous 2D COFs and Macrocyclic Compounds: From Hydrogen Storage to Li-ion Batteries. (<i>Sridhar Sahu</i>)	58
Unveiling newly modelled Janus Nb_2COS MXene as a Promising Anode for Alkali Metal-Ion Batteries: A DFT Investigation (<i>Chaithanya Purushottam Bhat¹, Debashis Bandyopadhyay*</i>)	58

Insights into Inversion Symmetry Breaking in 2D Materials: Piezoelectricity and Spin-Orbitronics (<i>Abir De Sarkar^{a,b}</i> ,)	59
Leveraging Data-driven Approaches and Density Functional Theory to Accelerate Novel Materials Discovery (<i>Koushik Pal^{1,*}</i> ,)	60
GC Jain prize talks	
MRSI-ICEM 2025	61
Modified 2D MoS ₂ and SnS ₂ flakes for Sensing Applications (<i>Ashok Kumar (P19EE203)</i> , <i>Prof. Mahesh Kumar</i>)	61
Inorganic-Organic Heterostructure Devices for Enhanced Electrical Conductivity and Magnetism (<i>Neha Singh^a</i> , <i>Prakash Chandra Mondal^{*a}</i>)	62
Investigating the Interplay between Hot Electrons, Electric Field, and Thermal Effects in Plasmonic Black Gold-Ni Photocatalyst (<i>Rishi Verma</i>)	63
Next-Generation Sodium-Ion Batteries: Coupling Cathode Design with Operando Diagnostics (<i>Hari Narayanan Vasavan</i>)	63
Design of Functional Materials for Multiscale Energy Harvesting and Sensing Applications (<i>Dalip Saini</i> , <i>Dipankar Mandal</i>)	64
Design and Development of Hybrid Memristor (<i>Raj Saha</i> , <i>Udai P. Singh</i>)	66
Detection of Mycotoxin Using Electrochemical Biosensors (<i>Radhika S. Patil</i> , <i>Shivaji B. Sadale</i>)	66
Contributory Talk	
MRSI-ICEM	
2025	67
Symposium: A	67
Optical Properties of Cerium Doped Gd ₂ O ₃ -SrO-P ₂ O ₅ -SiO ₂ (GSPS) Glass for Scintillator Applications (<i>Anurup Das</i> , <i>Ashok K. Sahu</i>)	68
Experimental Investigation Combined with Physics-Based Modelling of Vacancy-Controlled Switching in V ₂ O ₅ /ITO Memristors (<i>Aparajita Mandal^{1,*}</i> , <i>Rupam Mandal^{1,2}</i> , <i>Tapobrata Som^{1,2,*}</i>)	68
Solid-State Phosphors from Coal-Derived Carbon Quantum Dots for White-Light-Emitting Devices (<i>Ashutosh Thakur^{1,2,*}</i> , <i>Priyanka Gogoi^{1,2}</i> , <i>Binoy K. Saikia^{1,2,*}</i>)	69
Synthesis Strategies of Various Zinc Oxide Nanostructures and Their Potential Applications (<i>Koteswara Rao Peta</i>)	70
Third-Order Nonlinear Optical, Thermal, Dielectric and Ferroelectric Characteristics of Tri-allylthiourea Cadmium Chloride Single Crystals (<i>Arun Rajan</i> , <i>and Sreekanth G</i>)	70
Mimicking Neural Complexity Leveraging the Metal-Insulator Transition in Rare Earth Nickelates (<i>M. C. Sahu</i> , <i>B. G. Ruiz</i> , <i>J. Tornos</i> , <i>L. Perez</i> , <i>C. Leon</i> , <i>J. Santamaria</i> , <i>M. Romera</i>)	71
High-Performance Zinc-Tin Oxide Semiconductor-Based Thin Film Transistors (<i>Ravindra Naik Bukke[*]</i> , <i>Ananay Sharma</i> , <i>Abhinav Agarwal</i>)	71
Photoluminescence Intensity and Polarization Enhancement in GaAs QW-Microcavity System (<i>Shailesh K. Khamari^{1,2+}</i> , <i>Geetanjali Vashisht¹</i> , <i>S. Porwal¹</i> , <i>V. K. Dixit^{1,2}</i> , <i>T. K. Sharma^{1,2}</i>)	72
Applications of Sol-Gel Synthesized Perovskite Zinc Titanate Photocatalysts (<i>Surajit Ghosh¹</i> , <i>Urmimala Naha²</i>)	73
Symposium: B	74
Electronic and magnetic attributes of highly correlated vanadium-oxides (<i>Dr. Ashutosh Kumar</i>)	75
Current redistribution induced anomalous Magneto-transport signatures in the Superconductor/Topological insulator (Mo/Bi ₂ Se ₃) heterostructure (<i>Edward Prabu Amaladass^{1,2a)}</i> , <i>Shilpam Sharma³</i> , <i>Awadhesh Mani^{1,2)}</i>)	75
Effect of diamagnetic Zn-substitution on Enhancement of Magnetization in Ni-ferrite nanop (<i>C.N. Anumol</i> , <i>M. Chithra^{1,3}</i> , <i>Baidyanath Sahu⁴</i> , <i>Subasa C. Sahoo</i>)	76
Symposium: C	76
Bimetallic coordination network for ultrahigh performance in supercapacitor energy storage applications (<i>Amanpreet Kaur</i>)	77

Green Halide Perovskites as Next-Generation Photocatalysts: A Rational Design Approach (<i>Anu Bala, David Willock</i>)	77
Strategies for effective enhancement of Thermoelectric power conversion efficiency of complex oxides (<i>Anuradha M Ashok*, Nithya davis, Navya John</i>)	78
METAL-ORGANIC FRAMEWORK FOR HYDROGEN PRODUCTION BY PHOTOCATALYTIC OVERALL WATER SPLITTING (<i>Ashish Kumar Kar¹, Edouard Vögtli¹, Vanessa Pimenta¹, Sergio Navalón², Hermenegildo García², Georges Mouchahamv¹, Christian Serre²</i>)	79
Ag doped ZnO/PVDF Composites: An Excellent Piezoelectric Energy Harvesting and Storage Material for Smart Wearable and Security Devices (<i>Barnali Dasgupta Ghosh*</i>)	79
Improved Piezocatalytic Performance of BaTiO ₃ -Based Heterostructure Nanocomposites for Environmental Remediation (<i>Chandra Shekhar Pati Tripathi^{1,*}, Mohd Ali¹, Renuka Singh², Debanjan Guin²</i>)	80
Synergistic Spin Polarization and Catalytic Enhancement in Transition Metal Oxide Under Magnetic Bias (<i>Dibyendu Ghosh^{1,2}, Krishnendu Roy¹, Soumyajit Maitra¹, and Praveen Kumar¹</i>)	81
Tailoring 2D nanostructures: Strategies for enhanced electrocatalytic hydrogen production (<i>Nisha T. Padmanabhan</i>)	81
UV absorption and photocatalytic properties of graphitic-carbon coated 8 mole% yttria-stabilized zirconia nanoplatelets (<i>A. Mishra and S. Biswas*</i>)	82
Next-Generation Semiconductor Heterostructures in Solar Fuel Production: Unveiling Trends and Underlying Mechanisms (<i>Srabanti Ghosh^{1,2}</i>)	82
Investigation of Hydrogen Evolution Reaction in Two-Dimensional Transition Metal Dichalcogenides Through Experimental, Theoretical DFT and Machine Learning Approach (<i>Sukanti Behera*, Avala Ramesh</i>)	83
Development and Characterization of Y-rich Zr–2.5Nb Alloys for Hydrogen Gettering Applications (<i>Y. Pushpalatha Devi^{1,2}, K. V. Mani Krishna^{1,2*} and R. N. Singh^{1,2}</i>)	84
Field driven orbital Hall conductivity in time reversal symmetry broken Weyl semimetals (<i>Pankaj Bhalla, Dayana Joy¹</i>)	84
Improved Tribo-performance of MoS ₂ functionalized MWCNTs hybrid reinforced epoxy composites for severe erosion conditions (<i>Arun Sam Varghese, Sreekanth M. S.*</i>)	85
Ultrafast Charge Carrier Dynamics in CsPbBr ₃ –PbSe Epitaxial Nanocrystal Heterostructures (<i>Rakesh Kumar Behera¹, Hirendra Nath Ghosh^{1*}</i>)	85
Symposium: D	85
A Smart Clay Biosensor: Luminescent Clays for On-Site Phosphate Detection (<i>A. Sunil*</i>)	86
Rapid detection of Punica granatum juice adulteration via Eco-friendly AgNPs synthesised from Zingiber officinale (<i>Aarti Jaiswal¹, K. N. Uttam², Raju Kumar Gupta^{1,2,3,4}</i>)	86
Biodegradable Radiopaque Microbeads for Trans-Arterial Chemoembolization for Hepatocellular Carcinoma (<i>Manju Saraswathy*, Jinsu Mariya Sam, Vidya Unnikrishnan Geetha, Rahul Ravi</i>)	87
DMSO-Free Tin Perovskites Solar Cells (<i>Debendra Prasad Panda¹, Antonio Abate^{1,*}</i>) . .	88
Direct 3D-Printed Aligners: Integrating Material Science and Digital Orthodontics for Next-Generation (<i>Prabhat Kumar Chaudhari^{1,*}, Abirami R², Ritu Duggal³</i>)	88
Fabrication of Gd-doped In ₂ S ₃ thin films prepared by nebulised spray pyrolysis for photodetector applications (<i>Kumar Haunsbhavi*, David E Motaung**</i>)	89
Chlorhexidine polymer-based electrospun local drug delivery scaffold for treating periodontitis (<i>Kunaal Dhingra*</i>)	89
Symposium: E	89
Operando probing of functional surfaces towards real-time monitoring of surface-analyte hybridization routes (<i>Nirman Chakraborty¹, Efrat Lifshitz² and Christian Hess^{1*}</i>)	90
Symposium: F	90
Laser ablation Synthesis for High Entropy Alloy Nanoparticle (<i>Ajay Tripathi^{1*}</i>)	91
Effects of doping and nanostructuring on magnetic and thermoelectric properties of multicomponent alloys (<i>Archana Tiwari</i>)	91
aterials selection and properties: Tailoring EMI shielding efficiency of polymer composites (<i>Manobalan S., Sumangala T. P.*</i>)	92

Symposium: G	93
Novel Processes for Development of Rare Earth Free Nanoscale Magnetic Materials with Tailored Morphologies for Permanent Magnets (<i>Durgamadhab Mishra*</i> , <i>Nishtha Vats</i> , <i>Sampat Raj Vadera</i>)	94
Sustainable Solutions for Next-Generation Electronics: The Role of E-Waste Recycling (<i>Neha Shukla*</i> , <i>Sharin Jaswal</i>)	94
Effect of Carbonate Substitution on Radiation Stability of Fluorapatites (<i>Rumu H Banerjee^{a,*}</i> , <i>Rohini Garg^b</i> , <i>Jaisri Sanwal^c</i> , <i>Kulwant Singh^{a,d}</i> and <i>Pranesh Sengupta^{a,d}</i>)	95
Magneto-electrodeposition of Ni-V alloy coatings for better corrosion protection (<i>Aishwarya S Suvarna</i> , <i>A Chitharanjan Hegde*</i>)	96
Effect of Ion Irradiation on the Corrosion Resistance Behaviour of SS 304L (<i>Gopinath Shit^{*,1}</i> , <i>Satyaprakash Sahoo²</i> , <i>S. Ningshen¹</i>)	96
Controlled Bi-directional Threshold Switching Behaviours for Random Number Generation Applications (<i>Dilruba Hasina^{1,2}</i> , <i>Aparajita Mandal¹</i> , <i>Mahesh Saini^{1,2}</i> , <i>Sanjeev Kumar Srivastava³</i> , and <i>Tapobrata Som^{1,2,*}</i>)	97
Symposium: H	97
Particle-to-wave-like crossover in thermal transport of materials: A Wigner formulation approach (<i>Anees Pazhedath^{1,2*}</i>)	98
Molecular Dynamics Simulation for Predicting the Physical Properties of Cured Hydroxy-Terminated Polybutadiene (HTPB) / Toluene Diisocyanate (TDI) System (<i>Renjith S. Pillai*</i> , <i>K. P. Vijayalakshmi</i> , <i>Deepa Devapal</i>)	98
Computational Insights into Biomarker Adsorption on Functionalized Ti ₃ C ₂ T _x MXenes for Neurodegenerative Disease Sensing (<i>Kunchanapalli Ramya*</i> , <i>Sabyasachi Mukhopadhyay</i>)	99
Harnessing Ferroelectricity for Multifunctional 2D Materials (<i>Nilakantha Tripathy</i> , <i>Rajeev Ahuja</i>)	100
Posters	MRSI-ICEM 2025101
Symposium: A	101
Optoelectronic properties of ZnO/NiO based Heterostructures (<i>Aiswarya Rath</i> , <i>Dr. Pratap Kumar Sahoo</i>)	101
Rabi splitting mediated dual electromagnetically induced transparency in a metamaterial (<i>Amit Halder</i> , <i>Kshitij V. Goyal</i> , <i>Ruturaj V. Puranik</i> , <i>Vivek Dwij</i> , <i>Srijan Maity</i> , <i>Kanha Ram Khator</i> , <i>Subhashis Ghosh</i> , <i>Bhagwat S. Chouhan</i> , <i>Gagan Kumar</i> , <i>Satyaprasad P. Senanayak</i> , <i>Shriganesh Prabhu</i> , and <i>Shovon Pal</i>)	101
Influence of thermal annealing on the resistive switching and neuromorphic behaviour of GaOx-based ReRAM devices (<i>Ankita Ghosh</i> , <i>Rupam Mandal</i> , <i>Aparajita Mandal</i> , <i>Tapobrata Som</i> ,)	102
Study of Charge-transfer(C-T) Electroluminescence in TAPC: TmPyPB Bulk-hetero junction OLEDs (<i>Arghya Saha</i> , <i>Debdutta Ray</i>)	102
Oxygen-Vacancy-Mediated Z-Scheme Charge Transfer in Mixed-Phase TiO ₂ @B-Doped g-C ₃ N ₄ Heterojunction for Photocatalytic Degradation of Antibiotics (<i>Arjun Behera</i>)	103
Plasmonic Electromagnetic Damping by Hofmeister Series: Does It Follow the Electrochemical Order? (<i>Barnali Saha</i> , <i>Sujit Kumar Ghosh</i>)	104
Solvent dependent crystal packing of a F-appended Schiff Base: Non-Linear Optical property and selective cation detection (<i>Bebina Swain</i> , <i>Basudeb Dutta*</i> , <i>Rojalin Sahu*</i>)	105
Large Area Film of Highly Crystalline, Cleavable, and Transferable Semi-Conducting 2D-Imine Covalent Organic Framework on Dielectric Glass Substrate (<i>Diksha Srivastava</i> , <i>Vipin Mishra</i> , <i>Showkat H. Mir</i> , <i>Jyotirban Dey</i> , <i>Jayant K. Singh</i> , <i>Manabendra Chandra</i> , <i>Thiruvancheril G. Gopakumar</i>)	105
Defect-Rich Wide-Bandgap Li ₂ ZrO ₃ Engineered for Multiple Functionalities through a Cation Doping Scheme (<i>Inderjeet Singh</i> , <i>Sachin Pal</i> , <i>Sitharaman Uma*</i> , <i>Rajamani Nagarajan*</i>)	106
Effect of Na Doping on the Power Conversion Efficiency of Cu ₂ ZnSnS ₄ Solar Cells (<i>John Paul</i> and <i>Sagar Agrawal*</i>)	107

2D MoS ₂ Self-Powered Photodetector with Broadband Photodetection and Polarization Sensitivity (<i>Khondram Bijoykumar Singh, Arup Ratan Pal</i>)	107
EDTA-assisted defect modification of scheelite-type NaEu(WO ₄) ₂ functional material for optoelectronic application and a prototype fabrication of red LED (<i>Kumar Riddhi-man Sahoo, Chandan Kumar Ghosh*</i>)	108
Effect of Post Annealing on Zinc Phthalocyanine Film Grown by Close Space Sublimation Method (<i>Laxman Singh</i>)	108
MoS ₂ /VO ₂ Based Heterostructure Device for Highly Responsive Infrared Photodetection (<i>Malti Kumari,Basanta Roul,S. B. Krupanidhi, K. K. Nanda</i>)	109
Dopant induced room temperature phase transition in vanadium dioxide thin films (<i>Mayank Dotiyal , Emila Panda</i>)	109
Studies of Nickel doped Copper Oxide nanosheets for optoelectronic device applications. (<i>Megha Rana, Riya Malik,Suraj P. Khanna, Ritu Srivastava, C. K. Suman</i>)	110
Phonons and Structural Phase Transition Study of Hybrid Organic-Inorganic Perovskite-based Molecular Ferroelectrics (<i>Monalisa Pradhan,Aiswarya Abhisek Mohapatra,Ashish Anand,Diptikanta Swain,Gopal K. Pradhan</i>)	111
Hierarchically Structured Co _{1-x} Ni _x O/Laser-induced Porous Graphene Nanohybrids for Photocatalytic Dye Degradation (<i>Mutcha ShanmukhaRao, ShradhaSuman, Benadict Rakesh , Ramasamy Sakthivel,Kamatchi Jothiramalingam Sankaran</i>)	111
Effect of reduced graphene oxide on solution combustion synthesized chromium oxide towards ethanol sensing (<i>Namitha N.N, A. Sree Rama Murthy*</i>)	112
Formulating Iodine-integrated SmTaO ₄ for Efficient Visible-Light-Driven Degradation of Fluorene: A Synergistic Rare-Earth–Halogen Approach (<i>Presenting Author: Netra Prova Baruah, Co-Authors: Haimyapriya Buragohain, Palash Jyoti Medhi, Prof. Ramesh Chandra Deka, Prof. Dirtha Sanyal, Dr. Biswajit Chowdhury, Prof. Deva-sish Chowdhury</i>)	113
Energy-Efficient Organic Bilayer Crossbar Memristor with Tunable Switching (<i>Nikhitha Rajan, Ayash Kanto Mukherjee</i>)	113
Tunable plasmonic response in Ag nanoparticle doped ZrN thin films (<i>Nikita Choudhary, Prasanna Das, Bivas Saha, Praveen Garg, Uday Deshpandey, R. Venkatesh and Mukul Gupta</i>)	114
Synthesis and Photoluminescence Properties of KPbFe _{2-x} (PO ₄) ₃ : xNd ³⁺ , x = 0.01, 0.05 and 0.1 Doped Phosphors for NIR-Emission (<i>Prabhakar Lalchand Yadav, Sathasivam Pratheep Kumar</i>)	114
2D SnS ₂ thin film-based Pyrophototronic Photodetector (<i>Prag Ranjan Das, Arup Ratan Pal</i>)	115
Stabilization of the black-phase of FAPbI ₃ perovskite by multi-dentate chelating agents (<i>Riju Paria, Anik Biswas, Ravichandran Shivanna</i>)	116
Sustainable and Self-Powered NiO/TiO ₂ p–n Heterojunction for High-Performance UV Sensing (<i>Samim Hossain , P Murugavel and Somnath C Roy</i>)	116
Terahertz Spectroscopy for Probing Intrinsic Optical Properties of Covalent Organic Frameworks (<i>Satyapriya Nath,Saiprakash Rout,Shriganesh S. Prabhu,Himansu S. Biswal,and Bishnu P. Biswal</i>)	117
Optimization of Metal nitride – based memristor for resistive switching and neuromorphic application through reactive sputtering technique (<i>Shanu Bandyopadhyay,Sreelakshmi N,Aparajita Mandal, and Tapobrata Som</i>)	118
Tuning nonlinear optical response of MoS ₂ monolayer by plasmonic effect with gold nanoparticles of different shapes (<i>Shruti Narayanan,Sugandh Sirohi,Lavudya De-vendra,Bhagyalarxmi Pothal,Manu Jaiswal,Gurvinder Singh,and Prem B. Bisht</i>) . .	118
Printed Ti ₃ C ₂ T _X MXene–High Entropy Oxide Hybrid Sensor for Selective Detection of Ammonia and VOCs (<i>Simma Shiv Prasad,Lakkimsetti Lakshmi Praveen,Kiran Manjappa,and Saumen Mandal</i>)	119
A Comprehensive Comparison On Photodegradation In Tertbutyl Carbazole Based TADF Materials For Efficient Designing (<i>Smarak Islam Chaudhury, Pachaiyappan Raja-malli</i>)	119

Third-Order Nonlinear Optical, Thermal, Dielectric and Ferroelectric Characteristics of Tri-allylthiourea Cadmium Chloride Single Crystals (<i>Arun Rajan, and Sreekanth G</i>)	120
Metal oxide microflower-based optoelectronic memristor for in-sensor computing applications (<i>Subhashree Sahoo, Aparajita Mandal, Shanu Bandyopadhyay, Pratap K. Sahoo, and Tapobrata Som</i>)	121
Versatile Metal Phthalocyanine-based Memristive Nanowire Network (<i>Sudeshna Maity, Aparajita Mandal, Prabhanjan Pradhan, Ankita Ghosh, Dinesh Topwal, Biplab K. Patra, and Tapobrata Som</i>)	121
Multiplexed On-Site Detection of Heavy Metal Ions in Water Using an IoT-Enabled Metal Chalcogenide Platform (<i>Suprabha S. Dixit, Sayali S. Harke, Pranava Bhamidipati, Aditya Jadhav, and Chitra Gurnani</i>)	122
Controlled hydrothermal synthesis of La-doped CdTe nanomaterial for enhanced optoelectronic applications (<i>Swikruti Supriya, and Ramakanta Naik</i>)	123
Negative differential resistance in reduced graphene oxide wrapped silicon nanorods: effect of illumination (<i>Sudipta Chakrabarty, Syed Minhaz Hossain</i>)	123
Tunable Photocatalytic and Luminescent Properties of CVD-Grown Boron Carbon Nitride Thin Films (<i>Reema Nayak, Rashmi Acharya, Aiswarya Rath, Subrata Jana, Pratap K. Sahoo, and Prasanjit Samal</i>)	124
Symposium: B	125
Angle-dependent growth of 2D MoS ₂ monolayer, bilayer by chemical vapor deposition method (<i>Abhishek Kumar Pandey, Ajay Kumar Mishra</i>)	125
Investigation of spin-wave dynamics in Co ₂ Fe _{0.4} Mn _{0.6} Si Heusler alloy by using Ferromagnetic Resonance technique (<i>Abinash Mishra, Baisali Ghadai, Kirti Kirti, Sucheta Mondal,</i>)	125
Tuning magnetic anisotropy and spin states in a correlated 4d itinerant ferromagnet through the proximity of geometrically designed polar metal (<i>Aditya Mehta, Harisankar S, Shweta G Bhat, Ketan S Navale, Krushna R Mavani, Debakanta Samal,</i>)	126
Non-trivial magnetic order in the frustrated spin-1/2 depleted-kagome antiferromagnet Cu ₇ (TeO ₃) ₂ (SO ₄) ₂ (OH) ₆ (<i>K. U. Akshay, Sebin J. Sebastian, Q.-P. Ding, Y. Furukawa, R. Nath,</i>)	127
Investigation of Magneto-Transport Properties in Si/Ta/FeMn Heterostructures Deposited by RF Magnetron Sputtering (<i>Amod Kumar, Aman Kumar Singh, Roshna S H, Prahallad Padhan,</i>)	127
Insights into the Electronic Structure of Parkerite Ni ₃ Bi ₂ Se ₂ (<i>Amritpal, Mukesh Kr Dasoundhi, Sanjoy Kr Mahatha,</i>)	128
Engineering Magnetic Anisotropy in Co ₂ FeAl Thin Films Through Columnar growth on Rippled and Flat Substrates (<i>Amruta A, Sharanjeet Singh, Anup Kumar Bera, Pooja Gupta, Sarathlal Koyiloth Vayalil, Benedikt Sochor, Dileep Kumar</i>)	128
Effect of thickness on Resistive Switching Characteristics of Hafnium Zirconium Oxide (Hf _{0.75} Zr _{0.25} O ₂) thin films (<i>Anita, Ashok Kumar,</i>)	129
Spin Hall conductivity, magnetoresistance, and nontrivial topology in BeAu (<i>Arka Bhowmick, Jaspreet Singh, V. Kanchana,</i>)	130
Evidence of relativistic field-derivative torque in nonlinear THz response of magnetization dynamics (<i>Arpita Dutta¹, Pratyay Mukherjee², Swosti P. Sarangi¹, Somasree Bhattacharjee², Christian Tzschasche³, Debankit Priyadarshi⁴, Kouki Mikuni⁵, Takuya Satoh⁵, Ritwik Mondal², and Shovon Pal^{1,*}</i>)	130
Griffiths-like Phase, Spin-phonon coupling and large exchange bias in disordered GdSrCoMnO ₆ (<i>Aswin Kumar Burma^{1,2,*}, Gyanti Prakash Moharana^{1,*}, Nawaz Sarif⁴, Hanuma Kumar Dara¹, Debendra Prasad Panda⁵, Sachindranath Sarangi^{1,2}, Diptikanta Swain³, Debakanta Samal^{1,2}</i>)	131
Experimental Observation and Microscopic Modeling of Skyrmion in Co/Gd Synthetic Ferrimagnetic Heterostructure (<i>Bhuvneshwari Sharma¹, Shaktiranjana Mohanty¹, Brindaban Ojha¹, Soumyaranjan Das², Sanjeev Kumar², Subhankar Bedanta^{1,3,*}</i>)	132
The Superconducting Diodes (<i>Biswajit Maharana, Kartik Senapati,</i>)	133
Spin Hall mediated Josephson Diode effect in Pt barrier (<i>Debashree Nayak, Kartik Senapati,</i>)	133

Interfacial modulation of magnetic anisotropy in infinite-layer cuprate/manganite heterostructure (<i>Digbijaya Palai^{1,2,*}, K. Lal³, D. Sahoo⁴, P. Sharma⁵, B. Samantray³, G. Tripathy^{1,2}, R. Soni⁴, N. Ganguli⁵, Z. Hossain³, D. Samal^{1,2}</i>)	134
Quantum Phases and Altermagnetism of a Bipartite Square-lattice in an Extended Hubbard Model (<i>Gaurav Chouhan^{1,*}, Dayasindhu Dey², Rajamani Raghunathan¹</i>) .	134
Quantitative Kerr microscopy in Epitaxial Fe Thin Films (<i>Gyana Ranjan Kar¹, Swayang Priya Mahanta¹, Rupalipriyadarshini Chhatoi¹, Esita Pandey¹, Subhankar Bedanta^{1,2,*}</i> ,)	135
Quantum dot and half-metal due to disruption by topological defects at edge of zigzag graphene nano ribbon (<i>Hemant Lohumi, Joydeep Bhattacharjee*</i>)	135
Effect of hybrid modes on the spin-torque efficiency in the FM/FiM heterostructure (<i>Jayita Paul¹, Kshitij Singh Rathore¹, Abhisek Mishra¹, Shubhansu Sahoo¹, Subhankar Bedanta^{1,*}</i>)	136
Persistence of Incommensurate Charge Ordering in Ligand-Disordered 1T TaSeTe (<i>Jyoti Sharma¹, Sambit Choudhury¹, Hemant Singh¹, Kai Rossnagel^{2,3}, Sanjoy Kr. Mahatha^{1,*}</i>)	137
Magnon mediated spin pumping by coupled ferrimagnetic garnets heterostructure (<i>Kshitij Singh Rathore^{1,*}, Anupama Swain¹, Pushpendra Gupta¹, Abhisek Mishra¹, Gary Lee², Jinho Lim³, Ramanathan Mahendiran², Axel Hoffmann³, Subhankar Bedanta^{1,4}</i>)	137
Investigation of magnetic and magneto-transport properties in non centrosymmetric antiferromagnetic semimetal GdGaSi (<i>Manikantha Panda, Prabuddha Kant Mishra, Sonali S. Pradhan, V. Kanchana, Tapas Paramanik</i>)	139
Synthesis and Characterisation of Single Crystals of Type-II Dirac semimetal 1T-PdSeTe (<i>M. Yadav, P. Das, K. Yadav, S. Patnaik</i>)	139
Chiral Phonon in XY type 2D layer magnet CrCl ₃ (<i>Mrinal Deka, Prahlad Kanti Barman, Ashutosh Srivastava, Shaunak Sarkar, Prasanta Kumar Mudulli, Abhishek Singh, Abhishek Misra</i>)	140
Joint Wannier Centers (JWCs) in Topological insulators and heterostructures: topological transition from the perspective of chemical bonding (<i>Nabendu Mondal, Joydeep Bhattacharjee,</i>)	140
Turning Superparamagnetic Nanoparticles into Ferromagnetic at Room Temperature via Molecular Functionalization for Magnetic Memory Applications (<i>Neha Singh, Anurag Pritam, Vikram Singh, Konstant Katin, Jonas Fransson, Prakash Chandra Mondal</i>)	141
Comparative Investigation of Exchange bias in Fe ₃ O ₄ @NiO Core shell Structure by varying Shell thickness. (<i>Nilja George, Shamili Bandaru, Sabyasachi Chakaraborty, Siddhartha Ghosh</i>)	142
Correlated Structural, Magnetic, and Transport Behavior in Ce ₂ FeAl ₃ (<i>Nilofar Kurawle, Smita Borole, Sudhindra Rayaprol</i>)	142
Strong Correlations in Rare-earth Intermetallic Compounds (<i>Payel Shee, Chia-Jung Yang, Tanaya Halder, Nainish Tickoo, Shishir Kumar Pandey, Ashis Kumar Nandy, Anamitra Mukherjee, Ruta Kulkarni, Arumugam Thamizhavel, Manfred Fiebig, Shovon Pal</i>)	143
Microwave synthesis of BiAgOTe Nanosheets for Photoresponse Properties (<i>Prabhukrupa Chinmay Kumar, Ramakanta Naik</i>)	144
Strong Correlations in Rare-earth Intermetallic Compounds (<i>Prakriti Mishra, Muhammed Ali A V, H. S. S. Ramakrishna Matte</i>)	144
Determination of Topological Characteristics in Single Crystals of WTe ₂ by Magnetoresistance Measurements (<i>P. Das, D. Das, P. Kumar, M. Yadav, S. Patnaik</i>) . . .	145
Emergent Non-collinear Magnetism in Cu-based Layered Hybrid Perovskites (<i>P. Biswal, Sagar Sarkar, S. N. Sarangi, Arvind Kumar Yogi, Subhendra D. Mahanti, G. Tripathy, Ashis K. Nandy, Diptikanta Swain, D. Samal</i>)	146
Temperature-induced spin-reorientation transition (SRT) in FeCoB/Pt multilayers with perpendicular magnetic anisotropy (<i>Rahul Vishvkarma¹, Md. Shahid Jamal¹, Pooja Gupta², Mukul Gupta¹, and Dileep Kumar^{1,*}</i>)	146

Optimization of Bi ₂ Se ₃ /MoSe ₂ Heterostructure for a Tunable Interfacial Vibration Mode (<i>Rashmi Ranjan Das, Pratap Kumar Sahoo</i>)	147
Interface-induced spin-orbit coupling mediated weak antilocalization effect in La _{0.7} Sr _{0.3} MnO ₃ thin films on (001) oriented Si substrate (<i>Rasmi Ranjan Mohapatra, Santosh Kumar Sahu, Sandip Kumar Padhi, Umesh Kumar Sinha, and Prahallad Padhan</i>)	148
Magnetic Hardening via Strain in Co ₂ FeAl Heusler Alloy Flexible Films (<i>Rupalipriyadarsini Chhatoi¹, Swayang Priya Mahanta¹, Shubhransu Sahoo¹, Soubhagya Dash¹, Abhisek Mishra¹, Esita Pandey¹, Subhankar Bedanta^{1,2}</i>)	148
Evolution of electronic structure in Weyl semi-metal Mo _x W _{1-x} Te ₂ (<i>Sambit Choudhury¹, Jyoti Sharma¹, Amritpal¹, Raman Sankar², Sanjoy Kr Mahatha^{1,*}</i>)	149
Interface-induced enhanced magnetic anisotropy and observation of dual magnetoresis- tance in LSMO thin films on (001) Si substrate (<i>Sandip Kumar Padhi, Santosh Kumar Sahu, Rasmi Ranjan Mohapatra, Umesh Kumar Sinha, and Prahallad Pad- han</i>)	150
Development of a Time-Resolved Magneto-Optical Kerr Effect (TR-MOKE) Setup for Probing Ultrafast Spin Dynamics in Magnetic Heterostructures (<i>Saumya Prasad Jena, Subhankar Bedanta</i>)	150
Exploring Local Structural Distortion and Magneto electric Behavior in Skyrmion Host Cu ₂ OSeO ₃ (<i>Sayari Ghatak^{1,2}, Abhishek Das^{1,2,3}, Subhadeep Moulick⁴, Sudip Ghosh⁵, A. Sunderasen⁵, Atindra Nath Pal⁴, Dinesh Topwal^{1,2}</i>)	151
Proton Irradiation Studies on Bi _{1.95} Sb _{0.05} Se ₃ Topological Insulator Thin Films (<i>Shiv- ani Soni^{1,2}, Akhilesh Kumar^{1,2}, Edward Prabu Amaladass^{1,2,*}, Jegadeesan P¹, S. Amirthapandian^{1,2}, Kishore K. Madapu^{1,2}, Ramanathaswamy Pandian^{1,2}, Awad- hesh Mani^{1,2}</i>)	152
Artificial Synaptic Behaviour of Ag/Ti ₃ CNT _x /PMMA/ITO-Pet Nanocomposite Thin Films (<i>Shraboni Ray¹, Pranab Kumar Sarkar^{1,*}</i>)	153
Enhanced electrochemistry at Ti ₃ C ₂ T _x MXene edge (<i>Shubham B. Upadhye¹, Gopal Pradhan², Pranati Nayak^{1,*}</i>)	154
Quantitative Evaluation of Spin-Orbit Torque Efficiency in Mn ₂ Au Antiferromagnet- Based Heterostructures (<i>Shubhransu Sahoo¹, Abhisek Mishra¹, Manik Kuila¹, Soub- hagya Dash¹, Kshitij Singh Rathore¹, Jayita Paul¹, Subhankar Bedanta^{1,*}</i>)	154
Study of β -W/CoFeB Bilayer Device for Spintronic Application (<i>Sonali Patanjoshi¹, Vijay Kumar^{2,3}, and Alope Kanjilal^{1,*}</i>)	155
LARGE INVERSE ORBITAL HALL EFFECT IN Cr/Pt/Co ₄₀ Fe ₄₀ B ₂₀ THIN FILM HETEROSTRUCTURES (<i>Soubhagya Dash¹, Manik Kuila¹, Shubhransu Sahoo¹, Abhisek Mishra¹, Subhankar Bedanta^{1,*}</i>)	155
Orbital glass behaviour and local symmetry breaking in charge-transfer insulating CoFe ₂ O ₄ (<i>Soumya Shephalika Behera¹, Arvind Kumar Yogi¹, Rajeeb Rawat¹, V. R. Rao Medicherla^{2,*}, Parasmani Rajput^{3,4}, Archana Sagdeo^{5,4}, Vasant Sathe¹, and R. J. Choudhary^{1†}</i>)	156
Soft Magnetic Composites of Fe-Alloys and Mn-Zn Ferrite: Structural and Magnetic Properties for Advanced Electronics (<i>Sriram Jeyaram, R. Justin Joseyphus[*]</i>)	157
Quantum criticality in the Frustrated Kondo Screened Two-Impurity Model (<i>Sukalyan Deb, Abhirup Mukherjee, Siddhartha Lal[*]</i>)	157
Growth Optimization of MoS ₂ and Influence of Au Plasmonic on Excitonic Luminescence (<i>Surjyakant Mangaraj[*], Ankita Dey, Rashmi R. Das, Pratap K. Sahoo[*]</i>)	159
Correlation of crystal field distribution with magnetic properties in (Ca, Ga)-substituted strontium hexaferrite (<i>Sushree Nibedita Rout¹, Babaji Charan Sahoo², Sher Singh Meena², Manoranjan Kar^{1,*}</i>)	159
Electric field driven nanoscale memory in π -bonded organic molecules and inorganic quan- tum dot hybrid system (<i>Suswapna Mukherjee^{1,2}, Sudipto Chakrabarti^{1,2,*}</i>)	160
Influence of Graphene and Antimony Underlayers on Magnetization Dynamics in FeCo Thin Films (<i>Swayang Priya Mahanta^{1,#}, Antarjami Sahoo¹, Mitali Swain¹, Abhisek Mishra¹, Laura N. Serkovic-Loli^{2,3}, L. Avilés-Félix^{2,4,5}, and Subhankar Bedanta^{1,6,*}</i>)	161
Symposium: C	161

Optimisation of conditions for the hydrothermal synthesis of phase-pure Zeolite-W using Kaolin for the extraction of ReO_4^- (surrogate for $^{99}\text{TcO}_4^-$) (<i>Abhinash Maharana, , Hrudananda Jena</i>)	161
SrO and Nb_2O_5 Modified Phosphate Glass Network: A Candidate Host Matrix for Radioactive waste Immobilization (<i>Abhiram Senapati, S. Balakrishnan</i>)	163
Spacer Cation Induced Tunable Piezoelectricity in 2D Halide Perovskite for Energy Harvesting Applications (<i>Abhirup Chatterjee, Sreya Das, Soumen Maiti, Tufan Paul, Pulak Pal, Kalyan Kumar Chattopadhyay</i>)	164
Development of Supramolecular Metallogels of Chiral Bisnaphthyl Bipyridine Derivatives for Dye Degradation Application (<i>Abinash Dalai, Tumpa Gorai</i>)	164
Layer-Engineered Capacitive-Coupled Organic Memristor Based on PEDOT:PSS-Ion Gel Bilayers (<i>Aditya Ashutosh Dash, Pukhraj Prajapat, Vaivhab Kandwal</i>)	165
Oxygen-Vacancy-Engineered $\text{LaFeO}/\text{FeOOH}$ an S-Scheme Heterojunction for Sono-Photo-Fenton Degradation and Water Splitting (<i>Anshumika Mishra, Kulamani Parida</i>)	165
All-inorganic lead-free triple perovskites for two-terminal analog memristor-based artificial synapses (<i>Anuj Kanti Nath, Pranab Kumar Sarkar</i>)	166
Enhanced Piezoelectric Performance in Ion-exchanged Silver Niobate GlassCeramics: A Lead-Free Alternative for Energy Harvesting Applications (<i>Anwasha Dutta, Swagata Banerjee, Pounomi Bera, Md Amira, S. Wazed AlibShrabanee Senc, Atiar Rahaman Mollaa</i>)	167
Theoretical Investigation of B_2Cas an Anode for Post Lithium Ion Batteries (<i>Apoorva, Pankaj Kandwal</i>)	167
Structural, Morphological and Electrochemical Investigation of Mn and Mo Doped BiPO_4 for Energy Storage Applications (<i>Brintha T A, Sathasivam Pratheep Kumar</i>)	168
Turbostratic Twisted Graphene Bilayer Structures Detected in a Carbon Material Obtained from Coal and Supercapacitor Application (<i>Debashis Sarmah, Abhishek Hazarika, Binoy K Saikia</i>)	169
GeSnSbTe_2 : Structural Analysis and Prospects for Thermoelectric Performance Enhancement (<i>Debidatta Mohanty, Dinesh Topwal</i>)	169
Evolution of microstructure, magnetic, and electrical properties of novel double-layered Ruddlesden-Popper Perovskite $\text{Sr}_3\text{NiNbO}_{7-\delta}$ (<i>Deepankar Das, Chandana Rath</i>)	170
Next-Gen Clay Nanocomposites for Mercury Remediation (<i>Akkiraju Sai Santosh Sri Narayana Raju , Nemallapalli Madhusudhan , A. Sunil</i>)	170
Transition-Metal-Incorporation in NiCo_2O_4 Spinel Framework as Superior Oxygen Evolution Catalysts (<i>Amba Sankar K N, Debashrita Mahana, Mohan S, Amreen A. Hussain</i>)	171
A Family of Methylene Bridged Fully Functionalized Polynitroarenes and Tetrazole-based Energetic Materials (<i>Amit Bijlwan, Dheeraj Kumar</i>)	172
Gas Sensing by RGO Wrapped Fe_2O_3 Nanorod (<i>Ananya Mohanty</i>)	172
Energy-Saving Multifunctional Electrocatalyst Based on NiAl LDH MXene Heterostructure for HER, OER, and Hydrazine Oxidation Reaction (<i>Anjeli Sunny , Kanagaraj Rithanya , Alagarsamy Pandikumar</i>)	173
Composite Nanomaterial as Nanofillers for Enhanced Electroactive Phase of PVDF Piezoelectric Sensors Applications (<i>Ankur Verma, Pritha Dutta, Ashutosh Kumar Singh, Subash Cherumannil Karumuthil</i>)	173
High Temperature Thermal and Melting Properties of Multivalent and Offstoichiometric Mixed Actinide Oxides (<i>Arindam Chakraborty , Partha Sarathi Ghosh, Niharendu Choudhury</i>)	174
Chemical Vapor Deposition of Copper Selenide (Cu_2Se) on copper foil for Supercapacitor application (<i>Arshad Ahamed A, Rasik Manve, Jatis Kumar Dash</i>)	175
Ni Incorporation in Fe-Mn Based Prussian White to Subdue Octahedral Tilt Distortion and Jahn-Teller Distortion (<i>Ashwani Tyagi , Sreeraj Puravankara</i>)	175
TiO_2 thin films grown by atomic layer deposition (ALD) for photocatalytic reduction of CO_2 (<i>Aswathi P K</i>)	176
Hydrothermally Synthesized VS_2/MoS_2 Nanocomposite for Green-Hydrogen Evolution Reaction (<i>B. Dandasena, R. Naik</i>)	177

Asymmetric bridging site CoSeTe as a Co-catalyst on C,S-Doped g-CN for Superior Photocatalytic Hydrogen Generation (<i>V. Bharathi Mohan, M. Sathisha</i>)	177
Sustainable Water Purification Novel Nanozirconia-Intercalated Clay composite for Fluoride Remediation (<i>Bhargava Nithin T, Reddi Jagadeesh, Nemallapalli Madhusudhan, A.Sunil</i>)	178
DFT-guided graphene and graphene oxide in NiO: Engineering charge transfer process for optimized supercapacitor and electrochromic operation (<i>Bhumika Sahu, Love Bansal, Rajesh Kumar</i>)	179
Two-dimensional [Co(btbbH) ₂ (dpe) ₂].DMF metal-organic framework-derived low-cost nanocomposites for electrochemical nitrate reduction for ammonia production (<i>Biplab Kumar Manna, Amrutanshu Praharaj, Manjunatha Kempasiddaiah, Sudip Barman</i>)	179
NiCo LDH derived mesoporous Se doped NiCoP nanoflower architecture having regional defects for improving oxygen evolution reaction (OER) (<i>Dipti Prava Sahoo, Kulamani Parida</i>)	180
Unravelling the Oxygen Reduction Reaction Activity under Acidic Medium Using Designed N-doped Graphene Catalyst (<i>Dipti Ranjan Panigrahi, Santosh K. Singh</i>) . .	180
Tuning thickness of Molybdenum Nitride thin films for improved electrochemical sensing (<i>Divya Choudhary, Ankita Agrawal, Uday Deshpande, Mukul Gupta, Debalaya Sarker, Soumyendu Roy</i>)	181
Polyoxometalate-loaded reduced Graphene Oxide-modified Metal Vanadate catalysts for Environmental Pollutant Remediation. (<i>Gajiram Murmu, Dr. Sumit Saha</i>)	182
Enhancing Energy Density of Tailored 2D Nb ₂ C MXene/CoNb ₂ O ₆ Hybrids for Lithium-Ion Hybrid Capacitors. (<i>K. Gurunathana, V. Bharathi Mohana, M. Sathish</i>)	183
Tailored Nanoparticle Organic Network Membranes for Hydrogen Generation (<i>Jeebanjyoti Mohapatra, Saswati Mishra, Satyabrata Sahoo, Adithyan Puthukkudi, Sankalpa N. Panda, Simantini Nayak, Bishnu P. Biswal</i>)	183
Electrochemical Deposition of NiCo LDH on Diverse Substrates for Improved Electrocatalytic Oxygen Evolution Activity (<i>Kanagaraj Rithanya, Anjeli Sunny, Alagarsamy Pandikumar</i>)	184
Double-encapsulated red-emitting formamidinium lead halide perovskite nanocrystals for fluorescent sensing and lighting applications (<i>Kajol Sahoo, Latika, Ramakanta Naik, Saikat Bhaumik</i>)	185
Photolithographic patterning of metal halide perovskite nanomaterials for advanced anti-counterfeiting devices (<i>Latika Juneja, Saikat Bhaumik</i>)	185
Integrated SERS Detection and Photocatalytic Degradation of Microplastics: A Dual-Strategy Approach Using Ag-Cu Nanoparticles and ZnTi-Layered Double Hydroxides (<i>Madhusmita Nanda, Gracy Nag, Dipti P. Das, K. Kamali</i>)	186
Green synthesis of a magnesium single-atom catalyst from Spinacia oleracea chlorophyll extracts for sustainable electrocatalytic nitrate reduction to ammonia (<i>Kanhai Kumar, Karuna Kar Nanda</i>)	187
Graphite supported Ni-Co-P: A Promising Electrocatalyst for Hydrogen Evolution (<i>Loganathan Kanishga, Subramanian Rajalekshmi, Alagarsamy Pandikumar</i>)	187
Solution-Processed Cs ₃ Bi ₂ I ₉ -PMMA Composites for Flexible Memristive Devices (<i>Karabi Kanchan Borgohain, Asim Roy</i>)	188
Electromechanical and Computational Insights into Bent Core Liquid Crystal-Infused PVDF Composites for Improved Piezoelectric Performance (<i>Kaustav Jit Bora, Supreet Kaur, Aloka Sinha</i>)	189
Piezoelectric Mono-elemental Black Phosphorus for Pressure Sensing Applications (<i>Kavya Bodhi T K, and Subash Cherumannil Karumuthil</i>)	189
Harnessing Cobalt-Based Heterostructures For The Efficient Removal Of Nitrofurantoin Via Peroxymonosulfate activation (<i>Keerthi Valsalan, Triveni Rajashekhar Mandlimath</i>)	190
Role of V ₂ O ₅ in Modifying the Sintering Kinetics and Electrical Characteristics of Lead-Free BNT-BT-KNN Ceramics (<i>Kiran Kumar Padhi, Swarup Kundu</i>)	191
Enhancing the Longevity of Perovskite Solar Cells via Spacer Cation Engineering (<i>Km Sakshi, Soumyendu Roy</i>)	192

Wheat-Bran Derived Carbon Activation via Green Activation: A Structural and Electrochemical Insights of Supercapacitor Application (<i>Kuldeep Kumar Kushwaha, Pratiksha Singh, Sumit Kumar Chaudhary, Dr. Devendra Singh Negi, Dr. Pranay Ranjan, Dr. Achchhe Lal Sharma</i>)	192
Design and Development of High-Performance Silicon-Based n-i-p Heterojunction Photoanode for Large-Scale Photoelectrochemical Water Splitting Application (<i>Kumar Shubham, Mukhesh K. Ganesha, Ashutosh K. Singha</i>)	193
Enhancing charge transfer dynamics through S-scheme based WS ₂ /SCN photocatalyst for simultaneous O ₂ reduction reaction and crystal violet degradation (<i>Kundan Kumar Das, Kulamani Parida</i>)	194
Engineering Non-Centrosymmetric Bismuth-Based Photocatalyst and Investigation of Their Influence on Mixed Pollutant Degradation (<i>Logamithrai D, Raveena P V, Anitha Christy Antony, Debabrata Sarkar</i>)	195
Development of MOF-Based materials from lean resources (<i>Manaswini Karsharma, Mamata Mohapatra</i>)	196
Computational Engineering of KCaX ₃ (X = Cl, Br, I) Halide Perovskites: Unveiling their Potential in Energy Conversion and Optoelectronics (<i>Mathivarsini P, Mahalakshmi P, Punithavelan N, Sudharsan J</i>)	196
Phonons and Structural Phase Transition Study of Hybrid Organic-Inorganic Perovskite-based Molecular Ferroelectrics (<i>Monalisa Pradhan, Aiswarya Abhisek Mohapatra, Ashish Anand, Diptikanta Swain, Gopal K. Pradhan</i>)	197
Phonons and Structural Phase Transition Study of Hybrid Organic-Inorganic Perovskite-based Molecular Ferroelectrics (<i>Monotosh Dalapati, Dipak Samanta</i>)	198
Integrating Hydrothermal Synthesis and Cold Sintering for Ultra-Low Energy Processing of High-Density BaTiO ₃ Ceramics (<i>Montek Mohapatra, Partha Sarathi Mondal, and Arvind Pandey</i>)	198
Scalable Osmotic Energy Harvesting using Two-dimensional MoS Membranes (<i>Mukesh Kumar, Simran Nasa, Akshitha, Samriddhi Kushwaha, Sumanth Sekhar Samal, Manoj Varma, Pramoda K. Nayak</i> ,)	199
Synthesis of a Novel Zirconium-Kaolin-reduced Graphene Oxide Composite for Multi-pollutant Adsorption from Water Samples (<i>Nemallapalli Madhusudhan and A. Sunil</i>)	200
Tuning Structural and Electronic Properties of AgSnSbTe ₃ via Doping for Enhanced Thermoelectric Performance (<i>Nevin Noble, Dinesh Topwal</i>)	201
Binary-Ternary complex Oxide nanoflower: Pulse Reverse electrodeposited electrode for designing supercapacitor prototype (<i>Nikita Ahlawat, Rajesh Kumar</i>)	201
Eco-Friendly Water Cleanup: Nanotitania Composites for Sustainable Dye Degradation. (<i>Veerababu N, Abhiprayas Sahoo, A. Sunil</i>)	202
Synergistic Effect of NiSb ₂ O ₆ and rGO Nanocomposites for High-Performance Charge Storage Applications (<i>Parul, Surjit Sahoo, Satyajit Rath, Saroj Kumar Nayak</i>) . . .	202
Harnessing Dual Ambient Energies: Magneto-Pyroelectric Hybrid Harvesters for Modern Electronics. (<i>Parvathy Ravindranath, Dalip Saini, Dipankar Mandal</i>)	203
Double-modified (Ag & Al) manganese with sufficient energy and power density for thermistor and supercapacitor applications (<i>Piyali Biswas, Manoranjan Kar</i>)	203
Flexible and wearable piezoelectric nanogenerator based on three-phase composite film for energy harvesting and mechanosensing (<i>Pounomi Bera, Susmita Kundu, Shrabanee Sen</i>)	204
A Non-Enzymatic Glucose Sensor Based on AG Modified Electrode (<i>Pratiksha Singh, Kuldeep Kumar Kushwaha, Sumit Kumar Choudhary, Pranay Ranjan, Devendra Singh Negi</i>)	205
Two-dimensional Titanium Carbide MXenes for Efficient Water Electrolysis (<i>Pritish Kumar Behura, Teresa Dong, Peter Berg, Jasneet Kaur</i>)	205
Impact of Temperature Variation on Functional and Electromechanical Properties of Lead-Based Ceramics (<i>Priya Choudhary, Nita Dilawar Sharma, Ashok Kumar</i>) .	206
Sulfonamide-derived Covalent Organic Frameworks (COFs) serving as efficient additives in polyethylene oxide (PEO) to enhance ionic conductivity (<i>Priyanka Bhardwaj, Neha, Anshuman Dalvi, Madhushree Sarkar</i>)	207

Cost-Effective and Durable AlN/Al/AlN Multilayer Coatings for Energy-Efficient Window Applications (<i>P. Hemani ,E. Panda</i>)	207
Binary vs. Ternary MOF-on-MOF Architectures: Engineering Charge Dynamics for High-Efficiency Solar to Chemical Conversions (<i>Priyanka Priyadarshini,Kulamani Parida</i>)	208
Solvent-Controlled Self-Assembly and Chiral Induction in Pd(II) Coordination Cages (<i>Raghunath Singha,Dipak Samanta</i>)	208
Electronic structure and electrical properties of Bi _{1-x} Mn _x FeO ₃ thin films. (<i>Rajat Kumar Tripathy, Subhajit Nandy, A Kathirvel,C. Sudakar</i>)	209
Porous W ₂ N Fibrous-Nanograins and TiN Nanopyramids Framework for High Energy Density Flexible Asymmetric Supercapacitors (<i>Rajesh Kumar, Bhanu Ranjan, Davinder Kaur</i>)	210
Radiation Assisted Chemically Synthesized Tin Oxide Nanoparticles Towards Solid-State Supercapacitor (<i>Rajulal Sahu, M.C. Rath, Sangeeta J. Keny, Babasaheb R. Sankapal</i>)	210
Facile Hydrothermal Synthesis of ZnFe ₂ O ₄ Nanoparticles with high specific Surface area for High Performance Supercapacitor Application. (<i>Rasik Manve, Arshad Ahamed A, Jatis Kumar Dash</i>)	211
From Charge to Waves: Fabrication and Fractional Dynamics Analysis of CuMnO ₂ Symmetric Coin-cell Supercapacitor for Low-Frequency Oscillator application (<i>Raushan Kabir</i>)	211
Developing Rh _{2-y} Cr _y O ₃ Cocatalysts to Outperform Platinum in Semiconductor-Based Photocatalytic H ₂ Evolution (<i>Raveena P V, Logamithrai D, Anitha Christy Antonysamy, Debabrata Sarkar</i>)	212
Engineering Cation Vacancy Defects on LaNiO ₃ for Efficient Oxygen Evolution Reaction (<i>Ravi K. Kunchala, Rohit Ranjan Raut Ray, Srijoti Mukherjee, Ashok K. Ganguli</i>)	212
Superpower from Nature and Nanostructure: A Dual-Engineered Deformable Supercapacitor for Portable Electronics (<i>Ritik Mohanty, Kulamani Parida</i>)	213
Layered Nb ₂ C and NiCo ₂ O ₄ Nanocomposites for Enhanced Charge Storage in Supercapacitors (<i>Riya Malik, Megha Rana, Suraj P. Khanna, Ritu Srivastava, C.K.Suman</i>)	214
Synergistic Integration of NiNbO and NbC MXene for Advanced Lithium-Ion Capacitor (<i>R. Robin, M. Sathish</i>)	215
Impact of Growth Conditions on the Structural and Magnetic Properties of -Fe ₃ xN Thin Films (<i>Rohit Kumar Meena, Nakshatra Ranjan Pal, Rajeev Rawat, Mukul Gupta</i>) .	215
Designing Defect-Rich Cobalt Oxide Nanostructures by Selective Cation Dissolution: A Template-Free Approach for Water Oxidation (<i>Rohit Ranjan Raut Ray¹,Ravi Kumar Kunchala², Ashok Kumar Ganguli^{2*}</i>)	216
Dual Functionality of Prussian Blue and Manganese-Doped Prussian Blue Materials for High-Performance Supercapacitors and Flexible, Low-Cost Screen-Printed Glutathione Sensors (<i>Roshni Begum¹, Chandan Kumar Ghosh^{2,*}</i>)	217
Magneto-Responsive Carbon:SPION Integrated Conducting Gel for Self-Powered Wearable Triboelectric Sensors (<i>Saira Bano^a , Ranbir Singh^{a,*}</i>)	217
Tuning Lattice Thermal Conductivity through Selenium Substitution in Bi ₂ Te ₃ Alloys (<i>Sambit Kumar Prusty¹, Prahallad Padhan²</i>)	218
Investigation of Lattice Thermal Conductivity in SrSnO ₃ : Combining Experiments, Theory, and Machine Learning Methodology (<i>Santosh Kumar Sahu, Rasmī Ranjan Mohapatra, Sandip Kumar Padhi, Prahallad Padhan</i>)	219
Employing Coumarin Framework for the Development of Insensitive Energetic Materials (<i>Satyabrata Sahoo^a, and Dheeraj Kumar^{a*}</i>)	219
Harnessing the mechanical and magnetic energy with PMN-PT/Ni-Mn-In based flexible piezoelectric nanogenerator (<i>Satyam Shankhdhar^a, Diksha Arora^a, Habeebur Rahman^a, Rajesh Kumar^a, Bhanu Ranjan^a, Kumar Kaushlendra^a and Davinder Kaur^{a,*}</i>)	220
Improved Ionic Conductivity and Phase Stability in Sm and W Co-Doped La ₂ Mo ₂ O ₉ Electrolytes (<i>Saurabh S. Shiwankar^{1*}, Smita A. Acharya¹</i>)	221

Volume Percentage Doping Effects of Fe ₃ O ₄ Nanoparticles in P(VDF-TrFE) Matrix: Enhanced Magnetoelectric Coupling in Nanocomposite Films prepared by solution casting method (<i>Sawan Kumar Bhakar^{1,2}, Srinibas Satapathy^{1,2,*}, Pratik Deshmukh^{1,2}, Bhumnika Sharma¹, Shovan Kumar Majumder^{1,2}</i>)	221
Electrospun Highly Porous N-doped Carbon Nanofibers for High Performance Supercapacitor Application (<i>Sayak Roy^{1,2}, Prajnashree Panda^{1,2}, Sudip Barman^{1,2*}</i>) . . .	222
Nanostructure Engineering of Pt-Shell-Decorated PdPt Alloy for Highly Efficient Oxygen Reduction Catalysis (<i>Silpa Subhalaxmi, and Kakali Maiti*</i>)	223
Piezopolarization Induced High Rate Solar N ₂ -to-NH ₃ Conversion in Vacancy Engineered AgCu-Modified BiFeO ₃ (<i>Simanta Ranjan Barik, Kulamani Parida^{*1}</i>)	223
Color tunable CsPbX ₃ @MOF nanocomposites as a temperature sensor and stable electrospun microfibers for fabrication of down-converting WLEDs (<i>Smaranika Ray¹, Saikat Bhaumik^{1,2,*}</i>)	224
Exploring the Reactivity of Oxygen and Ozone in C ₂ N Monolayer and its Photocatalytic activity for Water Splitting: A First Principles Study (<i>Soumendra Kumar Das¹, Lokanath Patra², Prasanjit Samal³, Pratap K. Sahoo³, and Sridhar Sahu¹</i>)	224
Vacancy-Tailored low-dimensional 2D perovskite inspired Halide CsAgBr ₂ for Next-Generation High-Performance Supercapacitor (<i>Sreya Das, Abhirup Chatterjee, Pulak Pal, Soumen Maiti and Kalyan Kumar Chattopadhyay</i>)	225
Simple and Template-free Approach for Synthesis of High Surface Area and Defect NiO from Olivine Precursor for Efficient Water Oxidation (<i>Srijoti Mukherjee, Ravi Kumar Kunchala, Ashok Kumar Ganguli</i>)	226
Multicomponent entropy stabilized ceria based rare earth oxides for photocatalytic hydrogen production and dye degradation applications (<i>Subhajeet Sen and Srinivasan Nedunchezian</i>)	226
Tailoring Gold Corroles via Regioselective Nitration: Near Infrared Emission, Singlet Oxygen Sensitization, and Photocatalytic Oxidation of Sulfides (<i>Subhajit Kar, Tanmoy Pain, Riddhi Chakraborty, Pravansu Panda, Narayan Ch. Jana, and Sanjib Kar</i>)	227
EVAPORATION-DRIVEN HYDROVOLTAIC DEVICES: HARNESSING ENGINEERED CARBON FOR SUSTAINABLE ENERGY (<i>Subham Kumar Subudhi and Alagarsamy Pandikumar</i>)	228
Influence of Nanoconfined Gold Nanoparticles on Phase Transformation and Enhanced Pyroelectric Response in PVDF Nanofibers (<i>Sudip Naskar, Dipankar Mandal</i>) . . .	228
Self-powered PVDF@MoSSe based TENG enabled Wireless Braille Typing System with Integrated Auditory Feedback for Assistive Communication Systems (<i>Supravat Ghosh, Partha Pratim Ray</i>)	229
Electronic Charge Transportation in Plasmonic NrGO/NiFeTb LDH@Cu Heterostructure for Enhanced Photoelectrochemical Water Oxidation (<i>Susanginee Nayak, Kulamani Parida</i>)	230
Pseudocapacitive nanoparticles of cadmium hydroxide – cobalt hydroxide composite electrodes for supercapacitor application (<i>Swapna Rout, Babasaheb R. Sankapal</i>) . . .	230
Oxy – hydroxyl manganese tungsten anchored on multi-walled carbon nanotubes with hybrid surface architecture towards flexible solid-state device grade supercapacitor (<i>T. Kedara Shivasharma, Babasaheb R. Sankapal</i>)	231
Micro-sampling of dilute analytes using metal-organic framework (<i>Tilottama Baisakhi, KM Archana Yadav, Ritesh Haldar</i>)	231
Self-sacrificial template-induced fabrication of sustainable micro-junction towards energy conversion and storage (<i>Upali Aparajita Mohanty, Kulamani Parida</i>)	232
From Nano to Wearable: Multimodal Energy Harvesting Using Axially Confined Chalcogenide in Ferroelectric Polymer (<i>Utsa Sarkar, Hari Krishna Mishra, Ajay Kumar and Dipankar Mandal</i>)	232
Stability and Thermal Transport Features of Cubic HfO ₂ and MgO ₂ Monolayers: A DFT Approach (<i>Vaishnavi S, Mahalakshmi P, Punithavelan N, Sudharsan J B</i>)	233
Neuromorphic Performance of Organic FeFETs Using Novel Ferroelectric Compounds: Towards In-Memory Computing (<i>Vanshaj Vidyan</i>)	234

Piezopolarization Induced High Rate Solar N ₂ -to-NH ₃ Conversion in Vacancy Engineered AgCu-Modified BiFeO ₃ (<i>Simanta Ranjan Barik, Kulamani Parida</i>)	234
Deciphering the S-scheme Carrier Transfer Dynamics at CdS-ZnCdS Heterojunction for Enhanced Hydrogen Evolution: An Ultrafast Approach (<i>Atal Swathi Patra¹, Himanshu Bhatt¹, Rakesh Kumar Behera¹, Nitika Kharbanda², Ipsita Parichha¹, Chetandipta Mahanta¹ and Hirendra N. Ghosh^{1*}</i>)	235
Symposium: D	235
2D h-BN Reinforced Protein Scaffold/Films for Biomedical and Thermoelectric Applications (<i>Bitopan Boro, Devasish Chowdhurya</i>)	235
Sericin–polyethylene glycol hydrogel as an innovative excipient for progesterone delivery: formulation development, characterization, molecular docking and toxicity evaluation (<i>Dona Deb, Deepjyoti Kalita, Mojibur R. Khan, Kamatchi Sankaranarayanan</i>)	236
Development of a Simple and Efficient Method for the Micropatterning of Silk Fibroin (<i>Heena B. Choudhary, Srinivasa K. Prasad, Ramendra Kishor Pal</i>)	237
Ligand-Dependent Regulation of Copper Nanocluster–DNA Binding and Its Relevance in Targeted Biology (<i>Joyoti Ghosh, Chinmayee Patra, Debabrata Chakraborty, Debraj Koiri, Sumit Kumar Pradhan, Moloy Sarkar</i>)	238
Wound Healing Activity of Nanocellulose-Graphene Oxide Hydrogel by Excision Model in Rats (<i>Monica Chingchuilin Gonmei, Mareeshwari Paramasivan, Madhan Jeyaraman, Devi M, Evelyn Sharon S, Athirai Chelladurai, Roop L Mahajan, M K Padmanabhan, Rajeshwari Hari, Chithra Lekha P</i>)	239
MXene as a new candidate for Photoacoustic Transducers for High-Resolution Diagnostic Imaging (<i>Neelkamal Das, Shivam Rakhoulia, Nagendra Singh, and Samir Kumar Biswas</i>)	240
A Covalent Organic Framework-Based Triad Sensor for Early Turner Syndrome Diagnosis (<i>Neethu K M, Paresh Mohanty, Neelam K, Sunetra Mondal, Satinath Mukhopadhyay, Gunjan Verma, Sugam Kumar, Rijo Rajeev, Parikshit Moitra</i>)	240
Stimuli-Responsive Defective NaNbO _{3-x} /CuIn ₂ S _{4-y} Binary Hybrid for Photo-Chemodynamic Antimicrobial–Antibiofilm Therapy (<i>Newmoon Priyadarshini, Kulamani Parida</i>) .	241
Activated Carbon/PNIPAM Nanocomposite Hydrogel Derived from Rice Straw for Effective Dye Adsorption (<i>Onkar Nath, Amul Jain, Koushik Mahata, Sanjib Banerjee</i>)	242
Rapid detection of fatty acids using gemini lipidoid based sensor: Application in quality checking of edible oils and profiling bacterial drug resistivity (<i>Pradipta Behera, Rita Ghosh, and Mrinmoy De</i>)	242
Design and development of Chitosan-Based Conductive Hydrogels for Biocompatible and Self-Healing Human–Machine Interfaces (<i>Salaman Ahamad, Shaista Fatima, Gourav Manik, Ankush Kumar</i>)	243
How Dental Biomaterials Wear under Saliva and Temperature Changes (<i>Prabhu Prasad Tripathy, N.L. Parthasarathi, Saralasrita Mohanty</i>)	244
Cost-Effective porous metal oxides and mixed metal oxides coatings for Ti- 6Al-4V biomedical implants (<i>Sarmistha Bhattacharjee, Kartikey Chaturvedi, Priya Mahato, Superb Misra, Emila Panda</i>)	244
Laser-scribed graphene microelectrode for non-enzymatic glucose detection (<i>Sarojini Prusty, Dr. Pranati Nayak</i>)	245
Development of Physically Crosslinked PVA–Gelatin Hydrogels Loaded with Piperine for Enhanced Wound Healing Applications (<i>Shaista Fatima, Salaman Ahamad, Sham Sundar Ravindranath</i>)	245
Synthesis of ZnO-TiO ₂ Heterojunction Nanocomposite for Dye Removal and CO ₂ Adsorption (<i>Shivam Kumar, Dr. Sarathi Kundu</i>)	246
Silk Fibroin-PEDOT: PSS Composite Coatings for Enhanced Stimulation Performance of Silver Microelectrodes with Neural Interfaces (<i>Sohini Das, Heena Bholaram Choudhary, Srinivasa Prasad K, Ramendra K Pal</i>)	247
Active Particles Knead Three-Dimensional Gels into Porous Structures (<i>Sourav Mukherjee, Martin Cramer Pedersen, Amin Doostmohammadi, Chandana Mondal, Kristian Thijssen</i> .)	248

Biom mineralization, Antifungal, Antibacterial and Cytotoxicity Investigation of Larnite/Nano Titania Composite via Sol-gel Combustion Method (<i>Subhashree Praharaj , Madhvesh Pathak</i>)	248
Active Ornstein-Uhlenbeck particle under stochastic resetting (<i>Uma Shankari M , Mamata Sahoo</i>)	249
Bioconversion of Paper Mill Wastewater into Bioplastic using a Novel strain isolated from soil (<i>Dimple Singh , Vibhore Kumar Rastogi</i>)	250
Rhodamine-Appended Fluorescent Probe for Selective Iron Sensing and Theranostic Applications of the corresponding Iron Complex (<i>Debadutta Samal¹, Basudeb Dutta, Rojalin Sahu^{2*}</i>)	250
Symposium: E	250
Fused Hollow Cathode Plasma Source for Plasma-Enhanced Chemical Vapor Deposition of Carbon Nanostructures (<i>Anannya Bordoloi, Arup Ratan Pal</i>)	251
Ex-situ XRD Analysis of Phase Transitions in P2-Type $\text{Na}_{0.67}\text{Ni}_{0.33}\text{Mn}_{0.67}\text{O}_2$ for Symmetric Na-ion Batteries (<i>Ananya Kumar, Sreeraj Puravankara</i>)	251
Raman at the Frontier of 2D Materials Research (<i>Arpit Patnaik, Surender Kumar Sharma</i>)	252
Thermal phonon induced resonant Fano interaction in V_2O_5 under off-resonant excitation (<i>Deb Kumar Rath, Rajesh Kumar</i>)	252
Estimating dielectric function of quantum dots (<i>Harshavardhan Reddy Kalluru</i>)	253
Advanced Corrosion Protection Using In-Situ Synthesized Fe/Mg-Doped Polyaniline–Polyimide Composite Coating (<i>Sagarika Padhan, Sandeep Sekhar Pradhan, Jayanta Vishnu Bharati, Harekrishna Panigrahi, Tapan Kumar Rout, Smrutirekha Mishra</i>)	253
Symposium: F	254
Self – Sterilizing Nanofiber Air filter for $\text{PM}_{2.5}$ Filtration (<i>Anitha Christy A, Raveena P V, Logamithrai D, Debabrata Sarkar</i>)	254
The Age hardenability and Colour differences of 22k gold micro alloyed with Sc, Zr and some rare earth elements (<i>Dayana Peter, G. S. Vinod Kumar</i>)	255
Tarnish Resistance Mechanism in Ag-4Cu-2.5Zn-1Ge novel Alloy: A Comprehensive Experimental and Computational Study (<i>Harsha K, Dr. G S Vinod Kumar</i>)	255
Multiple recycled triboelectric nanogenerators for smart waste management (<i>Nikhil RAM PATRA, Kaushik PARIDA, Yuvraj SINGH NEGI</i>)	256
Microstructural Evolution and Magnetic Properties of As Cast and Melt-Spun Co–Zr Alloys (<i>Sanjay Saini, A. P. Srivastava, S. Neogy</i>)	256
Structural, Magnetic and Thermoelectric properties of Al-Cu-Fe quasicrystal reinforced at various concentration of Sn and CNT (<i>Shradha Bhatt, Archana Tiwari</i>)	256
Study of bubble growth response in VCrFeNiCu High Entropy Alloy (<i>S. Vinitha, S. Abhaya, K. Suresh</i>)	257
A Novel Melt-Route Approach for the fabrication of uninterrupted and interrupted silver foams for jewellery applications (<i>Yadu Krishnan K T , G.S Vinod Kumar</i>)	258
Integrated PANI and Carbon Quantum Dots in UiO-66-NH_2 for Superior Conductive and Photoluminescent Sensing Performance (<i>Subrat Swain¹, Basudeb Dutta¹, Rojalin Sahu</i>)	259
Symposium: G	259
Phonon Dispersion in Superconducting NiBi_3 system (<i>Abhisek Sahoo, Dr. Pratap Kumar Sahoo</i>)	259
Enhanced EMI Shielding in Flexible Carbon Black/LSMO Reinforced PVDF Composites for Protection Against Electromagnetic Pollution (<i>Amar Dev, Piyali Biswas, S. K. Pradhan, P. Kour, and Manoranjan Kar</i>)	260
Ex-Situ Phase Evolution Study of Indigenous Lanthanum Carbonate Hydrate and Synthesis of Lanthanum Oxide and Lanthanum Hydroxide (<i>Anant Kumar Gupta, Subhajeet Sen, and Srinivasan Nedunchezian</i>)	260
MOF-Derived Porous Carbons and Hybrids for Microwave Absorption: A Comprehensive Review (<i>Anjali Maheshwari</i>)	261
Defect-Driven Anharmonic Phonon Dynamics in Ag-Implanted Bi_2Se_3 (<i>Ankita Dey, Rashmi Ranjan Das, Sudhanshu Gautam, Arvind Kumar, Sunil S. Kushvaha, Tanuja Mohanty, and Pratap K. Sahoo</i>)	262

Rare Earth Elements in Coalmine Overburden: Future Possibilities for Recovery (<i>Binud Attry, and Binoy K. Saikia</i>)	263
Controlled micro and nanodome formation by proton irradiation on ZnTe thin film (<i>Kalyan Ghosh, Pratap K. Sahoo</i>)	263
Effect of Gamma Irradiation on Radiation Shielding, Thermal and Optical Properties of Bismuth Modified Barium Zinc Borosilicate Glasses (<i>Richa Mishra, P. Nandi, Haripriya T. R., Shilpa Pradeesh, Abhinav K. P., B. Sanyal, and A. K. Sahu</i>)	264
Magnetic Field Simulation for Ion Beam Transport and Implantation: Development using COMSOL (<i>Sannu Kumar Nayak, Pratap Kumar sahu</i>)	264
Surface Plasmon Resonance study of Au plasmonic structures with Cr adhesion layers (<i>Anushka Das, Abhisek Sahoo, Sudakshina Prusty, and Pratap K. Sahoo</i>)	265
Symposium: H	265
Effect of quenching rate on the electronic properties in Iron Phosphate glass (<i>Aishwarya K, Manan Dholakia, Sharat Chandra</i>)	265
Orbital Free Density Functional Theory Applied On Solids And Finite Systems (<i>Abhishek Bhattacharjee, Dr. Subrata Jana, and Prof. Prasanjit Samal</i>)	266
Structure, Bonding and Stability of Boron Substituted Tungsten Clusters (<i>Akshata M. Waghmare, Sajeev S. Chacko, Balasaheb J. Nagare</i>)	267
Structure-Property Relationship in Triazatruxene Based Donor Materials for Organic Solar Cells: A Computational Study (<i>Aman Kumar, Neha Agnihotri</i>)	267
Swarm Intelligence in Quantum Nanorobots for AI-Assisted Detection of Airborne Nanoplastics (<i>Anisha Sainandini Panda, Anouska Dash</i>)	268
Role of A cation on the electronic and magnetic properties of the double perovskites A_2TiMnO_6 ($A = Ca, Sr, \text{ and } Ba$): A first principles study (<i>Debarghya Dutta,, Amrita Bhattacharya</i>)	269
Transition Metal Decorated Boron-Doped Graphene Quantum Dots for Efficient Hydrogen Storage (<i>Deepak Kumar Palai, Neha Agnihotri</i>)	269
Strain-Tunable DMI and Skyrmion Stability in 2D TMDC's (<i>Dimple Rani, B. R. K. Nanda, and Prasanjit Samal</i>)	270
Orbitronics: Exploiting Orbital Angular Momentum of electrons for Future Spintronic Devices (<i>Hirashri Pathak, Munima B Sahariah</i>)	270
Spatial Density of Mayer Bond Order: Distribution of Electrons Shared and Retained by Atoms in Matter (<i>Joyeta Saha, Sujith Nedungattil Subrahmanian, Chandrima Chakravarty, Joydeep Bhattacharjee</i>)	271
Multifunctional properties of alkaline earth-based A_2BTiO_6 ($A = Mg, Ca, Sr; B = Hf, Zr$) double perovskites: a first-principles investigation for photocatalytic and thermoelectric applications (<i>Kanchan Rawat, Jagrati Sahariya, Amit Soni</i>)	271
Optimization of device parameters in Thermoelectric Generator for Enhanced Waste Heat Recovery in Industrial Systems (<i>Kunal Kishore, Tanmoy Maiti</i>)	272
DFT-based computational design of D- π -A- π -D type small molecule electron donors for organic photovoltaic applications (<i>Modhurima Bhuiya, Neha Agnihotri</i>)	272
Ultrasonication-Assisted Synthesis of Benzimidazole Derivatives Using Green-Synthesized ZnO Nanocatalyst: Experimental and DFT Insights (<i>Nehal Telange, Omkar, Prachi A. Patil, Gurumeet C. Wadhawa, Paresh S. Gaikar</i>)	273
Dynamical stability of U_3Si : A DFT+U study (<i>Prasanta Kumar Maharana, Gurpreet Kaur, Sharat Chandra</i>)	274
Spin-Polarized DFT investigations of Hf-based half-Heusler alloys for Spintronic and Optoelectronic applications (<i>Pratiksha Meena, Sudharsan J B, Nithyanandan Kana-garaj*</i>)	274
Data-Driven Identification of High-Performance Thermoelectric Materials Using Supervised Learning (<i>Rahul Ghosh, Prasenjit Sen, Joydeep Bhaattachajee</i>)	275
Ground state of classical Heisenberg model with DMI and Anisotropy (<i>Ruma Khatun</i>) .	275
Computational Insights into the Adsorption and Detection of SF_6 Decomposition Gases on Ruthenium-Decorated Silicon-Doped Graphene Quantum Dots (<i>Saurav Kumar, Neha Agnihotri</i>)	276

Biaxial Strain Induced Modulation of Rashba Splitting and Hydrogen Evolution Reaction in AgBiP ₂ Se ₆ Monolayer (<i>Shilendra Kumar Sharma, Sudip Chakraborty</i>)	276
Sponsors	279
Author Index	291
Keyword Index	301

MRSI Awardee Lectures

MRSI-ICEM 2025

MRSI International Medal

2D and 3D Phases of Boron-Carbon-Nitrogen

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The ternary phase space consisting of boron, nitrogen and carbon shows a number of thermodynamically stable phases of binary and ternary compositions. There has been significant amount of work in the past on optimizing conditions to grow these phases and understanding their stability. This talk will focus on our long time pursuit of some of these interesting materials that have compositions of C, BN, CN and BCN. The effort in synthesizing hexagonal as well cubic phases of these compositions will be discussed with the goal of achieving 2D and 3D structures with specific applications in mind.

Keywords: binary -ternary compositions, C, BN, CN, BCN.

MRSI Distinguished materials scientist

Exploring Emerging Magnetic Materials

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R& D on advanced magnetic materials have led to some of the most important technological advances. The rational design of magnetic materials enables one to tailor magnetic properties for specific applications. A tremendous effort is on in finding suitable magnetic materials for magnetic memory devices, sensors applications, magnetic refrigeration, permanent magnets, spintronics, high permeability device applications, bio-medical applications, quantum technology applications, etc. We have been working on a variety of technologically important emerging magnetic materials, such as rare earth magnets, molecular magnets, spintronics materials, low-dimensional magnetic materials, and quantum magnetic materials. Our work focuses on various magnetic phenomena and effects viz. magnetization reversal, exchange bias reversal, magnetic proximity effect, large magnetocaloric effect, multiferroic properties, quantum magnetism, and spin quantum entanglement. It is essential to gain fundamental understanding of material's magnetic properties for rational design of such materials and to translate the research findings into realistic technological applications.

Keywords: Magnetic materials, magnetization reversal, exchange bias, magnetic proximity effect, magnetocaloric effect, multiferroics, quantum magnetism, spintronics.

MRSI CNR Rao prize lecture

My encounter with superconducting materials

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Superconductivity has remained one of the most intriguing and evolving frontiers in condensed matter physics since its discovery over a century ago. Since then, the quest for atmospheric and room-temperature superconductors has continued till date and is often termed the "Holy Grail" of physics. In this talk, I will take the audience through my personal and scientific journey with superconducting materials, from the early days of exploring conventional and high-T_c systems to the more recent adventures with topological and quantum materials. Beginning with the excitement surrounding the discovery of MgB₂ and the subsequent quest to enhance its performance through chemical doping and nano-engineering, the narrative moves through the fascinating world of iron-based superconductors, where magnetism and superconductivity coexist in delicate balance. The journey then extends to non-centrosymmetric and topological superconductors such as Pd-doped Bi₂Te₃, SnAs, and related compounds, where spin-orbit coupling and Dirac physics open new possibilities for realizing exotic Majorana quasiparticles. While going through this journey, I will also skim through some of the recent misfires in the quest of room temperature superconductivity including LK-99, however they have generated hope to bring the "Holy Grail" to reality very soon. Through this encounter, I hope to share how decades of engagement with superconductivity have shaped not only our understanding of materials, but also our approach to doing science by itself.

Keywords: Superconductivity, Iron-pnictides, Topological Superconductivity, BCS and Hydride superconductors.

MRSI Distinguished lectureship

Layered organic molecules for energy generation and storage

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Inorganic semiconductors such as binary and ternary oxides and sulfides are well known for their applications in hydrogen generation and other green technologies. They have also been widely employed as cathode and anode materials in energy-storage devices such as batteries and supercapacitors. However, their efficiency and capacity are often limited due to inherent theoretical constraints and synthesis-related complexities.

In our work, we have demonstrated the use of organic molecules for both solar hydrogen production and lithium-ion battery applications. 1,3-Pentacenequinone (PQ), an intermediate in the synthesis of the organic semiconductor pentacene, was prepared through a single-step, solvent-free solid-state reaction at room temperature under ambient conditions, which is notably simple and unique. Owing to its good thermal stability and strong visible-light absorption, PQ was utilized as a photocatalyst for solar-driven hydrogen production. Remarkably, we observed a high hydrogen evolution rate of 4848 $\mu\text{mol/h/0.1 g}$, corresponding to a quantum efficiency of 6.8%. Furthermore, coupled semiconductor photocatalysts consisting of 6,13-pentacenequinone/TiO₂ (PQ/Ti) in various weight ratios exhibited enhanced hydrogen-generation performance.

Our group has also explored organic cathode materials, taking advantage of the ability to design molecules with tailored theoretical capacities. Benzoic naphthalenetetracarboxylic diimide (NTCDI) was successfully synthesized and employed as an organic cathode for lithium-ion batteries, delivering good capacity and cycling stability. Additionally, a solid polymer electrolyte was

developed through the hybridization of PGDMA, PEO, and CTA, and used as the electrolyte in lithium-ion cells. The fabricated cells demonstrated strong electrochemical performance. In summary, our studies highlight the significant potential of organic materials in both energy generation and energy storage applications.

Keywords: Graphene, 2D Materials, Silicene, Phosphorene, MXenes, MoS₂, Germanene, Pseudo Jahn-Teller, Topological Insulators, Spin-Orbital Coupling

MRSI Annual prize

Critical Minerals Extraction by Functional Metal–Organic Frameworks (MOFs)+

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Critical minerals (CMs) are those minerals that are essential for economic development and national security. In 2025 Indian government have launched the National Critical Mineral Mission (NCMM) to establish a robust framework for self-reliance in the critical mineral sector, and identified a list of 30 critical and strategic minerals. These are essential for the advancement of many sectors, including high-tech electronics, telecommunications, transport, and defence. Currently extraction or processing of CMs are happening in a few geographical locations in the world, which may lead to supply chain vulnerabilities and even disruption of supplies. For that there is an urgent need for development of sustainable and efficient extraction technologies of CMs in our country. Recycling of CMs from secondary sources such as e-waste, lithium-ion battery scrap, and end-of-life vehicle parts is also strongly encouraged with incentive scheme under the NCMM. Advanced function porous materials—like metal–organic frameworks (MOFs), related porous materials, have recently emerged as transformative platforms for efficient extraction technologies of different metal ions, due to their tuneable pore environments, high surface areas, and ion-exchange properties. In this lecture I will talk about some of the examples of MOFs and related porous materials, developed in our laboratory, which can efficiently extract some of the critical minerals from solution, demonstrating, potential use of the materials for extracting critical minerals from primary and secondary sources.

Keywords: Minerals Extraction, MOFs

MRSI Annual prize

Development of Advanced Materials and Technologies for Energy

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Presently, major share of the energy generated and used in the world is from fossil fuels resulting in CO₂ emissions causing global warming. Moreover, the demand for energy is ever increasing due to the increase in population and improved quality life. In order to meet the ever-increasing demand for energy without significant increase in CO₂ emissions, there is a need to harness the renewable as well as nuclear energy and increase the efficiency of thermal power plants. The challenge with renewable energy is its continuous availability which can be stored and can be supplied to the grid as per the demand. Nuclear energy is another option for clean energy generation, but it is not being widely adopted due to nonavailability of nuclear fuel and associated operational complications. The economics, safety, reliability, and efficiency of both advanced fission and future fusion energy systems will ultimately depend on developing new high-performance structural materials that can provide extended service under extremely hostile conditions. Presently, thermal power plants are operated at 550-600°C with an efficiency of 37% and need to be operated at higher temperatures to increase the efficiency which again requires materials that can withstand and perform at those temperatures.

Automotive sector is yet another set which significantly contributes to CO₂ emissions. India is aggressively driving for the adoption of electric vehicles replacing internal combustion vehicles. Efforts are being carried out for the establishment of domestic supply chain for the manufacture of materials and batteries for electric vehicles (EVs) under mission mode to achieve the target of 30% of the vehicles manufactured must be electric by 2030. Lithium-ion batteries (LIBs) are playing a vital role worldwide for EV applications owing to high energy/power densities and are being imported by all EV manufacturers. However, due to tropical Indian conditions, high temperatures and lack of adequate quality controls, the imported LIBs cause many fire accidents. To alleviate these problems, there is a need for development of technologies for the manufacture of electrode materials for Li-ion batteries. Among the cathode chemistries used in LIBs, Lithium ferrous phosphate (LFP) cathode material has a safer chemistry because it avoids self-oxidation and thermal runaway due to strong covalent bond between P and O in PO₄ structure of LFP.

ARCI has undertaken development of materials for nuclear reactors, thermal power plants and Li-ion batteries. The presentation discusses about the research carried for the development of materials and components and about the technologies to produce these materials for the above applications.

Keywords: Energy efficiency, Electric vehicles (EVs), Lithium-ion, batteries (LIBs)

MRSI Medal Lecture

Eco-friendly Recyclable and Reprocessable Advanced Polymer–Carbon Nanocomposites for Radiation Shielding: Addressing Environmental Pollution and Health Protection

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The rapid expansion of nuclear energy, aerospace missions, medical imaging, and defense technologies has intensified the need for lightweight, efficient, and sustainable radiation shielding materials. Conventional metal-based shields, particularly those using lead, offer excellent attenuation performance but suffer from toxicity, high density, and non-recyclability, creating serious environmental and health concerns. Therefore, the development of alternative materials that are both effective and eco-friendly has become essential. In this context, eco-friendly, recyclable, and reprocessable polymer–carbon nanocomposites have emerged as promising candidates for next-generation radiation shielding. These advanced materials combine the flexibility, durability, and low weight of polymers with the superior electrical, thermal, and radiation attenuation properties of carbon nanomaterials such as graphene, carbon nanotubes, and carbon black. The synergistic interaction between polymer matrices and carbon nanofillers enhances shielding through absorption, reflection, and multiple scattering mechanisms.

This work highlights recent advances in material design, synthesis methods, and structure–property optimization of polymer–carbon nanocomposites for radiation protection. Their recyclability and reprocessability enable efficient material utilization and circular manufacturing, reducing waste and environmental impact. Moreover, their non-toxic, corrosion-resistant, and lightweight characteristics make them suitable for portable, wearable, and space-limited applications. Overall, these eco-friendly polymer–carbon nanocomposites represent a sustainable and high-performance approach to radiation shielding, addressing both environmental and human health challenges. Their integration into defense, aerospace, healthcare, and electronic systems can significantly advance green materials technology and promote safer operational environments.

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Keywords: Radiation shielding materials, Polymer–carbon nanocomposites, Recyclable and reprocessable composites, Carbon nanomaterials, Carbon nanotubes.

MRSI Medal Lecture

Coatings for renewable energy applications

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The energy sector plays a crucial role in the emission of greenhouse gases (GHGs) due to the reliance on fossil fuels, which contributes to global warming. Wind energy is regarded as a powerful renewable energy source and is anticipated to become one of the main sources of electricity. Nevertheless, leading edge erosion (LEE) of wind turbine blades caused by impacts from solid particles, raindrops, hailstones, bird droppings, ice, and other factors poses a significant challenge for the wind energy industry, ultimately reducing annual energy output. As a result, the development of coatings for leading edge protection (LEP) of wind turbine blades has emerged as a vital area of research and development over the past two decades. Composite coatings formulated with ceramic oxides and cellulose within polyurethane and epoxy resin matrices have been created on glass fibre-reinforced polymer (GFRP) substrates using the spray coating technique and have been evaluated for their resistance to solid particle and rain erosion. It has been noted that the average erosion resistance of filler-reinforced coatings significantly surpasses that of corresponding resin and GFRP substrate.

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Keywords: GHGs, LEE, GFRP, renewable energy

MRSI Medal Lecture

Development of Light-Harvesting Materials for Optoelectronic Devices

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Energy is a crucial factor in driving social, economic, and industrial progress. Our daily energy consumption continues to rise gradually. In recent decades, rising energy demand has increased reliance on fossil fuels such as coal, petroleum and natural gas, releasing CO₂ and contributing to global warming. Small organic molecules with suitable photophysical and electronic properties have garnered attention in advanced technology applications, especially in photonic devices such as dye-sensitized solar cells, organic solar cells, emissive displays like OLEDs; electronic materials such as organic semiconductors, and security printing. Organic photovoltaics are gaining popularity as a cost-effective, color-tunable, and mechanically flexible renewable energy technology. Numerous research endeavors aim to develop novel organic materials and enhance their efficiency and durability. Our research group is focussing on producing stable organic molecules for diverse applications. In the upcoming event, I will present our progress on developing hole-transport materials for perovskite solar cells. The presentation will commence with a brief introduction to solar cells, followed by an exploration of industrial applications and the commercialization potential of dye molecules.

Keywords: Organic molecules, hole-transport materials, perovskite solar cells, organic photovoltaics, dye-sensitized solar cells, OLEDs, renewable energy.

MRSI Medal Lecture

From Designing of Advance Materials to End-of -Life Management of Waste Streams: Holistic Approach for Technologies and Applications Development

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During past several decades, the growth of science & technology, advent of nanotechnology, and ever-increasing demand for efficient materials, devices and/or instruments, has led to quest for design & development of novel materials. In this pursuit, advanced materials have emerged as a special class comprising entirely new compositions or existing materials engineered with tailored structures or size ranges, leading to unique or enhanced properties and functionalities. During these years, our group at CSIR-NPL has significantly contributed toward the development of wide spectrum of advance materials including conjugated polymers (e.g., polyaniline analogues); carbon nanomaterials (e.g., graphene analogues & carbon nanotubes); nanoparticles (e.g., metal oxides) and/or their combinations (e.g., composites, blends or hybrids), for applications in diverse areas, including but not limited to, electromagnetic interference shielding, microwave absorption, antistatics, corrosion protection, gas sensing, water purification, energy storage, self-cleaning surfaces etc. This talk will highlight our key contributions in these areas, supported by representative examples of materials, technologies, and applications. It is also worth mentioning here that, with lifestyle changes, unsustainable material consumptions & disposal; ever-shortening life spans of technologies/products; and relatively inadequate waste management, material recovery & recycling ecosystem; have collectively contributed toward pressing issues such as global warming, pollution problem, health hazards, fast depletion of material resources/reserves etc. As a result, the otherwise breakthrough materials & technologies, resulted in corresponding waste streams, with polymeric waste and E-waste as particularly more concerning categories. Accordingly, their management & disposal through development & implementation of efficient material or energy recovery practices, has become global challenge. The later part of talk also highlights our works related to the management and recycling of various polymeric wastes (e.g., conventional thermoplastics; pharmaceutical blisters, multilayer plastics or MLPs paper/plastic laminates etc.) as well as E-waste streams (e.g., PCBs, discarded batteries and solar panels), for realization of technologically important materials for various practical applications.

Keywords: Microwave absorption, Energy storage, Polymeric waste, E-waste.

MRSI Medal Lecture

Designing greener energy conversion system for a sustainable future

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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. 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/metal-air/peroxide batteries/hydrogen production in its legions of shortcomings or corrigible features. 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 batteries.
- Visualization of local electrocatalytic activity by SECM.

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

MRSI Medal Lecture

Non-noble Metal based Materials as Sustainable Heterogeneous Catalysts for Plastic Waste Upcycling to Multiple Value Added Products

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Chemical recycling of plastic waste has attracted attention from all around the world because it offers a sustainable solution to the problem of plastic waste accumulation and helps create a circular plastic economy. One of the sustainable methods of conserving resources and protecting the environment is chemical depolymerization or recycling of commercial plastics. In this regard, polylactic acid (PLA) is a widely used plastic material for three-dimensional (3D) printing of objects and for various other purposes ranging from agricultural films to food packaging. In the first work, the chemical depolymerization of PLA was investigated using Cu-CeO_2 as a catalyst, yielding methyl lactate (ML) as a selective product under mild reaction conditions. This environmentally friendly and cost-effective approach aims to achieve the closed-loop chemical recycling of PLA waste. The reaction conditions were optimized to attain good catalytic activity and product selectivity. The effectiveness and sustainability of the designed protocols were investigated by the evaluation of the green metric parameters, including environmental factor (E), energy economy coefficient (ϵ) and environment energy impact factor (ξ). This study offers a sustainable, low chemical input and eco-friendly method for the chemical recycling of waste PLA materials.

Secondly, the indispensable use of polyethylene terephthalate (PET) causes several environmental concerns due to its massive accumulation. The chemical upcycling of PET provides an attractive route for the conversion of PET waste into valuable compounds. Herein, a highly effective $\text{Ni}_2\text{P-SiO}_2$ catalyst was synthesized for the glycolysis of real PET waste bottles into bis(2-hydroxyethyl) terephthalate (BHET) using biomass-derived ethylene glycol. The developed $\text{Ni}_2\text{P-SiO}_2$ catalyst exhibits excellent catalytic efficiency and high BHET yields. A thorough optimization of the reaction conditions for PET glycolysis was performed to achieve maximal product yields at optimal reaction conditions. To assess environmental sustainability, green chemistry metrics and life cycle assessment (LCA) were carried out, which highlighted the advantages of the developed reaction protocol over traditional PET disposal methods. In addition, the obtained BHET monomers were subjected to hydrolysis to form terephthalic acid (TPA), which was further converted to terephthaloyl dichloride (TCL), an important value-added product used in the production of Kevlar. This integrated chemical upcycling process involving conversion of PET waste bottles to multiple value-added products using $\text{Ni}_2\text{P-SiO}_2$ catalyst has a potential to tackle the ever-increasing plastic waste problem.



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Keywords: Chemical recycling, PLA, PET, Upcycling, Ni₂P-SiO₂, Green chemistry, Circular economy.

MRSI Medal Lecture

Engineering Pt and Pd Single-Atom Catalysts on Semiconductors for Improved Photocatalytic Hydrogen Evolution and Oxygen Reduction Reactions

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The photocatalytic routes to energy conversion processes have attracted a great deal of research attention in recent years to find sustainable and highly efficient alternative energy as a substitute for exhaustible fossil fuels.[1-5] As a contribution to this field, this study presents eco-friendly, one-step hydrothermal and thermal polymerization methods for synthesizing atomically dispersed Pd and Pt single-atom catalysts (SACs) on CuCo₂S₄ nanosheets and N-rich C₃N₄, respectively, to enhance photocatalytic conversion of abundant molecules into value-added products. The PdSA–CuCo₂S₄ catalyst exhibits strong Pd–S coordination, reduced charge transfer resistance, and asymmetric charge distribution, achieving visible-light-driven H₂ production at 39,550 $\mu\text{mol g}^{-1} \text{h}^{-1}$ with 15.57% quantum efficiency and stable O₂-to-H₂O₂ conversion at 19,200 $\mu\text{mol g}^{-1} \text{h}^{-1}$. [6] Similarly, ultralow-loading (0.08 wt.%) Pt SACs anchored on C₃N₄ demonstrate a high H₂ evolution rate of 64,100 $\mu\text{mol g}^{-1} \text{h}^{-1}$ with 25.3% quantum yield, attributed to enhanced electron trapping and accelerated water reduction kinetics.[7] These strategies highlight the potential of SACs in advancing sustainable photocatalytic H₂ and H₂O₂ production by overcoming mass-transfer and electronic limitations.

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Keywords: single-atom catalysts, photocatalysis, hydrogen evolution, oxygen reduction reaction..

MRSI Medal Lecture

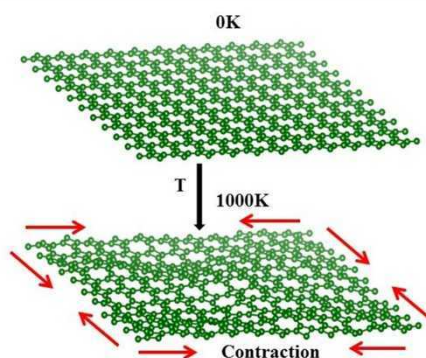
Buckling and Defects in Two - Dimensional Atomically Thin Monolayers

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Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other two-dimensional (2D) analogues like silicene, phosphorene, MXenes, MoS₂, and germanene have been recently isolated and characterized. One unifying theme among these new materials is that, unlike graphene, they are non-planar. The mode and measure of the buckling (puckering) from planarity depends on the local electronic structure. The effects of such ripples are manifold, particularly in their local reactivity to halogens and hydrogens along the more sp³ atoms. Pseudo Jahn-Teller (PJT) distortions are shown as a central unifying concept that explains the overall structural preferences of these systems.



The extent of buckling also leads to interesting and emerging phenomena, like phase transitions into Topological Insulators from normal semi-metals due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D monoatomic layers will be discussed in this lecture.

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Keywords: Graphene, 2D Materials, Silicene, Phosphorene, MXenes, MoS₂, Germanene, Pseudo Jahn-Teller, Topological Insulators, Spin-Orbital Coupling

MRSI Medal Lecture

Nanomaterials in Action: Translational Advances from Environmental Sensing to Biomedical Applications

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Nanomaterials have revolutionized modern science by bridging the gap between material innovation and translational applications in healthcare and environmental safety. This work integrates multiple nanomaterial-based platforms to highlight their potential across diverse domains. Two-dimensional tungsten disulfide (WS₂) combined with one-dimensional gold nanowires (AuNWs) yielded a highly conductive AuNW-WS₂ nanocomposite, demonstrating attogram-level sensitivity for monocrotophos detection via a simple screen-printed carbon electrode system. Complementing this, a silica alcogel-based chromagrid-lightbox, fabricated from recycled laboratory waste, enabled smartphone-assisted point-of-care colorimetric detection of pesticides—offering a sustainable, low-cost sensing alternative. Expanding into biomedical applications, a high-affinity aptamers against endosulfan was developed through SELEX and integrated into an electrochemical aptasensor with picomolar detection limits, validated using HPLC. Furthermore, micro-nanoarchitected silica fiber scaffolds combining pressure-spun microfibers and electrospun nanofibers exhibited enhanced fibroblast proliferation and accelerated wound healing in-vivo through synergistic biodegradability and ECM mimicry. Together, these studies underscore the transformative role of nanomaterials in enabling rapid environmental monitoring, point-of-care diagnostics, and regenerative medicine—paving the way for scalable, sustainable, and intelligent nanotechnology solutions for global health and environmental challenges.

Keywords: Nanomaterials, WS₂, Gold Nanowires, Aptasensor.

MRSI Medal Lecture

Surface modified nanostructured materials: Promising applications in analytical chemistry

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In recent years, the surface modified nanostructured materials (metal nanoparticles (NPs), metal nanoclusters (NCs), carbon dots (C-dots), MXenes and perovskite quantum dots (QDs)) crucial role in analytical chemistry for the analysis of wide variety target molecules (metal ions, anions, free radicals, biomolecules, drugs and pesticides) in various samples [1-3]. The surface modified nanostructured materials have opened new horizons in analytical chemistry to develop miniaturized analytical approach for assaying of various trace target analytes in real samples [4-7]. To support this, surface modified metal (Ag, Cu, Mo and Au) NPs and NCs were successfully integrated with UV-visible and fluorescence spectrometric techniques for selective and sensitive identification of multiple analytes at minimal volume of samples. Similarly, surface modified 2D nanostructured materials were integrated with fluorescence spectrometric technique for selective and sensitive detection of drugs and pesticides. Recently, ligand chemistry also play key role in fabricating water stable perovskite QDs for sensitive identification of free radicals, drugs and biomarkers in biofluids. These reports demonstrated that the surface modified nanostructured materials have greatly improved analytical features (selectivity, rapidity, sensitivity, and miniaturization) of UV-visible and fluorescence spectrometric techniques for molecular recognition, which favors to assay trace target analytes just like sophisticated analytical instruments. Glimpses of the surface modified nanostructured materials in UV-visible and fluorescence spectrometric techniques for chemical analysis will be presented.

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Keywords: Surface modified nanostructured materials, nanoparticles, nanoclusters, MXenes, perovskite quantum dots.

MRSI Medal Lecture

Stress-Induced Self-Organization of Nanostructures in Stretchable Matrices for Flexible Electronics

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Ensuring stable printed geometries under repeated stretching and bending cycles remains a critical challenge for ensuring the long-term mechanical integrity and electrical conductivity of flexible electronic devices. The increase in electrical resistance is mainly attributed to the dynamic restructuring of conducting nanofiller networks in the elastomer matrix, leading to instability of the interpenetrating conductive pathways under periodic stress. The in-situ stretching, annealing and concurrent conductivity measurements of nanocomposite films, along with synchrotron-based ultra-small-angle X-ray scattering have been used to elucidate the hierarchical evolution of nanofiller assemblies across multiple length scales. A wide range of polymers and conductive fillers with varying geometries and functionalities have been systematically explored to understand the intra- and intermolecular reinforcement mechanisms to mitigate shear stresses and delay network fragmentation. Insights into the non-bonded polymer-filler and filler-filler interactions as a function of the percolation threshold can facilitate the rational design of conductive ink formulations suitable for flexible and wearable electronic applications.

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Keywords: Conductive Nanocomposites, Stretchable Devices, Nanofiller Networks, Percolation Threshold, Elastomer Matrix, Wearable Devices, Mechanical Integrity, Synchrotron X-ray Scattering.

MRSI Medal Lecture

Structural Phase Transitions in Lead Free Ferroelectric Perovskite Oxides

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Ferroelectric oxides with a perovskite structure have attracted significant attention from the scientific community due to their intriguing fundamental physics and wide range of potential device applications. These ferroelectric materials are widely used in various electronic and optoelectronic devices because of their excellent dielectric, piezoelectric, pyroelectric, electromechanical coupling, and switchable ferroelectric properties. Structural phase transitions in ferroelectric materials are closely linked to changes in crystal symmetry. The use of group theory for understanding of the structural phase transitions in ferroelectric materials using both theoretical and experimental investigations is one of the interesting phenomena of condensed matter physics. The phase transitions in the ferroelectric materials are accompanied by a change in the symmetry due to external stimuli like chemical substitution, temperature, pressure, electric field, and also with swift heavy ions (SHI). The chemical modifications and fabrication of solid solutions are simpler and suitable

approaches to improve the functional properties of ferroelectric materials as per the requirements of device applications. It has been reported that enhanced ferroelectric and piezoelectric responses are observed around morphotropic phase boundary (MPB) compositions in ferroelectric solid solutions.

In the present investigation, we have considered the systematic investigation of structural phase transition phenomena in two lead-free ferroelectric systems, i.e., $(1-x)\text{Ba}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3 - x(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$ (BZT-xBCT) and $(\text{K}_{0.48}\text{Na}_{0.48}\text{Li}_{0.04})(\text{Nb}_{1-x}\text{Ta}_x)\text{O}_3$ (KNLNT-x), as a function of chemical compositions and temperatures. Both the series of ferroelectric materials (i.e., BZT-xBCT and KNLNT-x) have been prepared over a wide range of compositions. The compositional-driven structural phase transitions are investigated using X-ray diffraction (XRD) and Raman spectroscopic techniques. The temperature-dependent phase transitions are further examined from the temperature-dependent dielectric properties as a function of frequency. The dielectric, ferroelectric, and piezoelectric properties have exhibited maximum values at specific compositions, particularly in the phase co-existence region. To develop a clear understanding of the phase transition phenomena across various compositions and temperatures, phase diagrams are constructed using the room-temperature XRD, Raman, and temperature-dependent dielectric data. Finally, the enhancement of functional properties has been correlated with the crystal structure and discussed within the framework of morphotropic phase boundary (MPB). Symmetry mode analysis of structural phase transitions of ferroelectric materials will also be discussed to understand the atomistic origin of phase transitions by taking the example of simple ferroelectric perovskite oxides. The details of our results will be discussed during the time of presentation.

Keywords: Ferroelectric oxides, Perovskite, SHI, Piezoelectric properties.

MRSI Medal Lecture

Ionic Liquids and Deep Eutectic Solvents for Sustainable Sorption and Extraction Processes

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Ionic liquids (ILs) and deep eutectic solvents (DESs) are emerging as transformative materials in modern chemistry, offering a powerful platform for designing sustainable solvent systems with tunable structure, functionality, and performance. Their negligible volatility, wide liquidus range, and exceptional chemical and thermal stability make them highly attractive for energy-efficient sorption and extraction processes central to the circular economy.

This MRSI Medal Lecture will focus on the materials chemistry of ILs and DESs, highlighting how rational molecular design and structure–property correlations enable their optimization for targeted separations and resource recovery. Selected examples from our research demonstrate their effectiveness in selective metal extraction from electronic waste and spent lithium-ion batteries, biomass valorization, and wastewater purification, underscoring their role as sustainable materials for environmental and energy applications.

The lecture will further discuss the design strategies, synergistic interactions, and structure–function relationships that govern solvent performance, stability, and recyclability. By integrating materials chemistry principles with sustainable process development, tailored ILs and DESs emerge as key enablers of green separation technologies and sustainable innovation across the chemical and energy sectors.

Keywords: Ionic Liquids; Deep Eutectic Solvents; Sustainable Materials Chemistry; Sorption and Extraction Processes.

MRSI Medal Lecture

Ionic Liquid, Poly(Ionic Liquid) and Ionic Liquid Based Membranes: 'Green' Multi-Verse Materials For New Age Applications

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In response to the rising awareness of the environmental effects related to volatile organic compounds (VOCs), room temperature ionic liquids (ILs) have gained international acceptance as promising 'green' alternatives to VOCs. This acceptance is due to their advantageous properties, such as low vapor pressure, a wide liquid range, high stability against chemical and radiation, a broad electrochemical window, a high flash point, and a significant solubilizing characteristics of a diverse array of organic, inorganic, and polymeric materials. One of the most captivating aspects of ILs is their remarkable tunability. A slight modification in either the cationic or anionic components can result in considerable alterations in the physicochemical properties of the IL, which is why they are referred to as 'designer solvents.' When a structure–activity relationship is established for a particular property of ionic liquids, they can be adjusted accordingly. ILs are made up of large organic cations combined with organic or inorganic anions. The charge delocalization leads to a lattice energy that is too low for the system to exist as a solid crystal, thus remaining in a liquid state. Ionic liquids have been widely utilized in organic synthesis, sensor applications, electrochemistry, separation science, and membrane technology. At times, ILs demonstrate unique chemical phenomena that are not typically observable through conventional means. In functionalized ionic liquids, the selectivity and efficiency are enhanced by covalently attaching functional groups to the IL moieties. In ionic liquids, the mechanisms for extracting metal ions, the nature of bonding, and the kinetics and thermodynamics related to biphasic separation can be adjusted as required. Ionic liquids have also been explored for their selective dissolution of various oxides of f-block elements, enabling mutual separations with an exceptionally high separation factor. The polymerization of either ionic segment of the IL monomers can lead to the development of poly(ionic liquids) (PILs). These compounds exhibit the advantageous traits of both polymers and ionic liquids. They have been extensively utilized for the removal of dyes and other micro-pollutants from various aqueous industrial waste streams. Supported IL membranes and poly(ionic liquid) grafted or augmented membranes have been employed to achieve separations between aliphatic and aromatic homologues, such as hexane and benzene, as well as heptane and toluene, which cannot be accomplished through conventional sieving techniques. The interaction between the pi electron clouds of the aromatic components in the IL and the elements of interest serves as the driving force for this process. This membrane has also been utilized for the fractionation of regio-isomers, sugars, and dye molecules. The addition of a PIL brush has been found to enhance the antifouling properties of the membrane. The alternating cationic and anionic charges present on the PIL brushes enable the membrane to exert electrostatic repulsive interactions, thereby preventing the scaling of inorganic salts and minimizing adhesive interactions with micropollutants that possess surface charges. Additionally, a membrane with a PIL grafted polymer brush can create local perturbations in the presence of an external oscillating electrical field. The local perturbation can be externally adjusted based on the frequency of the oscillating electrical field.

Keywords: Ionic liquids, poly(ionic liquids), membranes, separation science, VOC alternatives, designer solvents, functionalized ILs.

MRSI Medal Lecture

Atomic-layered 2D MXenes: Materials driving innovation in sustainable development and clean energy solutions.

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Ti₃C₂-X MXenes have gained significant research momentum due to their 2D laminar morphology, which enables a wide range of functional applications. Realizing these potentials at scale requires the synthesis of high-purity MAX phase, the essential precursors for MXene production, through simple and cost-effective techniques. However, achieving pure MAX phase at atmospheric pressure and relatively lower temperatures remains a major challenge. Conventional synthesis routes, including liquid or solid-state reactions and pulsed laser deposition, have been explored to improve MAX phase purity. However, these often result in residual impurity phases, smaller grain size, low component density, secondary phases, irregular morphologies, and low overall yield. Such imperfections adversely affect the interlayer spacing and structural integrity of the resultant MXenes, thereby limiting their performance.

In this context, I will present our recent advances in synthesizing high-purity Ti₃AlC₂ MAX phases via a molten salt shielding solid-state synthesis (MS5) process conducted under atmospheric pressure. This approach effectively enhances the interlayer spacing and significantly improves the electrochemical performance of Ti₃C₂-F MXene electrodes. The incorporation of F-terminal groups expands the interlayer spacing, yielding a surface area of ~ 8.9 m²/g and providing more electroactive sites that facilitate efficient Na⁺ ion intercalation. Remarkably, an increase in MAX phase purity from 47% to 99% results in a substantial enhancement in specific capacitance. Furthermore, high-purity (i.e., >99%) Ti₃C₂-F MXene exhibits outstanding performance as an anode material for Na-ion batteries, maintaining excellent activity even at temperatures as low as -120°C. Beyond energy storage, it also demonstrates significant potential for green hydrogen generation through photocatalysis and serves as a promising catalyst for hydrogen storage applications.

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Keywords: MAX, MXenes, Energy Storage, Energy conversion, Sustainability.

MRSI Medal Lecture

Rashba and Excitonic Physics in Emerging Materials and Correlations with Light-Matter Interaction: A Computational Insight

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We have successfully correlated the Rashba splitting with Excitonic Radiative lifetime in lower dimensional condensed matter systems with different periodic confinements and interfacial configurations, which would certainly have tremendous impact in discovering the emerging optoelectronic materials based on the fundamental charge carrier recombination [1-3]. We have also envisaged the transition between Rashba, Rashba-Dresselhaus and Persistent Spin Textures in novel perovskite systems in the form of a quasi-2D confinement [4]. We continued our quest of Rashba splitting driven water splitting mechanism in inorganic perovskite materials [5,6]. The next part will be devoted to theoretical understanding of piezochromism, where hydrostatic pressure could be employed as an effective tool, giving rise to novel crystal structures and optical properties, while it has proven to be an alternative to chemical pressure [7,8]. Therefore, new functional materials with intriguing properties can be designed by exerting external pressure and strain. In this connection, the composition dependent transition between Frenkel Exciton to Wannier-Mott Exciton in inorganic perovskites will be discussed [9]. I will end my talk touching upon our recent successful endeavour of pre-intercalation mechanism in Li-ion battery, as recently appeared in Nature Materials [10].

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Keywords: Rashba Splitting, Excitonic Radiative Lifetime, Perovskites, Piezochromism, Frenkel Exciton, Wannier-Mott Exciton, Li-ion Batteries, Functional Materials.

Plenary Lectures

MRSI-ICEM 2025

Plenary Lecture

Circular Bio-Economy Driven Sustainable Materials: Future is now in Mitigating the Climate Change

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Materials are at the core of our economy. Building a more resilient, circular, and low-carbon economy is at the the world's recovery plan for sustainable materials move. Innovation in materials science & engineering must be integrated with climate for economic growth. A transition to low carbon economy requires circularity. Plastics and composites are inevitable in our day-to-day life and their use spans from packaging, housing structures, auto-parts, sports utility to electronics and a lot more. In 1950, the "Age of Plastics" began to replace natural materials and thereafter their production and use skyrocketed. "Plastic waste" is a global pollution problem in our changing world with microplastics (< 5 mm in size) even found in human blood and brain today. By 2050, annual plastic production is predicted to reach one billion tons from the present level of 450 million tons annually. Immediate and vigorous actions are required in reducing plastic wastes in mitigating the climate change. The single-use-plastic ban is a daily news headline; however, a "Second Age of Plastic" is imminent to reduce and eliminate plastic waste concerns through reduced carbon economy, referred to as "Sustainable Polymers". Sustainable polymeric materials are the wave of the future. Those materials can be designed and engineered from renewable resources, recycled materials, wastes and their hybrids. Two categories of materials: (i) biobased, biodegradable, and (ii) biobased non-biodegradable, recyclable polymeric materials can help in creating the circular economy of plastics. Biodegradable plastics show leading trends in sustainable packaging. Incorporation of more recycled plastics up to 25% in packaging and auto-parts are becoming the new market trend. This presentation will highlight the challenges and new opportunities towards a zero-waste plastics economy in supporting circular bioeconomy. The combination of circular economy with bioeconomy can lead to advanced sustainability in plastic materials world. The end-of-life solution for plastics must grow and should be expanded through government and industry leaders as well as policy makers.

Keywords: sustainable polymers, biodegradable plastics, biobased materials, recyclable polymers, microplastics, circular bioeconomy

Plenary Lecture

New Vibrational Spectroscopies based on Quantum Geometry of Electrons

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We first present an introduction to quantum geometry of electrons in periodic structures in terms of Berry phases and curvature, which cause bending of electronic trajectories that can be observed with transport measurements. Time-reversal and inversion symmetries of a periodic system however force the quantum phase space of its electrons to be flat with vanishing curvature. With first-principles theoretical analysis, we predict that coupling of dynamical excitations, such as phonons, with electrons can induce oscillations in the quantum geometric curvature with observable signatures in Hall measurements. Illustrating these ideas with examples of 2D materials, we propose a new kind of vibrational spectroscopy technique making system-specific predictions (R Bhuvaneswari et al 2024). This spectroscopy can be realized experimentally with scattering of

electromagnetic waves or using circuits. It can be employed in analysis of wider range of systems by interfacing them with a quantum material like graphene, thus opening up new kind of applications of quantum materials wherein they are used as a substrate to sense vibrations of a system in the neighbourhood. We present partial validation with experiments carried out by Deshmukh et al (2025). Work done in collaboration with R Bhuvaneswari and the group of Mandar M Deshmukh at TIFR Mumbai.

Keywords: vibrational spectroscopy, dynamical excitations,

Plenary Lecture

Frustrated Magnetism and Topological Electronic States in Noncentrosymmetric and Square-Net Rare-Earth Compounds

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Noncentrosymmetric (NCS) magnetic materials offer an excellent platform to investigate unconventional magnetic interactions and emergent spin textures arising from the competition between symmetric exchange and antisymmetric Dzyaloshinskii–Moriya interactions. In the Th_3P_4 structural family, the lack of inversion symmetry supports magnetic frustration and leads to unique magnetic responses, such as pronounced ZFC–FC divergence and frequency-dependent AC susceptibility. Our recent investigation on Nd_3Se_4 reveals a ferromagnetic transition at $T_c \approx 52$ K[1], accompanied by large ZFC–FC bifurcation and characteristic slow spin dynamics, indicating a complex frustrated magnetic landscape and opening prospects for exploring nontrivial spin textures in NCS systems.

Beyond noncentrosymmetric systems, square-net compounds have recently emerged as a fertile platform for realizing topologically nontrivial electronic states and unique transport behavior such as extremely large magnetoresistance, high mobility, and nontrivial Berry phase. Our recent studies on NdBiTe [2], NdSbSe [3], GdSbSe [4], and SmSbSe [5] reveal rich and tunable magnetic ground states strongly coupled to electronic transport. NdSbSe exhibits signatures of frustrated antiferromagnetism, GdSbSe demonstrates two distinct field-induced metamagnetic transitions whereas SmSbSe exhibits strong CEF-driven magnetic behavior with a clear Schottky anomaly in the specific heat. In NdBiTe , the observed rise in resistivity below the Néel temperature suggests strongly correlated fermions. We have extended our investigations to the RMX_3 family of rare-earth transition-metal pnictides, which also hosts a rich variety of magnetic ground states due to strong electron correlation, anisotropic exchange, and hybridization between 4f and conduction electrons. Our recent work on CeNiSb_3 reveals an intriguing coexistence of long-range ferromagnetic order with a spin-glass-like component at low temperatures.

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Keywords: ZFC-FC, NCS, frustrated antiferromagnetism

Plenary Lecture

Single-Quantum-Dot Devices for Photonic Quantum Technologies: Design, Deterministic Nanofabrication, and Application Perspectives

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The development of solid-state quantum emitters for practical quantum information technologies requires nanofabrication platforms that combine high precision with reproducible yield. Self-assembled semiconductor quantum dots (QDs) are among the most promising candidates due to their excellent optical properties. Yet, their inherently random spatial and spectral distribution poses a significant challenge for deterministic and scalable device integration using conventional lithography techniques.

In this talk, I present a flexible and deterministic nanofabrication approach that combines low-temperature cathodoluminescence spectroscopy with high-resolution electron beam lithography [1]. This iEBL technique enables highly precise positioning of single QDs within complex photonic nanostructures to maximize the device performance for instance in terms of the photon extraction efficiency and the Purcell effect. I will discuss the iEBL process and its role as an advanced technology platform for single-emitter devices, emphasizing its capability for scalable, high-yield fabrication.

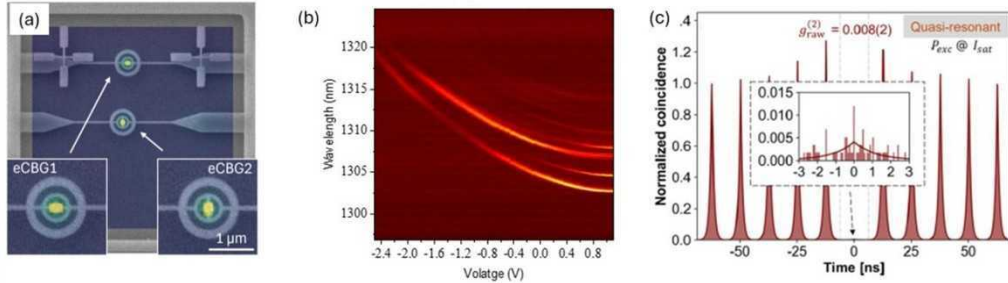


Figure 1: (a) Scanning electron microscopy image of two deterministically fabricated QD-eCBGs [2]. (b) Biasdependent micro-photoluminescence map of a Q-band QD-eCBG showcasing electrical control of emission [3]. (c) Autocorrelation histogram of a QD-eCBG with excellent single-photon purity of 99% [2].

Application examples include electrically tunable circular Bragg grating devices (eCBGs) for brightness enhancement and charge control [2, 3], as well as integrated QD-based quantum photonic circuits [4, 5]. These devices demonstrate electric control of the optical and quantum optical emission properties, near-unity singlephoton purity, and high indistinguishability, highlighting their potential for photonic quantum technologies.

This talk provides an overview of the design principles, deterministic fabrication strategies, and application perspectives of single-QD devices, illustrating the path toward scalable, high-performance solid-state quantum photonics.

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Keywords: iEBL, QDs, lithography, f single-QD device, flexible nanofabrication.

Invited Talks

MRSI-ICEM 2025

Degenerate transparent wide Bandgap semiconductors for multiplication applications

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The Fermi level (E_f), for some of the transparent conducting oxides (TCOs) known as degenerate semiconductors, is found within the conduction or above the conduction band, as is found in a metal. For example, such is the case when the wide bandgap semiconductor ZnO is doped with either Ga or Al. These doped semiconductors demonstrate properties that are more metal than semiconductor-like with the resistivity being proportional to the temperature. This class of semiconductor materials demonstrate remarkable properties of low-loss plasmonic materials because they do not have bound-state absorption transitions in their bandgaps, and their surface plasmon polariton losses can be even smaller, in the NIR region than those with conventional plasmonic materials at corresponding visible wavelengths. We will discuss the extreme tunability of these materials for optical manipulation and potential transformative applications, such as the electrothermal control of aluminum-doped zinc oxide /vanadium dioxide (VO_2) multilayered thin films, fabrication of Hyperbolic optical metamaterials, novel contacts for X- and gamma-ray detectors, electrothermal properties and memristors applications.

Keywords: TCOs, gamma-ray detectors, Hyperbolic optical metamaterials.

ions having magnetic properties gives rise to magnetic doped semiconductors. With the balance of optical and magnetic properties, these magnetic semiconductors are widely used in spintronics, bio-imaging and magnetic resonance imaging (MRI) applications. To facilitate their usage in bio applications, it is critical to synthesize water soluble magnetic QDs with stabilized structure while maintaining their optical and magnetic properties. Here in our work, we developed a facile substituted synthetic route to achieve Cr doped CdSe (Cr-CdSe) via a facile hydrothermal method. The effects of doping on the structural, optical, and magnetic properties of the Cr-CdSe were studied using X-ray diffraction, UV-Visible spectroscopy, photoluminescence lifetime. We then explored their chemical nature and morphology change with increase in doping concentration via X-ray photoelectron spectroscopy and transmission electron microscopy. Water soluble QDs have been used as a bio-imaging probe for the past few decades due to their strong fluorescence, photostability and improved tissue or cellular penetration. However, incorporating magnetic material into fluorescent entity harnesses the ability to control strengths of both modalities that enhance the diagnostic accuracy and facilitate its application in bio-systems especially in early accurate diagnosis. Finally, we demonstrate the competency of Cr-CdSe as a dual imaging probe with fluorescent cellular imaging and MRI applications [1-4].

Aqueous Based Ultra-Small Magnetic Cr-doped CdSe Quantum Dots as a Potential Dual Imaging Probe in Biomedicine.

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Substitution of semiconductor quantum dots (QDs) by a small number of transition-metal

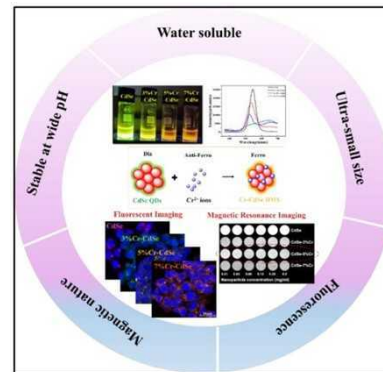


Figure 2: Graphical representation of Cr-CdSe magnetic quantum dots

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Keywords: MRI, CdSe, Potential Dual Imaging Probe

Emerging 2D borophene for photonics: Tunable nonlinear optical properties of iron oxide/borophene core shell nanostructure

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Borophene, a single-atom-thick boron sheet, has emerged as a promising member of the two-dimensional materials family, distinguished by its exceptional anisotropic properties and superior electronic tunability compared to isotropic graphene. Its electron-deficient nature leads to high thermal conductivity resulting in enhancement of the efficiency of energy storage devices. Two-dimensional borophene exhibits a broadband non-linear response in near-infrared and mid-infrared wavelengths. Its pronounced third-order nonlinear optical susceptibility and directional metallicity lead to advanced photonic applications including reverse saturable absorption, optical limiting, and ultrafast laser technologies.

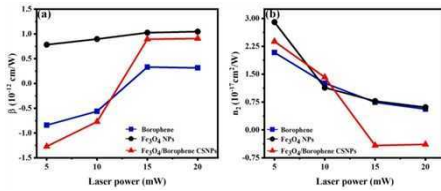


Figure 3: Variation of (a) β and (b) n_2 with laser power for borophene, Fe₃O₄ nanoparticles (NPs), and core-shell nanoparticles (CSNPs).

We will discuss the systematic investigation of power-dependent nonlinear optical characteristics in novel Fe₃O₄/Borophene core-shell nanoparticles (CSNPs). The nanostructures were synthesized via controlled chemical vapor deposition using sodium borohydride as boron precursor, followed by comprehensive characterization through XRD, FTIR, UV-vis spectroscopy, TEM, SEM, and EDX techniques. Vibrating sample magnetometry (VSM) revealed enhanced saturation magnetization of Fe₃O₄ nanoparticles upon borophene encapsulation, demonstrating synergistic core-shell interactions. Power-dependent Z-scan measurements utilizing ultrashort femtosecond laser pulses at 800 nm wavelength in open and closed aperture configurations revealed that borophene-coated Fe₃O₄ nanoparticles exhibit tunable nonlinear optical properties that enhance intrinsic borophene characteristics. Interfacial charge transfer mechanisms in these nanostructures play a key role in amplifying optical non-linearities. The pronounced anisotropy and metallicity of borophene, combined with magnetic core properties, create unprecedented performance in optical limiting applications.

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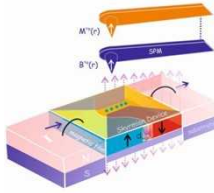
Keywords: Borophene, core-shell nanostructures, Non-linear optics

Creation and manipulation of magnetic spin texture in ferrimagnetic thin film system for application

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Next generation logic and memory technologies demands exotic material with tunable properties to have multi-functionality, room-temperature operation and energy efficiency. Topologically protected nano-scale spin textures, namely skyrmion, are found to be promising candidates for development of high-density data storage devices, spin-logic devices. I will present nanoscale magnetic properties of transition metal and rare-earth based ferrimagnetic thin film and their potential for room temperature skyrmion based application.



Ferrimagnetic system offers added advantage of nearly-zero skyrmion Hall effect and high-speed device owing to strong exchange field and measurable magnetic signal as opposed to antiferromagnetic counterpart. Our experimental findings are well supported by micromagnetic and atomistic spin dynamics modeling.

Keywords: ferrimagnetic, rare-earth, micro-magnetic.

Janus Sn on WS₂ and Beyond

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In this work, we study the growth and local electronic properties of Sn on the WS₂ surfaces by scanning tunneling microscopy (STM) and spectroscopy (STS) measurements, and by first principles ab-initio calculations. The growth of Sn on the WS₂ surface was carried out under

ultra high vacuum (UHV) conditions at room temperature (RT) for different coverages. The Sn grown layers exhibit almost similar atomic periodicity as the WS₂, indicating a stretched hexagonal surface lattice after Sn growth. LEED measurements reveal 1x1 surface symmetry after the growth without evidence of any extra spots in the diffraction patterns even after prolonged Sn deposition. This indicates a nearly commensurate growth of Sn on the WS₂ surface. Further STM measurements along with density functional theory (DFT) calculations, reveal the initial growth of Sn which is a case of substitutional doping at the top 'S' sites via the formation of monomers (U) and dimers (P) with the distance between two adjacent Sn atoms being 0.34 nm and 0.293 nm respectively [1]. STM and DFT studies validate the growth Janus Sn layer on the substrate. STS measurements display modulated in-gap electronic states of the Sn-WS₂ system [2]. The experimental realization of Janus structure of Sn and beyond, and the local electronic properties of the Sn grown surfaces, along with the theoretical calculations will be presented here.

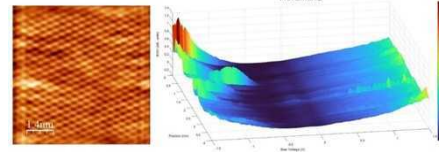


Figure 4: STM micrograph of the Sn grown surface and electronic structure mapping by STS.

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Keywords: LEED, DFT, STM

Tailoring of functional materials for multidisciplinary research

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Materials science is a highly interdisciplinary field that encompasses the study of the properties of matter and its diverse applications across various domains of science and technology. In recent years, the field has experienced a transformative shift, largely driven by the growing interest in nanomaterials. This shift has opened up new research directions, expanding the scope of materials science and enabling advancements in a wide range of industries, from electronics and energy storage to healthcare and environmental technologies.

In-situ polymerization and composite formation, combined with organic molecule-mediated complexation, represent two key reaction pathways for synthesizing metal-organic nanocomposite materials. These methods provide notable advantages in the field of synthetic material science, as they enable the effective integration of organic and inorganic components. Through functionalization, both components can interact at the molecular level, promoting enhanced synergy and facilitating more intimate contact. This approach not only improves the structural integrity and performance of the resulting materials but also opens up new possibilities for tailoring properties for specific applications. The presentation will explore the synthesis of hybrid materials and their applications across various fields, including catalysis, sensors, transport properties, organic transformation reactions and renewable energy research.

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Keywords: polymerization, functional materials, hybrid materials .

Multifunctional electrochromic materials and smart device

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The modern era is an era of science and technology that affects all aspects of life. The simplest physical manifestation of the term 'technology' takes place in the form of a simple and user-friendly device. The design and development of a smart device, capable of performing at its best, depends on the level of scientific understanding of the basic principles that make the actual backbone on which the technology relies. This leads to progressive development and research in electronics, materials science and related fields. An electrochromic device (ECD) is a perfect example of a smart yet very simple form of a device that can be useful for a range of applications, including electrochromism: the phenomenon of bias-induced optical modulation, shown primarily by at least one of the components in an ECD. This talk attempts to provide an update on different materials' regimes and highlights the basic requirements that a material must have to be suitable for use as the active component of an ECD. This gives the details of several electrochromic materials, and their electrochemical, electrochromic and other functional properties in brief. An attempt has been made to cover a subset of the vast superset of known electrochromic materials, which can be extended as a detailed comprehensive review in the future. Based on the type(s) of materials used in an ECD, device paradigms are defined, which have also been summarized through different device regimes, namely 'all-organic', 'all-inorganic' and 'hybrid'. To provide a glimpse, ECDs that are multifunctional and that show other functionalities like memory, and supercapacitive and sensing characteristics will also be discussed.

Keywords: electrochromic materials, supercapacitive, ECD

Interlayer Excitons and Ultrafast Dynamics in Twisted van der Waals Heterostructures

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Twisted van der Waals (vdW) heterostructures represent a rapidly evolving class of quantum materials in which interlayer coupling and moiré periodicity can be precisely tuned by varying the twist angle between adjacent two-dimensional (2D) layers [1,2]. This structural tunability leads to the formation of unique excitonic states, including long-lived interlayer excitons with spatially separated electron-hole pairs residing in different layers [3]. In this talk, I will discuss about the formation, relaxation, and recombination dynamics of interlayer excitons in twisted transition metal dichalcogenide (TMD) heterostructures such as MoSe₂/WSe₂ and MoSe₂/MoS₂ [3–5]. By employing ultrafast pump-probe spectroscopy, time-resolved photoluminescence, and temperature-dependent optical measurements, we uncover how twist-angle-induced moiré potentials modulate the exciton binding energy, diffusion behavior, and charge transfer rates across the interface. The comprehensive understanding of interlayer exciton formation and ultrafast dynamics presented here provides new insights into many-body interactions and non-equilibrium carrier processes in moiré-engineered 2D systems. These findings hold significant implications for the design of next-generation optoelectronic and valleytronic devices, including excitonic transistors, ultrafast photodetectors, and quantum light sources based on twisted vdW heterostructures.

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Keywords: vdW Heterostructures, Twist angles, Interlayer Excitons, Ultrafast Dynamics

Light–Matter Interactions, Contact Engineering and Single Defect Spectroscopy in Engineered 2D Heterostructures

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Two-dimensional (2D) materials and their hybrid interfaces provide a versatile platform for manipulating charge transport, excitonic processes, and light–matter interactions. This talk brings together three complementary directions. First, I discuss enhanced photodetection in 2D/0D and 2D/2D heterostructures, where graphene and TMDC devices exhibit tunable photoresponse driven by interface-mediated charge transfer, alloy engineering, and exciton–plasmon interactions. Second, I focus on ReS₂-based electronic and optoelectronic devices, where graphene-contacted ReS₂ FETs demonstrate nearly barrier-free carrier injection, reduced 1/f noise, and significantly enhanced photodetection enabled by van der Waals contact engineering. Building on this platform, I will present defect spectroscopy in ReS₂–hBN FETs, where ultraclean few-layer graphene contacts suppress disorder and allow direct observation of random telegraph noise from individual hBN defect centers. These single-defect signatures evolve into 1/f noise with increasing temperature, and statistical analysis attributes the traps to carbon-related substitutional defects. Third, I introduce 2D/organic hybrid heterostructures formed by spontaneous epitaxial growth of ultrathin vanadyl phthalocyanine (VOPc) on MoS₂, WS₂, and hBN. These systems exhibit tunable photoluminescence and hybrid charge-transfer

excitons, revealed by transient absorption spectroscopy and supported by XPS/UPS and DFT analysis. Interface-induced band alignment and molecular conformation emerge as new knobs for controlling optical and excitonic properties. Together, these results establish interfacial engineering across 2D/0D, 2D/dielectric, and 2D/organic platforms as a powerful strategy for uncovering new excitonic phenomena, enhancing photoresponse, and probing defect dynamics in quantum materials.

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Keywords: Light–Matter Interactions, HeterostructuresIT-B01, Single Defect Spectroscopy.

Disorder as a Lens: Unconventional Superconductivity in Infinite-Layer Nickelates

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The discovery of superconductivity in thin films of hole-doped infinite-layer (Nd,Sr)NiO₂ marked a significant step in the avenue of superconducting oxides [1]. Initially proposed as simple cuprate analogue with a square-planar structure and 3d⁹ Ni electron configuration [2], these materials were expected to closely resemble the cuprates. However, subsequent studies revealed notable differences in their electronic structure and hybridization landscape [3]. Nevertheless their experimental realisation provided a new platform to explore the physics of high-temperature superconductivity, generating significant interest. Since then, a variety of rare-earth and dopant combinations have been realized, also extending to the formally undoped parent phase. In parallel, recent advances in ma-

terials synthesis techniques and reduction methods have pushed T_c values even higher, reaching up to 35 K in Sm(Eu,Ca,Sr)NiO₂ thin films [4].

A central question is the symmetry of the superconducting gap structure in these materials. Probing this has remained an experimentally challenging task due to the thin-film geometry and surface degradation caused during the chemical reduction essential to stabilise the requisite Ni¹⁺ valence, which limits the applicability of techniques such as London penetration depth measurements via mutual inductance [5] or tunnel diode oscillator methods [6], single-particle tunnelling [7], photoemission spectroscopy [8,9], and thermal transport [10], often employed to investigate superconducting pairing symmetry.

To address this challenge, we employ high-energy electron irradiation to introduce controlled disorder in superconducting infinite-layer nickelate thin films and examine the effect of pair-breaking defects on superconductivity to elucidate the nature of the superconducting gap. Our results reveal a complete suppression of T_c and an increase in normal-state resistivity with added disorder, suggesting the presence of an unconventional sign-changing gap symmetry [11]. These observations provide valuable insights into the superconducting order parameter and electronic landscape of infinite-layer nickelates. More recently, we have extended these studies to also explore how these effects depend on choice of rare-earth ion, including Nd-, Pr-, and La-based nickelates.

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Keywords: pair-breaking defect, superconductivity, Nickelates

Realization of ZnO@ β -SiC Composite for Neuromorphic Computing

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Technological advancement of the memristor-based artificial synapse has attracted a considerable interest for neuromorphic applications. Current memristive technology is however more promising for metal oxide-based memristors, though it requires precise structural and chemical engineering. Here, we show a novel approach for realizing electroforming free non-volatile memory devices in rf magnetron sputtering grown ZnO@ β -SiC composite film. A switching from high resistance state to low resistance state is shown to be achieved at an extremely low voltage of ~ 0.1 V with a set/reset response speed of $\sim 40/50$ ns, where the device stability is found to be over 10^4 cycles with a retention of $\sim 10^4$ sec. This is shown to be associated with the formation of Zn₂SiO₄ nanocrystals in an amorphous layer as conformed by detailed structural studies followed by chemical and microstructure analyses. This is interpreted in terms of the formation and dissolution of conductive filaments made of oxygen ions, though involvement of Ag⁺ ions cannot be neglected in Ag/ZnO@ β -SiC/ITO device structure. The formation of conducting filaments has been confirmed by performing conductive atomic force microscopy. Moreover, the excellent synaptic properties such as excitatory post-synaptic current, pair pulse facilitation, potentiation/depression, and long-term memory/short-term plasticity have been established and discussed for sustainable development of the artificial intelligence with in-memory neuromorphic computing.

Keywords: Neuromorphic Computing, conducting filaments, synaptic properties.

Anomalous temperature-dependent Raman spectrum of van der Waals ferromagnet Fe_5GeTe_2

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Two-dimensional (2D) van der Waals (vdW) ferromagnet Fe_5GeTe_2 has attracted considerable attention owing to its high Curie temperature (T_C), large saturation magnetization, and complex magnetic behaviour, which arises in part from multiple inequivalent iron sites and intrinsic vacancies. Although several aspects of its intricate magnetic and structural properties have been explored through detailed experiments and first-principles calculations, many features remain under debate. In this work, we present a temperature-dependent Raman spectrum for bulk Fe_5GeTe_2 which shows an intriguing peak-shift anomaly near 150 K. We discuss the potential connection between this Raman anomaly, and the anomalous lattice expansion previously reported around 110 K. Furthermore, isothermal magnetization measurements reveal how this unusual lattice expansion influences the magnetic anisotropy in this vdW material. Together, these insights are expected to play an important role in guiding the use of Fe_5GeTe_2 in high-performance spintronic applications.

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Keywords: van der Waals magnets; magnetic anomalies; Raman Spectroscopy.

Anomalous Nernst and Hall Effects in Heuslers and Magnetic High-Entropy Alloys

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Understanding and controlling spin-dependent transport phenomena in complex magnetic materials has become a central theme in modern condensed matter physics and spintronics. Among these, the anomalous Hall and Nernst effects—both governed by the Berry curvature of electronic bands—serve as sensitive probes of symmetry breaking, topological characteristics, and scattering mechanisms in magnetic systems. The quest for materials that combine tunable electronic structure, thermal stability, and resilience to disorder has led to a resurgence of interest in multi-component intermetallics such as Heusler alloys and magnetic high-entropy alloys (HEAs). These materials represent a fertile platform where topology, entropy, and magnetism intersect, opening pathways for designing next-generation spin-caloritronic and energy-harvesting devices.

Recent advances from our group reveal how compositional complexity in Heusler and high-entropy systems can be exploited to design robust spintronic materials. In quaternary Heusler alloys such as CoFeVSb and CrRuXGe ($X = \text{Co}, \text{Mn}$), we demonstrate large and tunable anomalous Nernst effects (ANE) arising from both Berry-curvature and skew-scattering mechanisms, including polarity reversal linked to structural and magnetic transitions[1,2]. We find that nanocrystalline magnetic HEAs, such as CoCrFeNiGa , exhibit soft ferromagnetism with a high Curie temperature ($\sim 872\text{ K}$) and a large intrinsic anomalous Hall conductivity ($\sim 600\text{ S cm}^{-1}$) that persists despite significant chemical disorder[3]. These findings establish a unified framework connecting lattice symmetry, entropy, and topology to emergent spin-dependent transport, and point toward disorder-engineered materials capable of maintaining functionality under extreme conditions—key for scalable energy and information technologies.

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Keywords: Anomalous Nernst, Hall Effects, Heuslers

Proximate spin-liquid behaviour in the double trillium lattice antiferromagnets

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Quantum spin liquid (QSL) is a highly correlated but dynamically disordered state of spins characterized by the absence of magnetic long-range order (LRO) and is typically hosted by the frustrated magnets [1]. Trillium lattice formed by corner-shared triangular units provide an ideal platform for magnetic frustration in three dimensions (3D). In this talk, I'll present the proximate QSL behavior in $\text{K}_2\text{Co}_2(\text{SO}_4)_3$ where the magnetic Co^{2+} ions are embedded on a highly frustrated 3D double trillium lattice [2]. It undergoes a structural phase transition at $T_t = 125$ K from high-temperature cubic to low-temperature monoclinic phase with the three-fold superstructure. Magnetization and heat capacity consistently show the formation of the $J_{\text{eff}} = 12$ state of Co^{2+} below 50 K. In zero-field, $\text{K}_2\text{Co}_2(\text{SO}_4)_3$ shows signatures of static magnetic order formed below $T^* = 0.6$ K, but muon spin relaxation experiments reveal a large fluctuating component that persists down to at least 50 mK, reminiscent of QSL. Static order is completely suppressed in the small magnetic field of 1 T, and low-temperature heat capacity demonstrates the T^2 behavior above this field, another fingerprint of QSL.

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Keywords: antiferromagnet, QSL.

NV centers in diamond: Boosting quantum sensing through controlled implantation

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Nitrogen-vacancy (NV) centers in diamond have emerged as an important solid-state spin system for quantum sensing and metrology. In particular, the presence of optically addressable spin states along with the optically detected magnetic resonance (ODMR) characteristics makes it an attractive platform for room temperature quantum sensing applications.

However, the ODMR spectrum is governed by various properties like defect microstructure, spin-bath composition, and lattice strain. Hence, controlled creation of NV centers is key to develop a superior spin qubit-based sensing platform. In this regard, low energy carbon- and helium-ion implantation with variable dose has been carried out. Using SRIM software, it is possible to set different implantation-related parameters prior to the experiment where vacancy-generation profiles can be predicted, leading to tailored defect density and depth distributions. In the context of the present work, both ion species have been chosen carefully to enhance vacancy concentration within tens of nanometers in nanodiamonds. Subsequent characterizations were performed to understand the defects generated during ion-solid interaction. An indigenously developed ODMR setup for quantum sensing applications will be discussed. Furthermore, we will also revisit our effort of using the ion implantation technique for materials modification and characterization. We envisage that together, these advances will establish a pathway toward scalable, high-coherence NV-diamond quantum sensors for a robust nanoscale quantum sensing platform.

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Keywords: SRIM, ODMR, qubit.

Fish scale-based Nano Hydroxyapatite Reinforced Polylactic Acid Composite Blown Film

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In this study, nano-hydroxyapatite (n-HAp) was extracted from pink perch fish scales (PPFS) using a simple and efficient alkaline hydrolysis method. The obtained n-HAp was systematically characterized using XRD, FTIR, Raman spectroscopy, TGA, SEM, and TEM to confirm its structural, chemical, thermal, and morphological attributes. Subsequently, varying concentrations of n-HAp (0.25, 0.5, 0.75, and 1 wt.%) were incorporated into a polylactic acid (PLA) matrix via solution blending, followed by blown film extrusion. The effect of n-HAp incorporation on the thermal, mechanical, and biodegradation properties of the PLA-based composites was comprehensively evaluated. FTIR and Raman spectroscopy analyses confirmed the presence of chemical interactions between n-HAp and the PLA matrix in the blown films. Thermogravimetric analysis indicated an enhancement in the initial degradation temperature compared to neat PLA, which was attributed to the stabilizing effect of n-HAp. Differential scanning calorimetry revealed a reduction in both glass transition temperature and crystallinity, suggesting restricted polymer chain mobility and an increase in the amorphous phase. Mechanical testing demonstrated that lower concentrations of n-HAp notably improved the elongation at break, with the PLA-HAp 0.75 formulation exhibiting superior flexibility and enhanced ductility compared to neat PLA. Furthermore, a 180-day soil biodegradation study showed that the incorporation of 0.5 wt.% n-HAp accelerated the hydrolysis process by approximately 500%, significantly improving the overall degradability of the PLA-HAp composite film. These findings underscore the potential of n-HAp as a functional bio-filler for enhancing the performance of PLA-based composites, particularly in food packaging applications.

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Keywords: Polymer composite, Alkaline hydrolysis, Polylactic Acid, Hydroxyapatite, Blown Films, Biodegradable composite

Biocarbon Economy for the 2050 Net Zero Target: Strategies to Reduce the global Carbon Footprint

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Biocarbon (or biochar) is the solid product of the thermochemical conversion of biomass at high temperatures (600 C to 900-degree C) in the absence or a limited supply of oxygen. This is the material mainly responsible for the characteristic dark colour and high carbon content of terra preta “black soil”, a.k.a. “Amazonian dark earth”) found in the Amazon basin. The application of biocarbon has traditionally been limited to fuel, soil amendment, filtration and agriculture. Today, the application of biocarbon in materials has emerged as a flourishing new research area, thanks to the enormous role it can play in our transition to a circular carbon economy. These include composites, energy storage, super-capacitors and environmental remediation.

The biocarbon-based polymeric composites are manufactured through different processing methods including compression and injection moulding, 3D printing, extrusion, etc. The use of biocarbon based sustainable composites in automotive parts applications are quite vibrant recently. Use of biocarbon as a filler material in rubber and polyurethane matrix in replacing carbon black will be a major breakthrough in green manufacturing sector. Moreover, new arenas for the use of biocarbon in materials such as hydrogen safety, CO₂ capturing, catalysis, etc.

should be explored. Overall, biocarbon based materials can be very effective as one of the enabling strategies towards sustainable materials in advance manufacturing and a circular bioeconomy.

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Keywords: Biocarbon, polyurethane

Wearable Nanogenerators for Next-generation Electronics

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Advances in next-generation wearable electronic devices rely on the development of highly deformable, breathable and wearable energy generators to power these electronics. Textile-based wearable triboelectric nanogenerators (TENGs) have emerged as viable power sources for wearable electronics. However, achieving a high-performing textile-based nanogenerator while maintaining intrinsic textile properties such as stretchability, breathability, and conformability remains challenging. This issue is addressed by fabricating a record high-performing wearable, breathable, and stretchable nanogenerator using polarization-induced ultra-stretchable EVA/Nylon-11 micro/nano-fibers (1250%) as the triboelectric positive layer and polarization-induced ultra-stretchable EVA/PVDF/BA₂CsAgBiBr₇ micro/nano-fibers (1480%) as the triboelectric negative layer. The remarkable stretchability, breathability (1.15 Kg m⁻² d⁻¹), and high energy-harvesting performance (650 V, 19.5 μ A cm⁻²) are attributed to the mechanically-socketed structure of the aligned stretchable EVA microfibers with the polarized nanofibers, providing a universal framework for fabricating stretchable piezoelectric fibers. Compositional engineering and

polarization-induced surface charges, combined with triboelectric-induced surface charges, enhance performance compared to other wearable stretchable textile-based nanogenerators. Additionally, this nanogenerator functions as a stretchable self-powered pressure sensor with an ultra-wide pressure sensing range (0.05–500 kPa) and high sensitivity (2.5 V kPa⁻¹) even under deformations. To the best of our knowledge, PI-STENG excels among various stretchable self-powered pressure sensors regarding pressure sensing range and stretchability. The PI-STENG is also demonstrated as a machine learning-enabled intellisensor for workforce safety monitoring.

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Keywords: Nanogenerators, TENG, PI-STENG

Harnessing the advantage of defects to improve photocatalytic water splitting of 2D tertiary heterojunctions

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Hydrogen, due to its high energy density, has been projected as the most promising carbon-free green fuel. However, present industrial hydrogen generation is mostly based on the grey or blue process. For green energy, the electrochemical process of water splitting is at the forefront of commercial exploration; however, it requires a significant amount of electrical energy, which restricts its practical greenness. On the other hand, obtaining green H₂ via direct photocatalytic water splitting is the most cost-effective and straightforward method, but it suffers from sluggish reaction kinetics. In recent years, various heterojunctions, including p-n junction-based photocatalysts, have become attractive due to the improved catalytic efficiency. However, designing and fabricating such

heterojunctions is tricky to achieve a proper p-n junction interface. In this context, 2D materials offer a better opportunity for fabricating the desired composite catalyst due to their high surface area. Transition metal chalcogenides [1] & MXenes [2] are important new 2D materials that exhibit improved surface properties after exfoliation to 2D structures. Interestingly, defects in the 2D structure also played a significant role in tuning the band gap and influencing the catalytic properties. Both few-layered MoS₂ and Ti₃C₂ (MXene) 2D materials were explored for the synthesis of tertiary heterostructures by depositing cauliflower-shaped CdS and nano-sized Cu₂O on a 2D sheet by hydrothermal and precipitation techniques. MoS₂ is a potential semiconductor, whereas doped TiO₂ formed on the surface of Ti₃C₂ during hydrothermal treatment serves as a potential photocatalyst. XPS spectra of Ti2p and O1s confirm the formation of defect-enriched TiO₂ with sufficient oxygen vacancy on the surface of Ti₃C₂, which can serve as a potential photocatalyst. ESR and HRTEM analysis corroborate the presence of oxygen or sulphur vacancy in both the 2D materials. MXene-based heterojunction absorbs light in both the visible and NIR ranges of the solar light spectrum. Mott-Schottky analysis confirms the p-type nature of Cu₂O, thus facilitating the formation of the p-n junction. The rate of hydrogen evolution efficiency is found to be 11.5 mmol/g/h and 16.26 mmol/g/h on MoS₂-CdS-Cu₂O and (TiO_x)Ti₃C₂-CdS-Cu₂O, respectively, with good repeatability and long-term stability. The presence of defects promotes extended light absorption, thereby enhancing hydrogen efficiency. Efficient interfacial charge separation is achieved through proper interface formation, resulting in the suppression of hole-electron recombination in the tertiary heterostructure. Substantially increased hydrogen evolution on tertiary materials is discussed based on the proposed mechanism of dual p-n junction formation. The better efficiency of MXene-based tertiary junctions is explained by the high conductivity of Ti₃C₂ and extended light absorption up to the NIR range. Increased efficiency and stability of the developed noble metal-free catalyst are explained based on the synergistic effect of defect-enriched TiO_x and MoS₂ formation, extended solar light absorption, enhanced interfacial charge transfer on the 2D sheets and dual p-n junction formation.

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Keywords: photocatalyst, p-n junction, hydrogen evolution, MXene

Efforts Toward Developing High-Performance Aqueous Rechargeable Zn-Ion Batteries

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Zinc-ion batteries (ZIBs) are promising energy storage systems due to their safety, cost-effectiveness, and abundant resources. However, their practical application is hindered by the lack of stable, highperformance cathode materials. Vanadium-based compounds offer potential due to their structural versatility and multivalent redox chemistry, yet they suffer from sluggish ion kinetics and poor electronic conductivity. Here, we present a novel thermo-electrochemical activation strategy that transforms V₂O₅ into defect-rich ZnV₃O₈, significantly enhancing electrochemical performance. The activated cathode delivers an exceptional specific capacity of 302 mAh/g at 0.1 A/g (up from 73 mAh/g) and demonstrates ultralong cycling stability over 4500 cycles at 2 A/g. Electrochemical analysis reveals accelerated Zn²⁺ diffusion, while first-principles calculations emphasize the stabilizing effect of hydrogen intercalation. The activation process triggers a thermodynamically favorable phase transition to ZnV₃O₈, enabling improved ion storage, lower activation energy, and enhanced structural integrity. Ex-situ studies provide insights into the material's evolution during cycling. This work highlights thermo-electrochemical activation as a simple yet effective method for optimizing vanadium oxide cathodes, paving the way for high-performance ZIBs with superior energy density and cycling durability [1].

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DOI: <https://doi.org/10.1002/aenm.202502262>

Keywords: Zn-Ion Batteries, ZIBs, ZnV_3O_8 .

Integrating Biorefinery and Waste Management for Environmental Sustainability, Decarbonization and Circular Economy

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Biofuels are gaining attention as renewable energy sources to address the rising energy demands, fluctuating crude oil prices and greenhouse emissions from fossil fuels. Biofuels can be produced from various biogenic wastes through thermochemical, biological and hybrid conversion technologies. This presentation will highlight the candidacy of a wide variety of waste feedstocks such as lignocellulosic biomass (e.g., agricultural crop residues and woody biomass), municipal solid waste, food waste, waste plastics and biogenic wastes to produce carbon-neutral fuels and carbon-negative materials. The potential and performance of integrated waste-to-energy technologies, especially gasification, pyrolysis, torrefaction, and fermentation, will be discussed in this presentation. The strengths, weaknesses, threats and opportunities of biorefinery technologies to shape the future of energy requirements in the industrial manufacturing and transportation sectors will be reviewed. This presentation will discuss the current progress, challenges, and knowledge gaps in the research and development of biorefining technologies to produce clean hydrocarbon biofuels, biochemicals, and bioproducts from agricultural and forestry residues, as well as opportunities for the Indian and global bio-based economies. The systems thinking approach of “why, how and what” will be elaborated to demonstrate the value proposition of transforming wastes into valuable resources such as biofuels, biochemicals and biomaterials.

Keywords: NASA, DNA, Fluorescent Biosensor

Eu^{3+} -Doped Core-Shell Nanophosphor-Based Fluorescent Biosensor for Highly Selective and Sensitive Detection of Double-Stranded DNA

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Biosensors are analytical devices that integrate a biological recognition element with a signal transducer to detect specific analytes. They are widely applied in medical diagnostics, environmental monitoring, and biotechnology. Lanthanide-doped core-shell nanomaterials have attracted attention as luminescent probes; however, their biological applications remain restricted due to poor water solubility and limited biocompatibility. While the formation of core-shell structures can enhance optical performance, the mere presence of surface $-OH$ groups on silica is insufficient for effective biomedical use [1]. In this study, we report a simple and cost-effective strategy for synthesizing a water dispersible and biocompatible nanophosphor: chitosan-functionalized $Ca-Eu:Y_2O_3@SiO_2$ (CEY@ SiO_2 -CH). The synthesized nanomaterials were systematically characterized for their structure, morphology, and optical properties using standard analytical techniques. The CEY@ SiO_2 -CH nanophosphor serves as a highly sensitive and selective fluorescence sensor for double-stranded DNA (dsDNA). Upon binding with dsDNA, the material exhibits a pronounced “turn-on” fluorescence response, attributed to the antenna effect, where energy transfer from the DNA enhances europium ion luminescence. The sensor achieves a linear detection range of 0.1–90 nM with a remarkably low limit of detection (LOD) of ~ 16.1 pM under optimized conditions. Application in real sample analysis demonstrated excellent accuracy, with recovery rates of 101–105% and relative standard deviations (RSD) below 5.23% ($n = 3$). These findings highlight CEY@ SiO_2 -CH as a practical, sensitive, and portable platform for rapid optical detection of dsDNA, showing strong promise for biomedical diagnostics and environmental monitoring.

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Keywords: Core-Shell, Chitosan, Fluorescence, dsDNA.

Functionalized Spinel Ferrite Nanomaterials as a Unified Platform for Energy Conversion and Storage

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The development of cost-effective, high-performance electrode materials is vital for advancing multifunctional energy storage and conversion systems. In this work, we report the development of multifunctional iron-based bimetallic spinel ferrite nanoparticles, synthesized via a simple co-precipitation method, and demonstrate their dual capability in supercapacitive energy storage and electrocatalytic oxygen-reduction reaction (ORR) applications. By optimizing the composition and annealing conditions, we achieved tailored electrochemical properties in spinel-phase CuFe₂O₄ and NiFe₂O₄ nanostructures. The CuFe₂O₄ nanoparticles, annealed at 800 °C, exhibited a well-defined tetragonal spinel structure with a high specific capacitance of 911.1 F/g at 1 A/g, delivering an energy density of 12.97 Wh/kg and a power density of 3.92 kW/kg in an asymmetric device. The capacitor demonstrated excellent cyclic stability, retaining 77.26% of its capacitance over 5000 cycles, and maintained a Coulombic efficiency of 101.8%. Furthermore, the NiFe₂O₄ counterpart, optimized at 900 °C, showed a crystalline cubic spinel phase with a specific surface area of 62.1 m²/g, resulting in a specific capacitance of 136 F/g and stable performance over 3500 cycles. Its intrinsic redox activity further enabled efficient ORR catalysis, providing a platinum-free alternative for energy conversion, with strong electrocatalytic responses in alkaline media. Together, these findings demonstrate the structural tunability and multifunctionality of spinel ferrite nanomaterials. Their combined high surface area, redox-active centers, and phase purity position them as strong candidates for integrated

electrochemical systems that unify energy storage and conversion capabilities in a single material platform.

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Keywords: Spinel ferrites, Supercapacitors, ORR catalyst, Energy storage.

Manipulating molecular diffusion in nanoporous membrane

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Membrane-based chemical separation is widely regarded as a sustainable technology, offering reduced carbon footprint and lower energy consumption. Its primary challenge, however, lies in the inherent tradeoff between permeation and selectivity. In our research group, we have developed chemical strategies to overcome this limitation by controlling the microscopic motion of molecules within membranes constructed from nanoporous metal-organic frameworks. In this talk, I will provide a broader context and highlight two specific case studies where we demonstrated that simultaneous enhancement of both permeation and selectivity can be achieved by leveraging correlated adsorbent-adsorbate dynamics[1] and a photocharging [2] mechanism.

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Keywords: anoporous membrane, photocharging

Structure, Dielectric Property and Cation Dynamics in $\text{MA}_{1-y}\text{FA}_y\text{PbX}_3$ Perovskites

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Hybrid Organic-Inorganic Lead Halide Perovskites (HOIP) are represented by APbX_3 , where A is the organic cation e.g. MA $((\text{CH}_3\text{NH}_3)^+)$ or FA $((\text{CH}(\text{NH}_2)_2)^+)$, X is halide anion. We have investigated dielectric properties of the solid solution series, $\text{MA}_{1-y}\text{FA}_y\text{PbI}_3$ for various compositions with $1 \geq y \geq 0$. Through temperature dependent single-crystal and powder XRD, we could establish a structural phase diagram for these solid solutions. Most interesting finding in this system is that, structure and dielectric property are strongly correlated. To understand the dynamical nature of these two cations, namely MA^+ and FA^+ in APbBr_3 system, we have performed quasi elastic neutron scattering (QENS) experiments. We could establish that MA^+ exhibits 3-fold rotation around C-N axis and 4-fold jump rotation about C-N axis itself, in lowtemperature orthorhombic and high-temperature tetragonal/cubic phase, respectively. In contrast, FA^+ exhibits an isotropic motion throughout all the temperature range covering orthorhombictetragonal-cubic phases. Thus, through QENS experiments, we could realize the contrasting nature of these two cations. We report results of our thermoelectric properties and meta stable phase of $\text{MA}_{1-y}\text{FA}_y\text{PbI}_3$ with $1 \geq y \geq 0$.

Keywords:

DIKETOPYRROLOPYRROLE (DPP) derivatives: Materials design, Optoelectronic and Energy Devices

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Structural composition of the semiconducting materials profoundly impacts on the device stability in organic electronics and hole-electron pair extraction/transport properties.

We have embarked on the design and engineering of a series of small molecules and polymers based on diketopyrrolopyrrole (DPP) as core architecture. The C-H arylation, Stille and Suzuki coupling synthetic protocols have been adopted. Solution-processed organic electronic devices were constructed. Our investigation delves into the impact of chemical engineering on these meticulously crafted materials, employing a substitute identity approach. We have comprehensively examined their optical, physicochemical, and morphological properties. Remarkably, the introduction of these semiconductors has yielded tunable energy levels, upto NIR range absorbance with morphologically smooth surface and compact molecular packing. These findings underscore the potential of these DPP derivatives as promising candidates for optoelectronic devices, offering exciting prospects for future advancements in the field.

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Keywords: Diketopyrrolopyrrole, C-H arylation, opto-electronic properties, Energy devices

Conducting Filler Stimulated Polymer Nanocomposite-Based Smart Flexible Nanogenerator for Multiple Applications

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Advancements in modern technologies have surged the need for wearable sensors to track human body movements and generate artificial robots. However, the longevity of the energy sources powering these devices poses a persistent challenge. Polymer-based nanocomposites can be engineered to create nanogenerators as a natural and sustainable energy solution. Different kinds of ternary composites have been explored for nanogenerator fabrication. A piezoelectric nanogenerator (PENG) utilizing a composite material based on three-phase double perovskite nanoparticles, Polypyrrole (PPy), and polyvinylidene fluoride (PVDF) has been investigated for energy generation. Optimal performance was achieved with a 10 wt% LCuMO-2 wt% PPy-PVDF composite film, exhibiting an output voltage of approximately 20 V, a current of around $1.63 \mu\text{A}$, and a power density of approximately $14 \mu\text{W}/\text{cm}^2$ at $37 \text{ M}\Omega$. The PENG consistently delivered power and effectively charged commercial capacitors, highlighting its potential as a reliable and sustainable power source. This device also demonstrates its application as an epidermal sensor for monitoring skin motion and as a temperature sensor for medical and robotics applications.

It is observed that the electroactive β -phase, dielectric permittivity, saturation polarization, and output performance of the device improve with the incorporation of MnAl-alloy nanoparticles up to 7.5 wt% in the PVDF matrix. A MnAl-alloy-based optimized piezoelectric nanogenerator device was fabricated using a free-standing nanofiber mat (7.5 wt% MnAl-alloy) prepared via the electrospinning technique. The as-fabricated device channels charges generated by mechanical stress to the electrodes, resulting in an output voltage of approximately 16 V and an output current of around $7.1 \mu\text{A}$, yielding a power of $47 \mu\text{W}$ across a $4.5 \text{ M}\Omega$ resistor. Furthermore, energy harvesting from human movements such as jogging, knee bending, and walking was demonstrated for practical applications. A piezo potential of approximately 8 V generated during walking showcases the development of a self-powered pedometer. Tapping

the PENG charges a $0.1 \mu\text{F}$ capacitor up to approximately 1 V, demonstrating its potential to power small portable electronic devices. Overall, these devices not only generate electric power from natural mechanical energy but also enable multiple practical applications in wearable electronics and self-powered sensors.

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Keywords:

Development of Novel Nanomaterials for Molecular Diagnosis of Certain Rare Genetic Disorders

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We are developing new nanomaterials and conjugating them with suitably tuned complementary oligonucleotides targeting certain rare genetic diseases. These oligonucleotides are chosen based on their target binding energy and binding site disruption energy. The oligonucleotide-conjugated nanomaterials were characterized by various analytical techniques including UV-visible spectroscopy, fluorescence spectroscopy, X-ray diffraction, Raman spectroscopy, scanning electron and transmission electron microscopy. These nanomaterials are then used for molecular diagnosis of certain rare genetic disorders, namely Turner syndrome and rare blood genotypes. Changes in spectroscopic and/or electrochemical data were recorded to selectively detect the presence of targeted genetic material. In this talk, I shall be presenting the efforts being undertaken in my laboratory over the last year.

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Keywords: Covalent Organic Framework, Gold Nanoparticles, Complementary Oligonucleotides, Clinical Diagnosis, Rare Genetic Disorders.

Porous Hierarchical Functional Materials for Detection and Remediation of Food Toxins and Emerging Pollutants

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Emerging pollutants and food toxins have become significant global concerns due to their severe ecological and health impacts on humans. Addressing these challenges requires advanced materials capable of both detecting and removing such hazardous compounds. In this research, porous hierarchical and metal–organic framework (MOF)-based functional composites were developed for the sensing, quantification, and remediation of emerging pollutants (such as microorganisms, heavy metals, and organic dyes) and food toxins (including aflatoxins, ciprofloxacin, and hexavalent chromium). The synthesized materials,

possessing high surface area, porosity, stability, and magnetization, were thoroughly characterized using various techniques, including FE-SEM, HR-TEM, FT-IR, XRD, UV–Vis, and photoluminescence spectroscopy, to elucidate their structural and morphological properties. Due to their unique physicochemical properties and tunable porosity, these MOF-based composites have been successfully employed as multifunctional nanoprobe and nano-adsorbents for the selective, sensitive, and real-time detection as well as the effective removal of pollutants from aqueous and food matrices. Electrochemical (cyclic voltammetry and electrochemical impedance spectroscopy) and optical (photoluminescence) methods were employed to assess their sensing capabilities, with further validation through the analysis of real samples. Overall, this work demonstrates a novel and integrated strategy for designing multifunctional MOF-based nanomaterials with dual functionality for environmental remediation and food safety monitoring, offering promising potential for wastewater treatment and food quality assurance applications.

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Keywords: Metal–organic frameworks (MOFs), Porous hierarchical materials, Emerging pollutants,

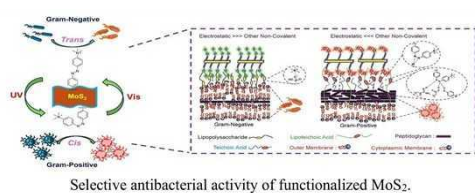
Selective Antibacterial Activity: Nanomaterials to Nano-assemblies

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Developing material-based antibiotics can be the most potent alternative due to the increasing resistance against conventional antibiotics. However, one of the important parameters in the development of antibacterial agents is Gram/strain selectivity, which is seldom explored in the case of nano-antibiotics. The multimodal action of surface-functionalized nanomaterials can exhibit strain-selective and enhanced antibacterial activity. Two-dimensional MoS₂ nanosheets (2D-MoS₂) have been widely used in many biological applications due to their distinctive physicochemical properties. In the past, it was theorized that chemically exfoliated MoS₂ can be modified using thiol chemistry. In this regard, we provided the first experimental evidence for this process using a facile solution-based method. By chemically engineering the ligands, we then showed the ability to modulate the surface of the MoS₂ sheets. In doing so, we have developed several strategies to demonstrate the ability to tune the surface of the conjugates for selective enzyme targeting, inhibition, and antibacterial activity. Those strategies are based on different proportions of positively and negatively charged functionalized ligands, tethered amino acids/peptides, conjugation of Ni-nanocluster, photo-controlled gating of selective bacterial membrane interaction, etc. Apart from Taken together, we have prepared simple and efficient Gram-selective 2D-MoS₂-based antibacterial agents, which can also be extended to other systems with antimicrobial properties. We have also developed selective antibacterial agents using nano assemblies such liposomal formulation and host-guest complexes.



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Keywords:

Salt-bridge mediated supramolecular systems with augmented catalysis

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Salt-bridge interaction, combining H-bonding and electrostatics between oppositely charged molecules, presents an important class of non-covalent interactions with strength more than either interaction alone. In biology, salt-bridges play a key role in governing peptides folding into their specific three-dimensional active protein structures and helps in molecular recognition towards drug molecules. Inspired by this biological paradigm, supramolecular chemists have increasingly turned to salt-bridges as a design principle to create robust functional soft materials. Our recent works demonstrate how salt-bridge can drive self-assembly across diverse synthetic platforms. In one study, we utilized a positively charged amphiphiles and ATP fuel to generate transient vesicular compartments through salt-bridge interactions between guanidium and phosphates of the respective entity.[1] These vesicles act as dissipative “glues,” temporarily enhancing catalytic reactions through enzyme anchoring and disassembles once the chemical fuel is consumed. Similarly, our other work reports an adaptive catalytic compartment emerged from ATP-driven salt-bridge formation with

cationic biguanide-based polymers.[2] The resulting liquid coacervate droplets selectively sequester G-quadruplex/hemin DNAzymes, significantly amplifying its catalytic performance. The system forms and disappears in response to ATP turnover. Furthermore, we employed salt-bridge interactions not to create compartments around a DNAzyme, but to construct a robust DNAzyme architecture itself, distinct from the conventional approach involving π -stacking of hemin.[3] Here, the DNA phosphate backbone interacts with platinum complexes bearing guanidinium head groups through salt-bridge interactions. This complexation promotes higher-order assembly and activates catalytic centers through metal-metal interactions, giving rise to potent light responsive oxidase-like activity. Notably, the high stability of these assemblies against nucleases in biological media positions them as promising candidates for photodynamic therapy. Together, these works show the potential of salt-bridge interactions as a versatile motif for constructing programmable supramolecular assemblies.

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Keywords: supramolecular, DNAzym, guanidium

Biomaterials for tissue repair: Essential factors and engineering techniques

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Hard-to-heal damaged tissues require innovative therapeutic strategies, and tissue engineering has emerged as a promising approach for their repair. Central to this field is the

development of *scaffolds*—engineered biomaterial frameworks that replicate the structural and functional attributes of native tissues. In particular, **ECM-mimicking injectable scaffolds for cell delivery and tissue repair** have gained significant attention for their ability to conform to irregular defects and provide a supportive microenvironment for regeneration. These scaffolds guide cell adhesion, migration, and new tissue formation by recapitulating essential extracellular matrix cues.

Designing such advanced scaffolds demands careful integration of biomaterial composition, biological signals, topographical features, biophysical properties, and morphological characteristics, each of which critically influences cell-material interactions. Through tailored fabrication and modification strategies, scaffold constructs can be optimized to promote healing in tissues with limited regenerative potential. This talk will highlight our scaffold engineering approaches and biomaterial innovations aimed at treating degenerative and chronic conditions, including osteoarthritis and non-healing ulcers.

Keywords: tissue repair, ECM-mimicking, regenerative potential.

Role of ultrasonication for material synthesis and environmental remediation

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Last few decades, ultrasound as a new and emerging technique, has been widely used for the synthesis of nano-materials that are used for the oxidation of various organic pollutants, production of hydrogen by photocatalysis, solar cell, fuel cell, etc. The frequency range of ultrasound from 20 to 500 kHz can be used to synthesize metal oxides, zero valent metal nanoparticles from metal precursors in aqueous condition in the presence of organic solvents, etc. In addition, the physical force (shear force) generated from ultrasound in liquid medium can be effectively used for the controlled synthesis of nano-particles with desired particle sizes, pore volume, pore diameter, etc. For example, particle size of nano-particles is substantially reduced while applying ultrasound during the synthesis of nanoparticles. Apart from reducing the size

of the particles, other physio-chemical characteristics and morphology of the particles are well controlled by using ultrasound. Recently, graphene oxide has been used as a potential solid support to hold the nano-particles and also enhances the fast transport of electrons. Metal and metal oxide nanoparticles with few layers of graphene oxide support is used for many application studies including solar cell, fuel cell, bio-sensors, photocatalysis and electrocatalysts, etc. It is proven that applying both low and high frequencies together (dual frequency) for the synthesis of metallic particles along with graphene oxide is considerably enhancing both the rate of reduction of metallic precursors and also improve high loading of metallic nanoparticles on graphene oxide. Those materials can be effectively used for complete oxidation of organic pollutants into carbon dioxide and water and also for the production of hydrogen by splitting of water through photocatalysis. Our group has developed a simple method to degrade organic pollutants effectively using light and sound along with photocatalysts (called sonophotocatalysis) and also for the production of hydrogen by photocatalytic splitting of water. Thus, both the pollution abatement and hydrogen production can be achieved by using photocatalysis.

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Keywords:

Understanding Materials at Near-Atomic Spatial Resolution: An Atom Probe Tomography Perspective

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The material degradation under extreme conditions of temperature, pressure, corrosive environment and irradiation limits the performance, life and safety of numerous components. To understand the materials response to these extreme conditions is of utmost importance, which eventually leads to better quality and safer materials. Most of the bulk properties of materials are governed by their microstructure. This microstructure can change drastically in response to the extreme conditions, thereby degrading the bulk material properties. Understanding the fundamental processes like clustering, precipitation, solute segregation at grain boundaries/dislocations, initial stages of phase separation need a special attention and that too at highest possible spatial resolution. Atom Probe Tomography (APT) is a very powerful technique to study these phenomena and provide unprecedented information of the materials at near atomic resolution.

Atom Probe Tomography (APT) is a microscopy and microanalysis technique that provides sub-nanometer resolution three-dimensional mapping of elements within a small volume of material [1]. Owing to its unparalleled capabilities, APT is being extensively utilized in various scientific fields, nano-electronics, materials science, semiconductor device metrology, geology, to name a few. Since its inception, APT is widely applied to the metals and metallic alloys, ranging from Fe-, Ni-based alloys to lately high entropy alloys. The power of APT to visualize low-Z elements like C, B and P at this scale is commendable. In nutshell, APT provides vital information about materials that no other technique can offer at this scale and spatial resolution.

In this context, this presentation will shed some light on the basic principle of APT technique along with the sample preparation for the same. Examples from the existing literature as

well as from my past and present work [2-5] will be presented to demonstrate the unique abilities of this technique.

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Keywords:

Ubiquitous isostructural phase transition in tin based alloys under compression

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One of the major motivations for the high-pressure structural investigation of condensed matter systems is to explore the structural phase transitions [see for example 1-4]. Recently with the availability of tools permitting to follow very systematically the pressure evolution of the structural parameters, it is possible to shed light on possible transitions which does not require a lattice symmetry change – generally termed as isostructural phase transitions. Pressure being an excellent external tool to controllably tune the bonding interactions permit to fine tune the electronic structure, several cases bring the systems to novel ground states permitting to host interesting collective excitations. Electronic topological transitions without requiring a bonding rearrangement is found in a number of systems (see for example in black phosphorus: [5]). Tin is a technologically important metallic system, thanks to its relatively low melting

temperature. This also allow tin to follow a variety of intermetallic compounds with vastly varying functional properties. We have recently investigated several such compounds under pressure: noncollinear AFM Mn₃Sn [6], the topological nodal line semimetal PtSn₄ [7], quasi-skutterudite superconductors [4,8] etc. Several of these systems are found to have the pressure induced isostructural phase transitions. Details about such investigations will be presented.

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Keywords: High-pressure; Diffraction; Raman spectroscopy; Superconductivity.

Molecular Origin of Piezoelectricity and Flexoelectricity in Crystalline Materials from Micro-XRD and Quantum Crystallography

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Mechanical brittleness and modest electromechanical coupling have long limited the practical deployment of molecular piezoelectric materials. In this talk, I will present our discovery of unusually high longitudinal piezoelectric coefficients in two mechanically flexible crystals derived from amino-acid analogues, and show how their piezoresponse is intimately governed by molecular packing. By integrating micro-focused X-ray diffraction (μ -XRD) with high-pressure crystallography (HP-XRD), we reveal the structural origins of their electromechanical behavior and establish a direct link between bending-induced lattice distortions and flexoelectric polarization. Flexoelectricity—polarization generated by strain gradients—remains largely uncharted territory in organic crystals, and our XRD-based framework provides a rare route to quantify it through spatially resolved structural mapping and stress-strain analysis. Further our new applications of X-ray quantum crystallography – with powerful new tools such as Hirshfeld Atom Refinement (HAR) and X-ray wavefunction refinement (XWR)[1] on the crystalline materials will also be discussed. Together, these insights not only deepen our understanding of structure-property relationships in soft crystalline materials but also outline a design paradigm where supramolecular helicity and mechanical flexibility converge to enable next-generation organic electromechanical systems.

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Keywords:

Exploring Molecules at Aqueous Interfaces Using Sum Frequency Generation Vibrational Spectroscopy

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Surfaces and interfaces play a crucial role in determining the physical, chemical, and functional properties of a diverse range of materials. Unlike bulk phases, where molecular arrangements are often isotropic and governed by long-range structural order, interfacial regions are inherently distinct: they break inversion symmetry, exhibit heterogeneous molecular environments, and often display unique dynamical behavior. These characteristics make surfaces and interfaces important sites for chemical reactions, charge transfer, molecular adsorption, and energy conversion processes. Consequently, understanding the molecular-level structure and dynamics at interfaces is essential for advancing several fields, including catalysis, electrochemistry, environmental chemistry, biophysics, and the design of advanced materials for device applications. Aqueous interfaces, in particular, have attracted sustained attention because water is a ubiquitous solvent and participates directly in numerous interfacial processes. At air–water or solid–water boundaries, the orientation, hydrogen-bonding structure, and solvation environment of water molecules differ markedly from those in bulk liquid water. Despite their importance, probing such interfaces with molecular specificity has historically been challenging due to the overwhelming bulk water signal and the spatial confinement of interfacial regions. Sum Frequency Generation Vibrational Spectroscopy (SFG-VS) has emerged as a powerful and inherently interface-specific spectroscopic technique capable of overcoming these challenges. As a second-order nonlinear optical process, SFG is allowed only in media lacking inversion symmetry—making it naturally sensitive to interfaces where symmetry

is broken. In an SFG experiment, the simultaneous interaction of an infrared (IR) beam resonant with molecular vibrations and a visible beam generates a sum-frequency signal that carries vibrational fingerprints of molecules localized at the interface. This provides direct access to molecular orientation, bonding configuration, ordering, and interfacial dynamics with monolayer sensitivity. In my talk, I will give detailed insight into the role of the hydrogen bonding environment of the interfacial water molecules in the evaporation process.¹ I would also highlight the spectroscopic signature of ion-specific water-macromolecule interactions in a complex ternary molecular system, as well as the role of ion-specific double layers in aqueous electrolytes.^{2,3}

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Keywords: Sum Frequency Generation Vibrational Spectroscopy, aqueous interfaces, hydrogen bonding, specific ion effect.

Novel oxide semiconductor particles and their composites for adsorptive and photocatalytic removal of dyes and pollutants from liquid phase

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Semiconductor oxide particles are an attractive class of materials for photocatalysis. Significant effort has been made in designing these materials active under visible radiation. Such designs can be useful in numerous applications such as treating environmental pollutants, hydrogen generation, and CO₂ reduction, under

solar light. Several oxides have shown potential for such functionality. We prepare composites of oxides of zinc, titanium, bismuth, and nickel using various routes such as sol-gel, polymer assisted synthesis and sol-electrospinning. Our key considerations in designing these particles are adsorption, bandgap, carrier lifetimes, and specific surface area. In this talk I will present some recent results from our group in preparing composites of semiconducting oxide particles and their efficacy in photocatalytic degradation of dyes, an important environmental pollutant.

Keywords: Oxide semiconductor, photocatalytic, CO₂ reduction

From Electronic Band Design to Solar Hydrogen: A Materials-Driven Green Energy Vision

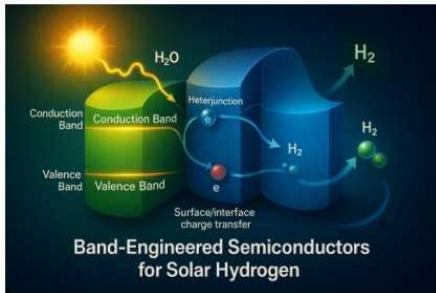
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Achieving a sustainable, carbon-neutral energy system demands breakthroughs in semiconductor materials capable of efficiently harvesting solar energy to produce hydrogen. Band-structure engineering is central to this transformation, enabling precise tuning of electronic energies to align redox potentials, facilitate charge separation, and suppress bulk recombination. In this talk, I will present how strategic band-edge modulation—through compositional design, defect engineering, and controlled doping—enhances carrier reactivity and selectivity for efficient solar water-splitting. I will also highlight recent progress in heterojunction and S-junction architectures, where interface-driven band bending and catalytic selectivity create built-in electric fields that significantly accelerate directional charge transport and overall hydrogen generation performance. These surface–interface designs, augmented by cocatalyst integration and optimized surface terminations, govern fast interfacial charge-transfer kinetics, improving proton-reduction and oxygen-evolution efficiencies. The convergence of novel semiconductor pairings, finely tuned interfacial energetics, and scalable surface engineering is progressively uplifting material performance toward emerging green hydrogen deployment targets. Ongoing innovations are transitioning

from fundamental discovery to early technology readiness, guided by materials-to-device co-development and durability validation. This talk will highlight a forward-looking roadmap that connects band structure innovation to solar hydrogen deployment, charting scientific and technological priorities to accelerate a green hydrogen future.



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Keywords: Band edge engineering, Heterojunction and S-scheme photocatalyst, Charge-Carrier Dynamics, Hydrogen Generation

Role of Chemical Pressure and Magnetic Disorders in Rare-earth Spin-Ices

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After the discovery of implications of Anderson's resonating-valence-bond (RVB) theory to high-temperature superconductors, frustrated magnetism developed wide-spread recognition. In these magnetically frustrated systems, low-temperature spin-dynamics are effectively controlled through dipolar and exchange interaction along with the crystal field effect. [1-4] Perturbation through the application of chemical pressure and magnetic disorder plays a crucial role in the spin dynamics of Rare-earth Titanates.

The dominance of the debilitation of exchange interaction over dipolar interaction is crucial parameter to decide the spin freezing in these systems. [5-8] The effect of both chemical pressure and magnetic disorder will be discussed taking up the Ising and x-y Pyrochlores. It will be shown that how these perturbations can be used for tuning the physical properties and sometime their robustness in a very subtle way. A theoretical study on these systems will also be presented.

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Keywords:

Defect tolerance & defect engineering in hybrid perovskite materials

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Defects are usually seen as imperfections in materials that significantly degrade their performance. However, lead perovskite materials have been found to be one of the most radiation resistant hard semiconductor material [1]. This exceptional defect tolerance is especially attractive for radiation detectors and spatial applications. We have controlled stress release in thin hybrid perovskite films with ion irradiation (protons) as a way to improve optoelectronic properties [2]. Ion irradiation allows local atomic diffusion and reorganization to a relaxed, optimal state. Moderate irradiation allows for improving the lifetime from about 450 ns to 1 μ s as measured with time-resolved PL, as a consequence of initial stress release (-0.2% after synthesis). In contrast, high irradiation fluence is shown to restore compressive strain leading to sample degradation, with lower lifetimes values (200 ns). Another very unusual phenomenon concerns the phase segregation occurring under light illumination between bromine-rich and iodine-rich regions. We have found a way to follow in-situ the photo-induced phase segregation using PL emission [3]. This mechanism was found to be defects-mediated as its kinetics increases by a factor of five for high irradiation fluence. The irradiation defects can also be revealed with low-temperature photoluminescence (PL) through bound exciton radiative recombination mechanisms [4]. This detailed investigation opens new perspectives for optimizing mixed-halide perovskite properties using ion irradiation techniques.

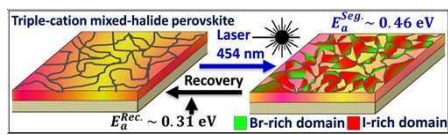


Figure 5: Schematic illustrating the reversible phase segregation process under light illumination in mixed halide (Br,I) halide perovskite. [3]

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Keywords: perovskite materials, photoluminescence, phase segregation.

Engineering Functional Surfaces with Low-Energy Ion Beams: Role of Surface Composition and Processing Parameters

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Ion beam processing has emerged as a powerful technique for the controlled synthesis, modification, and nanoscale engineering of materials. By precisely transferring energy and momentum, energetic ions can simultaneously alter surface morphology, microstructure, and composition, enabling atomic-scale tailoring of material properties.

In particular, low-energy ion beams offer a versatile route to induce self-organized nanostructures such as ripples, nanodots, and nanowires across polymers, semiconductors, and ceramics. These patterns arise from a dynamic balance between ion-induced sputtering, surface diffusion, and redeposition, leading to tunable structures with unique optical, electronic, and sensing functionalities.

This talk explores the ion-beam-driven surface structuring over large areas of polymeric, semiconductor, and ceramic materials induced by low-energy ion beam sputtering under oblique incidence. Recent experimental investigations on carbon, silicon carbide (SiC), silicon nitride (Si₃N₄), and germanium (Ge) reveal a rich spectrum of nanostructures—including ripples, nanodots, and faceted arrays—whose periodicity and orientation can be precisely tuned by controlling ion energy, fluence, and angle of

incidence. In carbon films, irradiation induces graphitic reorganization and anisotropic ripple formation; whereas in SiC & Si₃N₄, preferential sputtering and compositional asymmetry govern pattern regularity; while Ge exhibits highly ordered ripples formed through ballistic redistribution and defect-assisted diffusion.

The discussion will highlight the decisive role of surface composition and chemistry in influencing pattern evolution, stability, and wavelength selection. Understanding these underlying mechanisms not only advances the fundamental science of ion-surface interactions but also enables tailored large-area nanostructuring for next-generation applications in photonics, electronics, and sensing technologies.

Keywords:

Radiation effects on Energetic Materials and Devices

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Ion beams with energies ranging from a few kilo electron-volts (keV) to mega electron-volts (MeV) are utilized for materials analysis, modifications, and synthesis across various fields, including semiconductors, metallurgy, environmental studies, photovoltaics, nuclear reactor technology, and fusion energy materials. At the University of North Texas, we operate several dedicated ion accelerator facilities that provide proton and other heavy ion beams with low (keV) and medium (MeV) energies. These beams enable targeted irradiation of different layers within materials and device structures. Additionally, we have developed a novel and powerful scanning ion microprobe, which has a probing spot size of approximately 500 nm. This tool is used for characterizing elemental concentration, composition, and charge collection efficiency in various materials and device stacks.

In this presentation, we will highlight our capabilities in conducting quantitative microanalysis of a wide range of elements in next-generation photovoltaic devices and electronic materials. Our characterization techniques are relatively non-destructive and require minimal

sample preparation, allowing us to provide quantitative information about elemental compositional depth profiles, as well as the radiation tolerance of devices simulating outer space conditions. We will present examples of our research on irradiation-induced effects in electronics, photovoltaic devices, and nuclear materials [1-3]. This work has been advanced through extensive collaborations with key institutions in the United States, including the University at Buffalo, the University of Toledo, Arizona State University, the Rochester Institute of Technology, the National Renewable Energy Laboratory (NREL), and the National Aeronautics and Space Administration (NASA).

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Keywords:

Thickness Dependent Phase Transformation and Resistive Switching Performance of HfO₂ Thin Films

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Resistive random access memory (RRAM) devices are being investigated extensively for future nonvolatile memories using various transition metal oxides like NiO, ZnO, TiO₂, ZrO₂ and HfO₂ as the active material. Here, we have demonstrated the performance of RRAM device using HfO₂ thin films deposited by ion beam sputtering technique on p⁺⁺-Si (100) substrate with varying thickness from 10 to 30 nm. We

observe a structural transformation from orthorhombic to a dominant monoclinic phase with increase in thickness from 20 to 30 nm, although a small fraction of orthorhombic phase remains present in the later film. The phase transformation is accompanied with significant increase in the average grain size along with a decrease in the oxygen vacancy as observed from X-ray photoelectron spectroscopy. The performance of RRAM device fabricated using these films and the I-V characteristics show the bipolar forming-free resistive switching behavior in both films. Among the films, HfO₂ film of 20 nm thickness shows better switching behavior with an ON/OFF ratio of ~ 7.3 . The switching mechanism has been discussed on the basis of Ohmic and Poole-Frenkel conduction models¹.

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Keywords:

Ion beams in Organic–inorganic hybrid heterojunction devices

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Organic–inorganic hybrid heterojunctions represent a cutting-edge class of materials that synergistically combine the tunable electronic properties of organic semiconductors with the structural robustness and high carrier mobility of inorganic counterparts. This hybridization enables the design of multifunctional devices with enhanced performance across optoelectronic, sensing, and energy domains. Recent advances have demonstrated that ion irradiation serves as a powerful tool to manipulate the interfacial properties, defect states, and charge transport mechanisms within such heterojunction devices. By precisely tuning irradiation parameters—such as ion species, energy and fluence—researchers can engineer band alignment, induce phase transitions, and modulate conductivity, thereby unlocking new functionalities. The development of multifunction heterojunction hybrid diodes will be discussed for their implications for highly sensitive photodiodes

that can be very promising for efficient optoelectronic devices. An intriguing phenomenon of the negative differential resistance in conducting polymer-metal oxide hybrids is manifested to the electrical bistability has also been observed as an induced effect at low ion irradiation doses and explained by invoking ordering of the polymer chains and electric-field induced charge transfer mechanisms. The talk will be focused the fabrication strategies, irradiation-induced modifications, and application potentials of organic–inorganic hybrid heterojunctions, highlighting their promise in next-generation flexible electronics, photodetectors, and memory devices. The integration of ion irradiation as a post-synthesis tuning method paves the way for scalable, adaptive, and high-performance multifunctional systems that could be easily integrated into the existing silicon-based technology.

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Keywords:

Crystallization dynamics of Si and Ge in metal/semiconductor bilayer thin films under ion irradiation

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The crystallization of by solid-phase crystallization method usually takes place by annealing the amorphous-Si (a-Si) at a temperature of approximately 600 °C over a period of 24 h or more [1]. However, a-Si films and a-Ge in contact with some metals (Al, Au and Ni etc.) have been observed to crystallize to poly-Si films at a significantly lower temperature (below eutectic) [2-9], by a process known as metal induced crystallization (MIC). In present talk, the MIC of a-Si and a-Ge under thermal annealing and ion irradiation are presented. The c-Al /a-Si thin films have been prepared on thermally oxidized Si-substrates. A set of samples have been annealed at temperature ranges from 100 °C to 500 °C to achieve crystallization. Another set of similar samples have been irradiated at an elevated temperature of 100 °C using 100 MeV Ni⁷⁺ ions at fluences of 1×10^{12} ions-cm⁻², 5×10^{12} ions-cm⁻², 1×10^{13} ions-cm⁻², and 5×10^{13} ions-cm⁻². The crystallization of a-Si is observed at annealing temperature of 200 °C [4]. On the other hand, irradiation using swift heavy ion leads to crystallization of a-Si at significantly lower temperature of 100 °C [5-6]. In case of Ge, 50 nm a-Ge/50 nm Au have been prepared using e-beam evaporation and thermal evaporation techniques, respectively. The as-prepared samples have been irradiated with 100 MeV Ni⁷⁺ ions at different fluences of 1×10^{12} ions-cm⁻², 5×10^{12} ions-cm⁻², 1×10^{13} ions-cm⁻², and 5×10^{13} ions-cm⁻² at room temperature (RT) followed by thermal annealing at 300 °C leads to the crystallization of Ge [7]. However, the crystallization of Si is observed at room temperature under 500 keV Xe ion irradiation [8]. In case of Ge, the crystallization temperature was observed to be 125 °C using low energy ion irradiation [9].

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Keywords:

Computational Modeling of Materials for finding Glass-like Thermal Conductivity and Quantum Spin Liquid Candidates

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The Wigner transport equations for phonons have been developed along with first principles calculations to model and understand the glass-like thermal conductivity and developed Monte

Carlo based method to calculate spin-spin correlation functions and spin structure factors to predict various magnetic phases. We have modelled TlAgSe for finding its thermal conductivity as glass like, which was synthesized and investigated experimentally [1]. I shall also discuss the possible quantum spin liquid phases in dimer-based material, $\text{Yb}_2\text{Te}_5\text{O}_{13}$ and hyperhoneycomb random lattices, NaYbW_2O_8 with two compositions, which were synthesized and thermodynamical and μ -SR studies were carried out by our experimental colleague [2]. In fact, after finding the exchange constants, single ion anisotropy and biaxial anisotropy, our Monte Carlo based prediction of incommensurate phases at certain temperatures were confirmed for all the spin lattice systems. Furthermore, since the inelastic neutron scattering data is missing, we have verified our results with the experimental μ -SR data. Many more detail experimental and quantum theoretical studies are necessary to identify these as the elusive quantum spin liquid candidates.

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Keywords: Wigner transport equation, Density Functional Theory, Quantum Spin Liquid, Monte Carlo Simulation

Modeling Topology, Flat Bands, and High-Order van Hove Singularities in Quantum Materials

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High-order van Hove singularities (VHSs) represent a new class of electronic instabilities where locally flat dispersions produce faster-than-logarithmic divergences in the density of states. These singularities enhance electronic correlations and promote symmetry-breaking ground states. In this talk, I will discuss how

high-order VHSs emerge across diverse quantum materials and their connection to unconventional superconductivity and nematic order. I will present our theoretical modeling and workflow for predicting high-order VHSs in materials hosting correlated electronic states. Using the kagome metal CsTi_3Bi_5 as an example, I will show the prediction of these VHSs, their associated electronic features, and how they suppress charge order while favoring superconductivity and nematicity. Extending this framework to cuprates, nickelates, and the topological quasicrystal approximant $\text{Al}_{13}\text{Os}_4$, I will highlight how the order of VHSs serves as a predictive descriptor for discovering materials with correlated topological phases.

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Keywords: Topological quasicrystal approximants, Correlated electronic states, Predictive descriptors, Quantum materials

Accelerated Materials Design using Generative AI

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Discovery of advanced materials have played a crucial role in the progress of human technology and civilization. Basic sciences such as Physics and Chemistry are central to our modern approach to discovering new useful materials. In this approach, trial-and-error experimentation has been the paradigm of materials design and discovery. But this is time consuming, expensive and uncertain. Over the past couple of decades, materials discovery has accelerated via the high-throughput computation and experimental strategies. Yet, a comprehensive search of the chemical space to identify materials with

a desired set of properties is highly computation-intensive, and remains difficult.

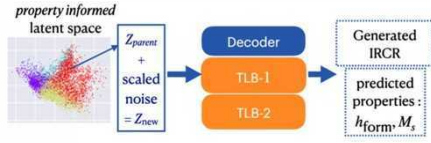


Figure 6: Constrained Variational Autoencoder MagGen for designing magnetic materials

In recent years, Machine Learning methods have emerged as an alternative to expensive first principles calculations. Broadly, two strategies have been used for search and design of advanced materials. In the first strategy, available materials data are used to train a series of ML models to predict material properties. These models are then used to hierarchically screen a set of new materials to identify the ones that satisfy the desired set of properties. The second strategy is to ‘inverse’ design materials with a set of target properties using generative artificial intelligence (AI).

The above developments have been aided by two allied developments. The first is ML force fields, which allow materials simulations with first principles accuracy at the cost of classical simulations, and the second one is ML-aided materials characterization. All these developments have opened up unprecedented possibilities that did not exist even a few years ago.

In this broad backdrop, I will present our works on inverse design of rare earth free magnets using generative AI. I will end by pointing out some of the exciting new possibilities that have opened up because of these developments.

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Keywords: Generative AI, ML models, autoencoder.

First principles modelling and materials engineering at the gate stack of nanoscale MOS devices

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Silicon (Si) and its oxide (SiO₂) have been the workhorse of scaling driven semiconductor industry. Almost a decade and a half ago, the high-k metal gate was introduced (Intel in 45 nm and IBM in 32-nm technology nodes), wherein Hafnium oxide (HfO₂) together with Titanium nitride (TiN) were used in the gate stack as preferred high-k dielectric, and metal respectively. The performance of these scaled Complementary Metal- Oxide-Semiconductor (CMOS) devices (32-nm and beyond) rely on accurate control of materials in the bulk and at the interfaces in terms of chemical composition, nature of atomic species, and defects. The defects in gate oxides and at their interfaces influence the threshold voltage shift, and the mobility degradation. The chemical composition, and the nature of atomic species at the source/drain contact, and metal interconnects strongly impact the resistances. In this talk, we will discuss some of these fundamental problems in nanoscale MOS devices, and solutions through first principles-based modelling approach. Further, we will discuss about achieving the device performance targets through materials innovation, and engineering, using the first principles modelling based on the density functional theory.

Keywords: MOS devices, CMOS, materials engineering

Functionalized Porous 2D COFs and Macrocyclic Compounds: From Hydrogen Storage to Li-ion Batteries.

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Porous two-dimensional covalent organic frameworks (2D COFs) and macrocyclic compounds are emerging types of lightweight, crystalline materials. They show great promise for hydrogen storage and use in lithium-ion batteries. Their tunable pore structures, large surface areas, and stable π -conjugated backbones allow for efficient gas adsorption and reversible ion transport.

In hydrogen storage, utilising tailored pore sizes, heteroatoms, and functionalized channels in 2D COFs and macrocycles enhances adsorption enthalpies and improves both gravimetric and volumetric capacities under real-world conditions. For lithium-ion batteries, these materials create clear ion-diffusion pathways, redox-active sites, and strong frameworks that support fast charging and discharging, along with long-lasting stability.

We focus on how macrocyclic units, such as para-cyclophane (PCP), cycloparaphenylene (CPP), and calixarenes, facilitate the creation of selective host-guest interactions. Meanwhile, 2D COFs offer structured, extended pore networks that allow for high-capacity storage.

We use multi-scale simulation methods, including density functional theory, molecular dynamics, and grand canonical Monte Carlo, to design and explore the structure-property relationships that affect hydrogen storage and lithium-ion battery performance. This combined computational approach provides valuable insights that facilitate the rational design of molecules, resulting in lightweight, high-capacity materials for future hydrogen storage systems and high-performance lithium-ion batteries.

Keywords:

Unveiling newly modelled Janus Nb₂COS MXene as a Promising Anode for Alkali Metal-Ion Batteries: A DFT Investigation

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Two-dimensional (2D) Janus MXenes have attracted significant attention as next-generation anode materials for alkali metal-ion batteries owing to their intrinsic dipole moments, asymmetric structures, and excellent electrochemical properties. In this study, we investigate the newly designed Janus Nb₂COS monolayer as a potential anode for Li-, Na-, and K-ion batteries using first-principles density functional theory (DFT) calculations. Structural stability was confirmed through phonon dispersion analysis and *ab initio* molecular dynamics (AIMD) simulations performed at 350 K, both of which demonstrated the robustness of Nb₂COS under thermal perturbations. The adsorption behavior of multiple alkali metal ions (up to 36 per unit cell) was systematically explored, revealing strong binding energies and stable configurations. To gain insight into charge transport, the nudged elastic band (NEB) method was employed, showing favorable diffusion barriers that support efficient ion mobility. Furthermore, the electrochemical performance was evaluated through open-circuit voltage (OCV) calculations, which indicated the suitability of Nb₂COS for stable and reversible ion storage. Importantly, the intrinsic asymmetry of the Janus structure facilitates enhanced ion adsorption and intercalation, thereby improving charge storage efficiency.

Overall, Nb₂COS combines high thermal and structural stability with excellent charge storage capability, low diffusion barriers, and favorable OCV values. These findings highlight its potential as an efficient MXene-based anode material for Li-, Na-, and K-ion batteries, offering a promising direction for advanced energy storage technologies.

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Keywords: Alkali metal-ion batteries, Density functional theory, Phonon stability, Open-circuit voltage, Nudged elastic band.

Insights into Inversion Symmetry Breaking in 2D Materials: Piezoelectricity and Spin-Orbitronics

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Breaking of inversion symmetry leads to the emergence of several important properties in 2D materials, such as piezoelectricity, valleytronics and spintronics. For instance, HfN₂ monolayers [1] exhibit valleytronic properties complementary to those in single-layer MoS₂, while the conflux of valley Hall effect, Rashba effect and piezoelectricity is observed in Janus MXSiN₂ (M=Cr, Mo, W; X=S, Se, Te) [2], h-NbN and h-TaN monolayers [3]. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers [4]. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS₂/BP [5] and MoSSe/BP vdWHs [6]. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated [7] together with strain

tunability in ultrahigh shear piezoelectricity in superflexible non-van der Waals graphitic ScX monolayers (X = P, As, Sb) [8]. Ferroelectricity in AlXY (X=S, Se; Y=Cl, Br, I) monolayers [9] will be presented along with sliding ferroelectricity in ZrX₂ (X=Cl, Br, I) bilayers [10].

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Keywords:

Leveraging Data-driven Approaches and Density Functional Theory to Accelerate Novel Materials Discovery

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Technological advancement often relies on the development of advanced materials. Therefore, the discovery of new materials with desired properties is an important but challenging task as trial-and-error methods of synthesizing novel compounds in the laboratory can be extremely labor, time, and cost-intensive. Computational methods combined with autonomous design strategies have the potential to reduce all three factors, significantly. In this talk, I will focus on the rapid discovery of a class of energy materials using advanced computational methodologies. First, I will show how the rational design of an automatic workflow can accelerate the discovery of thermodynamically sta-

ble compounds based on high-throughput density functional theory calculations. Then, I will demonstrate how a machine-learning model based on the crystal graph convolutional neural network can help discover the unsuspected compounds in the same family of materials, that would otherwise be difficult to do in conventional ways. Recent experimental validation of some of our predictions underpins the success and usefulness of computationally guided materials design approach. I will also show how data-driven screening strategy helps us to discover new high-performance photovoltaics in some of the experimentally known compounds, providing new avenues for research and exploration. Lastly, I will briefly discuss efficient materials innovation strategy that can be achieved through the design of a closed-loop autonomous infrastructure capable of performing discovery, synthesis, and characterization of novel materials.

Keywords: Novel Materials, DFT

GC Jain prize talks

MRSI-ICEM 2025

Modified 2D MoS₂ and SnS₂ flakes for Sensing Applications

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The emergence of two-dimensional (2D) transition metal dichalcogenides (TMDCs), particularly SnS₂ and MoS₂, has sparked significant interest in the field of advanced materials due to their unique layered architecture and atomic-scale thickness [1,2]. These materials exhibit exceptional electrical, optical, and chemical properties, rendering them highly suitable for a wide range of applications, including sensors, photodetectors, and various optoelectronic devices [3,4]. However, the full potential of SnS₂ and MoS₂ is often hindered by common challenges such as large-area controlled growth, limited optical absorption in pristine materials, and slow response and recovery times attributed to inefficient charge transfer dynamics [5]. To address these challenges, we employed a thermal chemical vapor deposition (CVD) technique to optimize the growth conditions for high-quality SnS₂ and MoS₂ films. By systematically adjusting parameters, we achieved vertically aligned structures and uniform layers, laying the groundwork for enhanced device performance. Comprehensive characterization techniques, including scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and photoluminescence (PL), were utilized to analyze and confirm the structural, morphological, and optical properties of the synthesized materials. Based on the results from these analyses, we propose a detailed growth mechanism in which in-plane SnS₂ and mixed MoS₂ flakes act as a seed layer for the initial development of

vertically aligned SnS₂ and MoS₂, ultimately leading to the formation of an interconnected three-dimensional network of these flakes. We developed a highly sensitive gas sensor based on vertically aligned SnS₂ flakes, which exhibited exceptional selectivity toward NO₂ over various other toxic and combustible gases [6]. The sensor demonstrated stable performance and strong selectivity, supported by electronic structure calculations. To further enhance gas sensing capabilities, we implemented defect and interface engineering techniques, specifically inducing optimal sulfur vacancies in the SnS₂ lattice through nitrogen plasma treatment [7]. This vacancy engineering significantly improved electronic conductivity and increased the active surface area for gas adsorption, resulting in a remarkable sensitivity to NO₂ and complete recovery at 120°C. In parallel, we explored the functionalization of mixed MoS₂ flakes for NO₂ gas sensing. Recognizing the limitations of pristine MoS₂, which suffers from low response and slow recovery times, we modified the material through nitrogen doping and decoration with silver nanoparticles. The resulting nitrogen-doped MoS₂ (N-MoS₂) and silver-decorated nitrogen-doped MoS₂ (Ag-N-MoS₂) sensors exhibited substantial improvements in NO₂ sensing performance. Notably, the Ag-N-MoS₂ sensor demonstrated nearly double the response of pristine MoS₂ at 100°C, illustrating the synergistic effects of nitrogen doping and silver decoration. Finally, we investigated the application of MoS₂ in optoelectronic systems through the development of a self-powered broadband photodetector utilizing a van der Waals heterostructure composed of MoS₂ and WS₂. The fabricated heterostructures exhibited enhanced responsivity, detectivity, and response times compared to pristine MoS₂, showcasing the potential of these materials in next-generation optoelectronic applications. Furthermore, the anticipated chal-

lenges and future perspectives in the rapidly evolving research on SnS₂ and MoS₂ for sensing applications are similarly explored.

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Keywords: Sensing, gas sensor, selectivity.

Inorganic-Organic Heterostructure Devices for Enhanced Electrical Conductivity and Magnetism

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This thesis introduces a new way to think about magnetic-oxide nanoparticles not as static materials, but as platforms that can be reprogrammed at the molecular level. Instead of treating covalent grafting as a surface add-on, the work proves that aryl diazonium chemistry can rewrite the electrical and magnetic behavior

of oxide nanoparticles by forging strong carbon–metal interfaces. [1][2] These interfaces reshape charge flow, spin ordering, anisotropy, and the entire energy landscape at the nanoscale, offering a level of control that traditional surface modification cannot achieve. Across the thesis, four advances stand out. First, a fully covalent organic–inorganic heterostructure (ITO–EB–ZnFe₂O₄) shows a dramatic 67,978-fold increase in electrical current, demonstrating how sequence-controlled molecular layers slash interfacial resistance and enable low-power conduction routes. [3] Second, aryl-functionalized Fe₃O₄ nanoparticles undergo a striking transformation from insulators to semiconductors. This shift arises from efficient charge exchange between mixed-valence Fe ions and π -rich aromatic rings, introducing a new paradigm for tuning conductivity in oxide systems. [4] Third, 8-Q-CuFe₂O₄ hybrids deliver a high-performance all-solid-state supercapacitor with 418 F g^{−1} capacitance and strong cycling durability, showcasing the practical reach of covalent molecular interfaces in energy-storage architectures. [5] Finally, covalently engineered CoFe₂O₄ nanoparticles exhibit enhanced room-temperature magnetism—higher coercivity, remanence, and blocking temperature—enabled by reduced surface spin disorder and weakened interparticle coupling. This offers a scalable pathway toward molecule-encoded magnetic memory materials. [4] Together, these findings establish covalent molecular grafting as a powerful design principle for the next generation of functional nanomaterials. Beyond advancing the fundamental science of interfacial coupling, the thesis delivers hybrid architectures that push the boundaries of miniaturized electronics, energy storage, and spintronic technologies.

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Keywords: Heterostructure, Electrical Conductivity, Magnetism

Investigating the Interplay between Hot Electrons, Electric Field, and Thermal Effects in Plasmonic Black Gold-Ni Photocatalyst

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The sustainable conversion of CO₂ into value-added products using sunlight offers a promising route to mitigate greenhouse gas emissions while producing renewable fuels and chemicals. Plasmonic catalysis, which exploits localized surface plasmon resonance (LSPR) in metallic nanomaterials, concentrates electromagnetic fields, generates energetic “hot” charge carriers, and local heating, which facilitates bond activation under light. However, their broader application is limited by the narrow light absorption of conventional plasmonic nanoparticles and an incomplete mechanistic understanding of how light drives plasmonic catalysis. This thesis advances plasmonic photocatalysis for CO₂ reduction by developing black gold–Ni (DPC-C4-Ni) catalysts that unite the broadband absorption of plasmonic black gold with the catalytic activity of Ni nanoparticles. Under visible light, this antenna-reactor catalyst achieved CO production rates of 2464 mmol g_{Ni}⁻¹ h⁻¹ with 95% selectivity, maintaining stability for over 100 h in continuous flow. Integrated catalytic kinetics, operando DRIFTS, FDTD simulations, and ultrafast spectroscopy revealed a predominantly hot-electron-driven mechanism. Sub-100 fs electron transfer from Au to Ni populates Ni d-band states, enabling selective CO formation. A superlinear power-law dependence on light intensity and enhanced kinetic isotope effects confirmed that non-thermal hot carriers, rather than photothermal heating, are the primary drivers, providing key mechanistic insights into plasmonic catalysis. A simplified, scalable synthesis for black gold was also developed, and the catalyst’s applicability was extended to challenging reactions such as

C–Cl bond activation, H₂/D₂ dissociation, and selective hydrocarbon hydrogenation. Further, applying an external magnetic field enhanced CO production by up to 140% by prolonging hot-carrier lifetimes, increasing mobility, and improving interfacial transfer efficiency, introducing a novel strategy for tuning plasmonic catalysis. By coupling high-efficiency CO₂ reduction with mechanistic understanding, this work establishes design principles for plasmonic catalysts that combine broadband solar harvesting, efficient hot-carrier utilization, and selective product formation, advancing the prospects for scalable solar-to-chemical CO₂ conversion.

Keywords: Hot Electrons, Electric Field, Gold-Ni Photocatalyst, LSPR.

Next-Generation Sodium-Ion Batteries: Coupling Cathode Design with Operando Diagnostics

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As the demand for sustainable energy storage grows, sodium-ion batteries (SIBs) are emerging as a promising alternative to lithium-ion systems, especially for large-scale and stationary applications. This presentation introduces a research program focused on developing better battery materials and understanding how they behave during operation.

The work centres on layered oxide cathodes, key components that store and release energy in batteries. By carefully adjusting the atomic structure and chemical composition, new materials have been created that offer improved energy output, longer life, and greater stability. One such innovation involves combining two structural phases (P3 and P2) and using aluminium to stabilize the material, resulting in a high-sodium cathode that retains 90% of its capacity after 200 charge–discharge cycles.

To understand how these materials degrade over time, advanced techniques such as operando synchrotron X-ray diffraction are used. These allow real-time observation of structural changes inside the battery while it operates, offering insights that traditional methods cannot provide.

Overall, this research establishes new design principles for stable, high-capacity SIB cathodes, contributing directly to the development

of low-cost, long-life batteries for grid and renewable energy storage.

Keywords: Sodium-Ion Batteries, Coupling Cathode

Design of Functional Materials for Multiscale Energy Harvesting and Sensing Applications

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Modern energy-harvesting-aided sensor technology can meet the growing demand for energy to power up portable and wearable devices. Harvesting energy from various environmental sources, such as temperature fluctuations, mechanical vibrations, and stray magnetic fields, may lead to energy autonomy that can reduce reliance on batteries. The present study investigates the selection of materials and device designs in a manner similar to constructing an efficient energy network, assuring effective harvesting of widely available waste energies using mechanical energy harvesters, hybrid nanogenerators, and functional materials.

Implementing this idea, the development of multifunctional energy harvesters has been developed to improve energy efficiency and sustainability by simultaneously capturing multiple forms of waste energy. In this context, a hybrid nanogenerator, i.e., a pyro-magnetoelectric nanogenerator (PyMENG) was developed to harvest waste magnetic and thermal energies simultaneously. It promptly stores thermal-magnetic energies in a capacitor that generates electricity at room temperature. Thus, in this work, a spin-charge-regulated pyro-magnetoelectric nanogenerator is devised with a composite of well-known ferroelectric P(VDF-TrFE) copolymer and ferromagnetic nickel-zinc ferrite. It exhibits superior pyroelectric response, improved thermal sensing, significant magnetoelectric coupling, and high magnetosensitivity. Notably, electrical poling treatment makes further improvements in pyroelectric and magnetoelectric response. It is a novel method for effectively harvesting waste thermal and magnetic energy offered from homes, factories, and electrical machines. Future self-powered technology may benefit from this sustainable approach. Further, the field of multifunctional energy harvesters is being expanded to open up

new possibilities for effective energy conversion and storage by exploring cutting-edge 2D materials with unique features. Strain-engineered quasi-2D tellurium (Te) nanosheets are synthesized to investigate their multiferroic properties. Due to quantum confinement and a symmetry-breaking effect, ferroelectric functionalities and a magnetic moment have been introduced in quasi-2D Te. The strain-induced magnetoelectric coupling in quasi-2D Te exhibits improved catalytic activity for the hydrogen evolution reaction (HER). A reduced HER overpotential is observed in the presence of a weak magnetic field, indicating improved catalytic efficiency, enhanced reaction kinetics, and exceptional long-term stability. These outstanding features make quasi-2D Te an ideal material for multiferroic devices, spintronics, and renewable energy conversion systems.

Furthermore, the investigation of flexible polymer alternatives presents a viable approach to overcoming the drawbacks of traditional piezoelectric materials for mechanical energy harvesting and pressure sensing. For example, although inorganic piezoelectric materials (e.g., lead zirconate titanate (PZT), barium titanate (BTO), lead zinc niobate-lead titanate (PZN-PT), etc.) hold a high piezoelectric coupling coefficient, however, due to their brittleness, rigidity, and toxicity, polymer materials (such as polyvinylidene fluoride-trifluoro ethylene (P(VDF-TrFE)) and polylactic acid (PLA)) are selected for this work. In addition, flexibility, lightweight, and biocompatibility are added advantages for fabricating large-area, shape-adaptive, wearable devices. However, polymers possess low piezoelectric coefficient that limits the mechanical energy harvesting and dynamic pressure sensing abilities. In this context, electrets have gained lots of interest in fabricating pressure sensors due to their adequate mechanosensitivity caused by ionized trapped air and injected space charge within porous structures. Hence, a 3D-printed thermoelectret-based mechanical energy harvester (3D-TEH) made of PLA has been developed for mechanical energy harvesting and sensing. It has been found that bimodal surface polarity is possible to achieve over the top and bottom surfaces of 3D printed PLA thermoelectrets, which enable a wide range of potential applications, such as mechanical energy harvesting for wearable biomedical sensors. Besides this, the enhanced surface potential leads to a giant longitudinal piezoelectric coefficient (d_{33}) of 350 ± 15 pC/N, which is typically 10 times higher than the best-known piezoelec-

tric polymer, P(VDF-TrFE). The as-developed 3D-TEH delivers an outstanding power density, which makes it a suitable candidate for the self-power pressure sensor. These sensors have high mechano-sensitivity and fast response time, making them ideal for real-time joint motion monitoring and foot-pressure mapping in biomechanical sensing applications.

Inspired by the experience from electret-based mechanical energy harvesting, a non-contact triboelectric nanogenerator (NC-TENG) was developed with the flexible single crystals of an organic compound ($C_{20}H_{13}NO_3$). It exhibited enhanced electrical performance surpassing that of earlier studied devices. It is successfully employed as a self-powered tactile sensor to monitor index finger joint movements at different bending angles. This investigation thus establishes the viability of using flexible organic single crystals for mechanical energy harvesting and touch sensing applications and could pave the way for their utilization in wearable devices.

Expanding the scope of energy harvesting, a unique electromagnetic harvester is established that efficiently uses aluminum foil to collect and recycle electromagnetic energy. By applying Faraday's induction principles, this harvester scavenges electromagnetic energy mostly wasted at factories, domestic appliances, and electrical gadgets. This is utilized for a number of useful uses, including charging smartphones, powering up calculators, and LED illumination.

This thesis covers mechanical, thermal, electromagnetic, and catalytic applications and focuses on building new energy-harvesting and sensing systems by mixing diverse materials and techniques, much like putting together the right tools for specific applications.

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Keywords: Functional Materials, Energy Harvest, Sensing Applications

Design and Development of Hybrid Memristor

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Resistive random-access memory (ReRAM)-based memristors are emerging as a leading class of non-volatile memory devices due to their simple metal-insulator-metal structure, scalability, and ability to switch between distinct resistance states through controlled filament formation and rupture. Despite advantages such as high speed, low power consumption, and multilevel storage capability, conventional ReRAM technologies face challenges including endurance degradation, non-uniform switching, retention instability, and high power demands. To address these limitations, this work proposes the fabrication and characterization of a hybrid ReRAM device integrating copper oxide (CuO) and gallium oxide (Ga₂O₃) as dual active layers. The interfacial coupling between CuO and Ga₂O₃ is expected to enhance filament confinement, improve switching uniformity, and increase the ON/OFF current ratio, offering better control over multilevel resistance states. The fabrication process will involve depositing a CuO thin film via a sol-gel route on fluorine-doped tin oxide (FTO)-coated glass, followed by RF sputtering of a Ga₂O₃ layer and aluminum top-electrode deposition through thermal evaporation. Structural and compositional characterizations will confirm film quality and phase formation. Electrical measurements using a semiconductor parameter analyzer will evaluate the hybrid device's resistive switching behavior. Based on the results, an

extended back-gate field-effect transistor (FET) configuration employing a LiF dielectric and the CuO/Ga₂O₃ heterostructure will be designed to explore memristive transistor functionality. The proposed hybrid oxide approach is anticipated to deliver improved endurance, stability, and switching reliability, making it a viable pathway for next-generation memory and neuromorphic computing applications.

Keywords: Hybrid Memristor, ReRAM, FET.

Detection of Mycotoxin Using Electrochemical Biosensors

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Mycotoxins in wine cause serious health risks and require strict monitoring. Conventional detection methods are slow and costly, and laboratory-bound. Rapid, portable electrochemical biosensors are needed to ensure efficient on-site wine safety. An electrochemical biosensor based on graphene sheets was developed. Sensor performance was optimised using advanced nanomaterials and electrochemical techniques. Wine samples were tested to evaluate sensitivity, specificity, and analytical robustness. The electrochemical measurements were carried out for bare methanol, PBS and for different concentrations of wine in the methanol and PBS. The Cyclic Voltammogram (CV) was recorded in the potential range of 0.6 to -1.2V for methanol at a scan rate of 20 mV/s. For the bath of PBS, CVs were recorded in the potential range of 0.8 to -1.15 V at the scan rate of 20 mV/S. The biosensor achieved low nanomolar-picomolar detection limits below regulatory thresholds. The biosensor provides a fast, sensitive, and practical tool for routine mycotoxin detection in wine.

Keywords: Mycotoxins; Ochratoxin A; Wine; Electrochemical Biosensors; Food Safety.

Contributory Talk

MRSI-ICEM 2025

Symposium: A

Optical Properties of Cerium Doped $\text{Gd}_2\text{O}_3\text{-SrO-P}_2\text{O}_5\text{-SiO}_2$ (GSPS) Glass for Scintillator Applications

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Scintillating glasses are extensively employed as radiation detectors for X-rays, gamma rays, and neutrons across numerous research areas and practical applications [1]. Phosphate glasses exhibit several advantageous properties, including good chemical durability, low melting temperatures, excellent physical characteristics, high optical transparency, and strong luminescence efficiency. Cerium-activated phosphate glasses have gained significant interest due to their promising applications in scintillation detectors [2]. In this study, Cerium doped $\text{Gd}_2\text{O}_3\text{-SrO-P}_2\text{O}_5\text{-SiO}_2$ (GSPS) glass was synthesized using melt-quenching technique. The density of the glass was determined using Archimedes' principle, yielding a value of 3.25 g/cm^3 . Unlike Ce^{3+} , which is optically active and contributes to luminescence, Ce^{4+} does not exhibit luminescence due to its closed-shell electronic configuration. Therefore, to probe the valence states of the cerium ions XPS experiment was carried out. Figure.33 shows the XPS spectra of Ce3d. The fitting of this spectra shows there are two peaks at 885 and 904eV which correspond to Ce^{3+} . There is no peak associated to Ce^{4+} . Figure 52 presents the photoluminescence (PL) emission spectra of the GSPS glass under 302nm excitation at room temperature. The sample exhibited broad emission bands ranging from 300 to 430nm, with the peak intensity centered around 334 nm. This emission feature is consistent with those reported for Ce-doped glass systems and are attributed to the allowed $5d \rightarrow 4f$ transitions of Ce^{3+} ions, which serve as the primary luminescent centers.

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Keywords: phosphate glass, scintillator detector, photoluminescence, cerium

Experimental Investigation Combined with Physics-Based Modelling of Vacancy-Controlled Switching in $\text{V}_2\text{O}_5/\text{ITO}$ Memristors

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Resistive switching in transition metal oxides is often governed by the interplay between oxygen vacancy (V_O) dynamics and interface energetics. In this study, we combine nanoscale conductive atomic force microscopy (c-AFM) with bulk device measurements to uncover the switching and negative differential resistance (NDR) behaviour of near-stoichiometric $\text{V}_2\text{O}_x/\text{ITO}$ memristors. At the nanoscale, spatially distributed V_O s drive variable-range hopping conduction accompanied by polarity-dependent N- and S-type NDR. In contrast, in bulk $\text{Ag}/\text{V}_2\text{O}_x/\text{ITO}$ devices, Ag-induced V_O accumulation near the top interface enables low-voltage switching ($\sim 0.3 \text{ V}$) and artificial synaptic plasticity ($\sim 0.2 \text{ V}$), obeying linear ion drift model and trap-limited transport across vacancy-depleted regions.

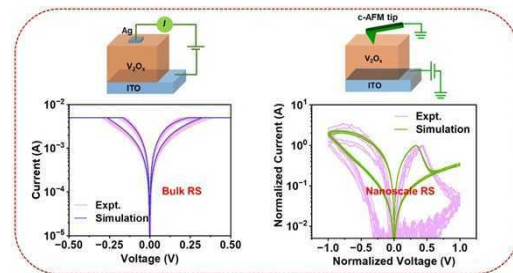


Figure 9: Experimentally obtained IV characteristics and corresponding simulated IV curves for $\text{V}_2\text{O}_5/\text{ITO}$ memristors probed under bulk and c-AFM method

A dynamic rate equation-based conduction model, incorporating voltage-driven trapping/detrapping kinetics and Joule heating-induced temperature rise, qualitatively re-

produces the observed hysteresis, bidirectional NDR, and cycle-to-cycle variability observed in the nanoscale devices. By linking nanoscale transport phenomena to bulk device operation, results demonstrate how growth parameter-dependent bulk V_O profile combined with electrode-mediated interface stoichiometry govern low-power, stable, and neuromorphic-relevant switching pathways in near-stoichiometric oxides.

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Keywords: resistive switching, rate equation, cAFM, oxygen vacancies

Solid-State Phosphors from Coal-Derived Carbon Quantum Dots for White-Light-Emitting Devices

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The development of low-cost and metal-free wide band gap solid-state phosphor materials is an important target for realizing the next-generation artificial lighting. Carbon quantum dots (CQDs), especially those derived from low-cost precursors such as coal, are suitable non-metallic semiconductors owing to their unique optical and chemical properties with low toxicity. However, these CQD nanomaterials with a size typically ≤ 10 nm exhibit aggregation-induced emission quenching behaviour upon drying to the solid state. To mitigate this issue, we have developed a process for synthesizing solid-state phosphors from coal-derived CQDs by embedding the CQD nanomaterials within an appropriate solid matrix. The process involved

a facile one-pot sol-gel method between coal-derived CQDs and an alkoxy silane compound under basic conditions.

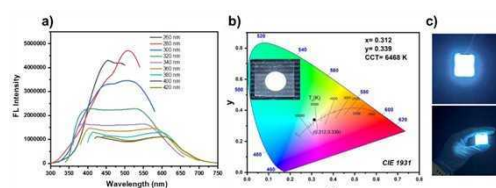


Figure 10: (a) Fluorescence spectra of a solid-state phosphor synthesized using coal-based CQDs. (b) CIE 1931 chromaticity diagram of the solid phosphor under UV irradiation shown in the inset. (c) A prototype white-light-emitting device.

The SiO_2/CQDs solid materials exhibited high-intensity white light emission (Figure 10a) when irradiated with UV light covering most wavelengths of the visible light spectrum. Such white light emission was not observed with a solid-state phosphor synthesized using commercial CQDs, highlighting the unique role of coal-derived CQDs. Detailed investigations suggested that the coal-derived CQDs co-doped with N and S heteroatoms and containing extremely small-sized and crystalline nanoparticles, favored the heterogeneous nucleation and rapid formation of SiO_2/CQDs solid-state phosphors. Coal-derived CQDs endowed a suitable band gap structure in a SiO_2/CQDs solid phosphor, causing high intensity white light emission with correlated color temperature (CCT) value of 6468 K and CIE chromaticity coordinates of (0.312, 0.339), for potential cool-white lighting applications (Figure 10b). A prototype of phosphor-converted white-light-emitting device (WLED) was fabricated (Figure 10c) using a representative SiO_2/CQDs solid phosphor in combination with a 365 nm UV LED chip, demonstrating practical applicability towards artificial lighting.

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Keywords: coal-derived CQDs, solid-state phosphor, WLED

Synthesis Strategies of Various Zinc Oxide Nanostructures and Their Potential Applications

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Zinc oxide (ZnO) is a wide bandgap (3.4 eV at room temperature) semiconducting material, it exhibits nanostructures in 0D, 1D, 2D and 3D with different shapes. These nanostructures are being used for novel applications which include optic, optoelectronic, catalysis and biomedical. However, there are many challenges involved to obtain stable nanostructures of ZnO. Hence many researchers are focused to overcome these challenges. In our work, various nanostructures of ZnO such as nano-rod, nano-disc, nano-flakes and nanoparticle structure were found while doping it in chemical synthesis process and studied their applications. Particularly, ZnO nano-rods studied for polymer LED applications. When ZnO nanorods integrated in MEH-PPV light emitting diode (PLED) there is enhancement in the luminance. It was observed that, luminance of ZnO nanorod/MEH-PPV LED increased by 20 % as compared to PLED without rods due to single waveguide effect in ZnO nano-rods. This strategy rectifies the problem of undesired total internal reflection at ITO/glass and glass/air interfaces. In addition, we successfully 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 core-shell structure. The core-shell SmO/ZnO hetero-junction NPs are used as photocatalyst to remove methyl green dye molecules from water. The dye degradation rate of Sm^{3+} ions doped ZnO NPs found was 91% which is 26 % higher than that of pristine ZnO NPs. We believe the cost effective synthesized stable ZnO nanostructures have great potential for various applications.

Keywords: ZnO nanostructures, photocatalysis, LEDs

Third-Order Nonlinear Optical, Thermal, Dielectric and Ferroelectric Characteristics of Tri-allylthiourea Cadmium Chloride Single Crystals

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Single crystals of tri-allylthiourea cadmium chloride (ATCC) were successfully grown by the slow evaporation solution technique and subjected to detailed optical, dielectric, nonlinear, and ferroelectric studies. To study the surface morphology of the grown crystals of ATCC, the scanning electron microscopy (SEM) images were recorded at magnification factors of 1500, 5000, and 10000 under an operating voltage of 20 kV. UV-Vis absorption analysis confirmed a wide transparency window in the visible region with a sharp absorption edge corresponding to an optical bandgap of 3.6 eV. The melting point of ATCC is at 113.36 °C and the onset decomposition temperature is at 228 °C. Nonlinear optical characterization using the single-beam Z-scan technique (532 nm, pulse width 4999.99 ps) revealed a two-photon absorption coefficient (β) of 10×10^{-12} m/W and a three-photon absorption coefficient of 4499×10^{-12} m³/W². Dielectric studies in the frequency range 100 Hz–1 MHz and temperature range 303–373 K were performed. The piezoelectric charge coefficient was measured, and the hysteresis loop of the ATCC crystal was traced using a PE loop tracer, with loop parameters such as remnant polarization (P_r) and coercive field (E_c) determined.

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Keywords: NLO, ATCC, Z Scan.

Mimicking Neural Complexity Leveraging the Metal–Insulator Transition in Rare Earth Nickelates

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Over the last decade, intensive academic and industrial research has focused on developing hardware that emulates the efficient way the brain processes information by exploiting the principles of parallelism, sparsity, and low power consumption— a field known as neuromorphic computing. This requires nano-scale devices capable of reproducing the main functionalities of neurons and synapses. The mechanisms of biological synapses can be emulated in hardware by leveraging non-volatile analogue resistance states provided by emerging devices such as ion-based non-volatile memories, drift and diffusive memristors, or synaptic transistors^{1,2}. In contrast, biological neurons are complex nonlinear dynamical units that encode information in the frequency of their output spikes and adapt their responses based on previous inputs, thereby exhibiting internal memory. Developing electronic nanodevices that efficiently reproduce such non-linear dynamical neuron functions³ is essential to unlock the full computational power of artificial networks. This remains a major challenge, as it requires electrically induced volatile resistive switching combined with internal memory for adaptive behaviour.

this work, we exploit the metal-insulator transition (MIT) in a NdNiO₃ nickelate device to implement dynamical neuron functionality. A planar two terminal device [Fig. 11(a)] is fabricated using photolithography on an 8 nm thick NdNiO₃ film grown using sputtering technique on a LaAlO₃ substrate. Upon reducing temperature, the device undergoes a Mott transition from metallic to insulating behaviour around $T_{MIT} \sim 100$ K. We show that the MIT can also be triggered electrically, in which case the device exhibits current-controlled negative differential resistance (CC-NDR)[Fig.11(b)]. In this regime, electrical pulses induce volatile resistive switching with threshold and relaxation dynamics strongly resembling neuronal spiking. After recovery of the original state, the device exhibits a longterm memory effect that naturally enable adaptive behaviour. Building on these mechanisms, we implement key neuronal func-

tionalties such as leaky-integrate and fire (LIF) spiking, sub-threshold firing, long-term relaxation and nociception. These results highlight the potential of NdNiO₃-based nanodevices for constructing intelligent and adaptive large-scale neuromorphic networks closely inspired by the non-linear dynamics of biological systems.

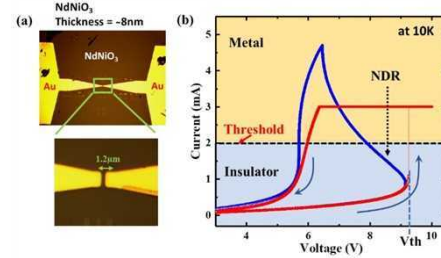


Figure 11: (a) Optical image of the planar two-terminal NdNiO₃ device. (b) Current-controlled negative differential resistance (CC-NDR) observed in the device under electrical excitation, evidencing the electrically driven metal–insulator transition (MIT).

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Keywords: Rare earth nickelates, Mott transition, Neuromorphic computing, Leaky integrate and fire

High-Performance Zinc–Tin Oxide Semiconductor-Based Thin Film Transistors

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Amorphous metal-oxide semiconductor (MOS) thin film transistors (TFTs) have become indispensable elements in modern large-area flat-panel displays, shaping the progress of display technology over the past decade. Their widespread adoption is largely due to a combination of exceptional properties, including

relatively high carrier mobility, excellent optical transparency, and uniform performance across large areas, and stable electrical operation. Among the various materials investigated, MOS such as indium-gallium-oxide (In-Ga-O), indium-zinc-oxide (In-Zn-O), zinc-tin-oxide (Zn-Sn-O), indium-zinc-tin-oxide (In-Zn-Sn-O), and indiumgallium-zinc-oxide (In-Ga-Zn-O) have been extensively studied as active n-channel materials, demonstrating significant potential for high-performance oxide TFTs. Despite these advancements, the reliance on indium and gallium poses economic and sustainability challenges. Both elements are scarce and costly, which limits their long-term industrial use in large-area electronic applications. To address this, alternative materials with comparable electronic performance are being explored. Tin (Sn) stands out as a particularly attractive candidate, as it is abundant, environmentally benign, and possesses electronic characteristics and ionic radii similar to indium. This makes it a viable replacement in the development of cost-effective and sustainable oxide TFTs.

In this context, amorphous zinc-tin-oxide (a-ZTO) thin films integrated into TFTs have shown promising results. Optimized a-ZTO TFTs demonstrate a high saturation mobility (μ_{sat}), a low subthreshold swing (SS), and an impressive ON/OFF current ratio (I_{ON}/I_{OFF}). Furthermore, these devices exhibit excellent bias stress stability and reliable performance under a range of environmental conditions, making them suitable for practical deployment in display backplanes. The superior electrical performance of a-ZTO TFTs is closely linked to the better quality of the films. High film density and smooth surface morphology contribute to reduced oxygen-related defects, resulting in improved conduction pathways for efficient electron transport. This, in turn, enhances the switching behavior and long-term operational stability of the a-ZTO TFT. The demonstrated performance and stability of a-ZTO TFTs highlight their strong potential as a next-generation semiconductor material. By combining affordability, abundance, and excellent electrical characteristics, a-ZTO stands as a leading contender to drive advancements in large-area flat-panel display technologies.

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Keywords: Semiconductors, Zinc-Tin-Oxide, Thin Film Transistors, Display

Photoluminescence Intensity and Polarization Enhancement in GaAs QW–Microcavity System

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High-quality microcavities are versatile platforms for applications such as quantum light sources, quantum electrodynamics, and quantum optomechanics[1]. In such structures, strong exciton–photon coupling has enabled phenomena such as polariton lasing and Bose–Einstein condensation, while weak coupling has led to Purcell enhancement and vertical-cavity surface-emitting lasers (VCSELs)[2,3].

In this work, we report our recent studies on such microcavities, where MOVPE growth is used to sandwich a GaAs quantum well (QW) between two

Al_{0.9}Ga_{0.1}As/Al_{0.1}Ga_{0.9}As distributed Bragg reflectors (DBRs) with reflectivity greater than 99%. The position of the QW is carefully chosen to coincide with the antinode of the optical field. The normal-incidence reflectivity spectrum exhibits a sharp dip at $\lambda_0 \sim 815.2$ nm (FWHM = 0.7 nm), indicating a high- Q cavity ($Q \approx 1164$) [Fig.12a]. The resonance wavelength can be tuned either by varying the angle of incidence, thus altering the perpendicular component of the light wave vector, or by changing the temperature, which modifies the effective cavity length [Fig.12 b,c].

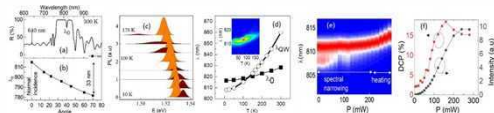


Figure 12: (a & b) Normal incidence reflectivity and its angular dependence, (c) evolution of deconvoluted PL peaks with sample temperature, (d) QW PL peak and Cavity resonance vs Temperature, inset is 3D PL spectra plotted as a function of Temperature, and (e) 3D PL spectra, (f) DCP and PL intensity plotted as a function of excitation power (P).

The interaction between the light confined in the cavity and excitons confined in the QW is probed through the enhancement of photoluminescence (PL) intensity over the temperature range where the cavity mode coincides with the exciton recombination energy. However, no clear anti-crossing between the exciton energy and cavity modes is observed, which is usually a sign of strong coupling [Fig.12 d]. This indicates that the system operates in the weak coupling regime. As the exciton and photon densities are increased by raising the incident light intensity, the PL intensity exhibits a super-linear increase with threshold-like behaviour and associated spectral narrowing [Fig.12 e]. Furthermore, we demonstrate selective excitation of a particular exciton spin state by injecting spin-polarized carriers in the barrier layer using circularly polarized light. The degree of circular polarization (DCP) of the emitted light also exhibits threshold-like behaviour at lower excitation intensities [Fig.12 f]. Such behaviours are not observed in bare QW structures without the two Bragg mirrors, confirming the influence of the microcavity on the excitonic recombination. Resonant excitation of spin-polarized electrons in the QW can shed more light on the spin coherence process. Details will be presented during the conference.

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Keywords: Micro-cavity, Exciton-phonon coupling, Purcell enhancement

Applications of Sol-Gel Synthesized Perovskite Zinc Titanate Photocatalysts

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The widespread use of antibiotics has led to their persistent presence in water bodies, promoting the spread of antibiotic-resistant bacteria (ARBs) and genes (ARGs), and posing serious environmental and health risks. Amoxicillin (AMX), a common β -lactam antibiotic, frequently escapes conventional treatment, contributing to ARB emergence even at low concentrations. Photocatalytic decomposition of such emerging contaminants using perovskite materials is one of the cost-effective and less-toxic methods. In this study, perovskite ZnTiO_3 photocatalysts were synthesized using the sol-gel method. Their photocatalytic performance was evaluated through the degradation of the emerging contaminant AMX. The effects of synthesis parameters, including calcination temperature, the amount of added polyvinylpyrrolidone (PVP), and ammonia, were systematically investigated. Specifically, calcination temperatures of 500, 600, 700, and 800°C, ammonia volumes of 750, 1500, and 3000 μL , and PVP amounts of 3g and 5g were explored. The resulting ZnTiO_3 photocatalysts were characterized by XRD, FE-SEM, BET, and UV-Vis spectroscopy. The materials exhibited a rod-like morphology and were responsive to ultraviolet light. Optimal photocatalytic activity was achieved with a calcination temperature of 700°C, 1500 μL of ammonia, and 5g of PVP. Additionally, the photocatalytic degradation of other pollutants—namely tetracycline (TC), methyl orange (MO), and methylene blue (MB) dyes—was assessed, further supporting the potential of perovskite ZnTiO_3 photocatalysts for the removal of emerging contaminants and organic pollutants in wastewater treatment applications.

Keywords:

Symposium: B

Electronic and magnetic attributes of highly correlated vanadium-oxides

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Vanadium-based oxides have significant impact to the field of material science over the decades. The startling nature of phase transition in vanadates is the major reason behind such enhancement in structural, electronic, and magnetic attributes. This is a first order reversible phase transition popularly coined as insulator-metal transition (IMT). In VO_2 , it is observed in the vicinity of 340 K whereas in V_2O_3 , the same is detected around 170 K. A vanadate belongs to either of the two families; Magneli ($\text{V}_n\text{O}_{2n-1}$) or Wadsley ($\text{V}_n\text{O}_{2n+1}$). However, V_6O_{13} is the only member of Wadsley family that exhibits IMT, on contrary, each member of Magneli family illustrates IMT. This temperature-dependent transition is quite susceptible to external influences such as doping, stress, irradiation, heat, etc. In particular, the hunt of securing ferromagnetism in vanadium-oxides is on peak for potential increase in data storage capability. Studies suggest the inducement of Cr has subtle sign of ferromagnetism in VO_2 . On contrary, the case of V_2O_3 is different in the sense where previously it was thought to be a system with half-spin. But now it is confirmed that $3d^2$ electrons are align in such a manner to have full integral spin. IMT in V_2O_3 has distinct magnetic domains as the so-called transition is seen as antiferromagnetic insulating state to paramagnetic metallic state. Further increase in temperature results in transition from paramagnetic metallic state to paramagnetic insulating state. Synchrotron-based X-ray techniques have confirmed that the inducement of Cr in VO_2 causes a shift in vanadium valency from $4+$ state to $5+$ state and under suitable condition, double-exchange interaction between Cr^{3+} - V^{5+} proceeds to support ferromagnetism. In a nutshell, vanadates fulfill the criteria of spintronics implementation.

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Keywords: VO_2 , V_2O_3 , Synchrotron, Ferromagnetism, Spintronics

Current redistribution induced anomalous Magneto-transport signatures in the Superconductor/Topological insulator ($\text{Mo}/\text{Bi}_2\text{Se}_3$) heterostructure

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Proximity-induced superconductivity in topological insulator/superconductor heterostructure systems is one of the proposed routes to realize topological superconductors for quantum computing applications. Here, we report the proximity-induced changes in the magneto-transport properties in $\text{Mo}/\text{Bi}_2\text{Se}_3$ heterostructures. Bi_2Se_3 thin films were deposited by magnetron sputtering on a SiO_2/Si substrate. It was partially covered with a 40 nm thick Mo superconductor using the shadow masking technique to create a step junction. The magneto-transport (MR) measurements have been performed simultaneously on two different regions of the sample—with and without the Mo top layer—in the temperature range $T = 4\text{--}10\text{ K}$ and in magnetic fields up to $B = \pm 15\text{ T}$. The temperature dependence of resistance measured at different magnetic fields, as shown in Fig.13(a), shows the typical superconducting signature with a T_C of $\sim 4\text{ K}$ on the Mo side.

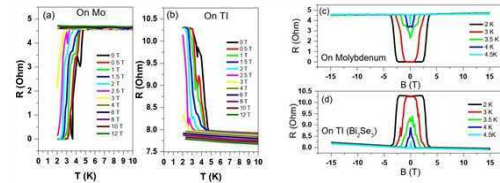


Figure 13: (a,b) Variation of resistivity with temperature on the Mo and TI sides of the $\text{Mo}/\text{Bi}_2\text{Se}_3$ heterojunction, (c,d) Magneto resistance data showing the weak antilocalization (WAL) signature, and the anomalous resistive variation in the heterojunction.

In contrast, on the TI side, an anomalous upturn in resistance is observed exactly at the superconducting transition, as shown in Fig.13(b). Upon increasing the magnetic field, the T_C shifts to lower temperatures as expected; similarly, the temperature corresponding to the anomalous upturn also shifts to lower T . Magnetoresistance data at 2 K show a sharp fall in resistance at 3 T (Fig.13(c)). MR measured at different temperatures exhibits a systematic reduction in critical field, as expected for a superconducting sample. The weak antilocalization (WAL) signature also coexists with the superconducting transition and becomes more prominent near 3.5 K, where superconductivity is suppressed. From our previous observations[1], these signatures are not due to scattering of Cooper pairs with surface electrons, as sometimes erroneously reported in the literature. Instead, these anomalous resistance changes arise from the redistribution of electron current in a heterojunction with a tilted superconducting electrode.

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Keywords:

Zn^{2+} concentration and was found to be in the range of 0.8318 nm–0.8428 nm. Grain size did not show any systematic behavior with the increase in Zn^{2+} concentration; however, it increased with increasing annealing temperature. At 300 K, the magnetization value (M_s) of the as-prepared sample increases with the increase in Zn^{2+} concentration up to $x = 0.2$, and the highest M_s value of 59 emu/g was observed. With further increase in Zn^{2+} concentration, the M_s value decreases. The annealed samples followed a similar pattern, and the highest value of 75 emu/g was observed for $x = 0.40$ in the 900 °C annealed samples. At 60 K, the highest magnetization of 111 emu/g with a coercivity of 18 Oe was observed in the present study for the sample annealed at 900 °C with $x = 0.50$. This property may find important application in the future. With the increase in diamagnetic Zn^{2+} concentration, ferrimagnetic to antiferromagnetic ordering associated with the transition from collinear to canted spin structure was observed in the sample.

Keywords: Ferrite; Substitution; Nanoparticles; Magnetization.

Symposium: C

Effect of diamagnetic Zn-substitution on Enhancement of Magnetization in Ni-ferrite nanop

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Zinc substituted Ni-ferrite, $\text{Zn}_x\text{Ni}_{1-x}\text{Fe}_2\text{O}_4$ ($0 \leq x \leq 1$) nanoparticles were synthesized by the sol-gel method and were annealed at 550 °C and 900 °C in air for 2 hours. The samples were characterized by XRD, Raman spectroscopy and FE-SEM. All the as-prepared and annealed samples were of spinel phase. The lattice constant increased with the increase in

Bimetallic coordination network for ultrahigh performance in supercapacitor energy storage applications

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Electrochemical capacitors (ECs), or supercapacitors (SCs), are gaining prominence for their high power density, excellent reversibility, long cycle life, and inherent safety. Bimetallic coordination polymers (CPs) have emerged as promising electrode materials due to the synergistic interaction between two metal centers, which enhances structural stability and introduces unique electrochemical properties. This dual-metal approach offers improved capacitance and conductivity; however, its application in supercapacitors remains underexplored, highlighting the need for further investigation into their design and performance. The bimetallic coordination polymer was synthesized hydrothermally and has been thoroughly characterized using various spectroscopic and structural techniques. The crystal structure reveals a network composed of one divalent Zn^{2+} ion, two monovalent Cs^+ ions (Cs1 and Cs2), two half BTC ligands, one coordinated water molecule, and three lattice water molecules. The Zn^{2+} ion adopts a tetrahedral coordination environment and bridges three Cs^+ ions (two Cs1 and one Cs2). Cs1 is connected to two Cs2 and two Zn1 ions, whereas Cs2 is linked to two Cs1 and one Zn1 ion, forming a robust 3D network. The electron synthesized from $\text{Cs}_2\text{Zn-COP}$ shows a maximum gravimetric capacitance of 1106.3 F/g at 1 A/g, whereas the ASC device prepared from this material also shows a maximum gravimetric capacitance of 107.1 F/g at a current density of 1 A/g. After comparing the energy and power densities of both SC and ASC devices from the bimetallic polymer, it has been concluded that they exhibit maximum energy density (i.e., 38.4 Wh kg^{-1} for SC and 29.2 Wh kg^{-1} for ASC devices) at a current density of 1 A/g. Moreover, both SC and ASC devices show maximum power density at increased current density (in the case of SC, 5009.6 W kg^{-1} at 20 A/g, and in the case of ASC, 6999.9 W kg^{-1} at 10 A/g). The structural features of this compound suggest its potential as an efficient electrode material for high-performance supercapacitor applications.

Keywords:

Green Halide Perovskites as Next-Generation Photocatalysts: A Rational Design Approach

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Traditional photocatalysts, such as metal oxides, can only absorb light in the ultraviolet range due to large band gaps, while transition metal sulfides with suitable band gaps have improper band gap edges for driving CO_2 reduction or water oxidation. In this context, low-cost lead-halide perovskites have attracted significant attention as possible heterogeneous photocatalysts¹ due to their tuneable band gaps, strong light absorption, long carrier lifetimes, long charge-carrier diffusion lengths, and low effective masses of charge carriers.

However, lead-halide perovskites raise environmental concerns because of the presence of toxic lead (Pb^{2+}) and their low stability under normal operating conditions of a photocatalytic reactor². *In this contribution, we apply density functional theory calculations to explore the stability and electronic structure of alternative materials based on Sn^{2+} . Stability is assessed under different chemical potential conditions, suggesting control through the synthesis conditions.*

It is found that under CsX -rich ($\text{X} = \text{I}, \text{Br}$ or Cl) chemical potential conditions (Figure 14 a), slabs with around 11 atomic layers of CsMX_3 ($\text{M} = \text{Pb}, \text{Sn}$; $\text{X} = \text{I}, \text{Br}, \text{Cl}$) along the [001] direction can be suitable candidates for enhancing the photocatalytic efficiency of TiO_2 or $\text{g-C}_3\text{N}_4$. Interestingly, selective slabs synthesized under MX_2 -rich conditions (Figure 14b) along the [001] and [100] directions show the possibility of finding suitable tin-halide layers appropriate for H_2 generation through water splitting and CO_2 reduction to useful products. Furthermore, we worked on suitable organic molecules that can couple energy states of inorganic and organic regions of layers to open up channels for charge transfer. We checked the stability of these hybrid layers at room temperature using AIMD simulations.

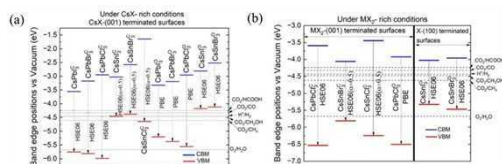


Figure 14: Figure:1 Alignment of band gap edges (red and blue lines) w.r.t. vacuum for stable layers under (a) CsX and (b) MX₂-rich conditions.

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Keywords: perovskites, Photocatalysts:

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Strategies for effective enhancement of Thermoelectric power conversion efficiency of complex oxides

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Thermoelectric energy conversion is gaining increasing importance due to its robust, durable, environment friendly and sustainable nature. In recent days oxide materials are explored specifically for harsh environment and mid-high temperature applications. When compared to the other well-known thermoelectric materials, oxides suffer from the disadvantages of low electrical conductivity and power factor. To overcome these challenges several strategies such as site selective doping, Nano structuring and compositing etc. are being carried out. The presentation involves the attempts to enhance the thermoelectric efficiencies of perovskite-structured lanthanum cobalt oxide (LaCoO₃), and spinel

ferrites of type AFe₂O₄ (A-Cu, Zn). These materials feature tunable bandgaps, enabling modulation of their carrier concentration through doping or thermal activation. Combined with a high effective mass of charge carriers, which contributes to enhanced thermopower and their robust thermal and chemical stability, these materials are capable of energy conversion in harsh environments at mid-high temperatures. Despite these favorable attributes, challenges such as low intrinsic electrical conductivity and strong carrier-phonon interactions persist, limiting their heat conversion efficiency. Therefore, it becomes imperative to explore targeted strategies such as cationic doping and composite formation to optimize their charge transport behavior and overall thermoelectric efficiency. This study is dedicated to investigating these approaches, aiming to advance LaCoO₃ and AFe₂O₄ (A-Cu, Zn) based materials as viable candidates for efficient thermoelectric applications.

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Keywords:

METAL-ORGANIC FRAMEWORK FOR HYDROGEN PRODUCTION BY PHOTOCATALYTIC OVERALL WATER SPLITTING

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Non-sustainable, fossil fuel-dependent processes still account for most of the worldwide hydrogen (H₂) production.[1] Among alternatives, photocatalyzed water dissociation into H₂ and O₂ is particularly appealing owing to its intrinsic sustainable nature.[2] However, up till now reported catalysts for light-driven water splitting still do not meet the techno-economical requirements for industrial implementation as they suffer from either a lack of solar-to-hydrogen conversion (STH) efficiency and/or stability under operation, require complex synthesis processes, and are in most cases inactive under visible-light irradiation.[3]

Over the last few years, metal-organic frameworks (MOFs) have drawn increasing interest as candidate catalysts, but most reported studies deal with either of the half reactions, i.e., the hydrogen and oxygen evolution reactions (HER and OER, respectively), thus requiring the use of sacrificial agents.[4] In this regard, the MOF2H2 project[5] is ambitious and aims to be a game changer in producing hydrogen from water through a more sustainable process—overall water splitting (OWS)—using non-noble MOF-based catalysts.

This project relies so far on two main families of MOFs. Inspired by nature, a MOF made of a multicopper-based metalloligand reminiscent of the active site of certain reductive enzymes was first selected and found to be an efficient catalyst for photo-induced water splitting reactions. Besides, specific Ti₁₂O₁₅-based MOFs[6] are also being explored. While the first studies demonstrated the high potential of these MOFs for HER and OWS,[7,8] deeper physicochemical and photocatalytic investigations are ongoing and driving the chemical modifications/optimization to reach higher performances.

In this communication, the concept of the MOF2H2 project will be presented as a whole. A specific highlight will be provided on the most recent advances leading to ground-breaking results in terms of H₂ photo-induced production. Finally, our ongoing work aimed at improving the MOF-based catalysts' performances will also be discussed.

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Keywords: metal-organic frameworks (MOF), photocatalysis, overall water splitting

Ag doped ZnO/PVDF Composites: An Excellent Piezoelectric Energy Harvesting and Storage Material for Smart Wearable and Security Devices

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Harvesting biomechanical energy through piezoelectric and triboelectric materials offers a sustainable pathway to power the next generation of smart wearable devices. Despite its potential, progress has been hampered by the difficulty of creating materials that are simultaneously low-cost, flexible, durable, and highly responsive. In this work, we present functionalized Ag-doped ZnO (f-Zn_{1-x}Ag_xO) integrating

into PVDF to prepare robust composites with exceptional energy storage and harvesting performance.

The filler was precisely engineered by doping ZnO with 2 wt% Ag, followed by surface functionalization with APTES, yielding f-Zn_{0.98}Ag_{0.02}O. This modification transformed the filler morphology from nanoflakes to aligned nanorods, markedly improving interfacial compatibility and polarization response. Incorporating an optimal 30 vol% of f-Zn_{0.98}Ag_{0.02}O into PVDF resulted in a remarkable energy storage density (W_{erc}) of $\sim 11.6 \text{ J/cm}^3$, which is nearly 39 times higher than pristine PVDF (0.3 J/cm^3) with an efficiency of 85% and significantly reduced dielectric losses.

Beyond superior storage performance, the composite delivered an impressive piezoelectric power density of $42.5 \mu\text{W/cm}^2$, ~ 56.7 times higher than neat PVDF, outperforming many recent systems fabricated using more complex strategies. A prototype piezoelectric nanogenerator (PENG) based on this composite successfully lit 26 LEDs and showed excellent responsiveness to diverse biomechanical stimuli and toy-induced motions.

Notably, the PENG also exhibited application potential in security technologies, producing distinct and reproducible electrical signatures under different mechanical inputs, making it suitable for integration into smart door locks and ATM authentication systems. Overall, these findings highlight the versatility and promise of our PVDF/f-Zn_{0.98}Ag_{0.02}O composites for next-generation energy harvesting and storage, security applications, and smart wearables.

Keywords: Piezoelectric, Doping, Composites, Energy harvesting

Improved Piezocatalytic Performance of BaTiO₃-Based Heterostructure Nanocomposites for Environmental Remediation

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The rapid discharge of dyes, pharmaceuticals, and microbial contaminants into aquatic systems poses severe environmental and health challenges, necessitating sustainable remediation technologies. Piezocatalysis, driven by mechanical energy, offers a promising green approach for pollutant degradation. However, conventional piezoelectric materials such as BaTiO₃ (BT) nanoparticles suffer from poor catalytic efficiency due to the rapid recombination of charge carriers. To overcome this limitation, we have designed and investigated two heterostructure nanocomposites: BaTiO₃-MoS₂ (BT/MS) and BaTiO₃/CuO (BT/CuO). In BT/MS composites, the optimal 1.0 wt% MoS₂ loading (BT/MS1) exhibited superior piezocatalytic activity, achieving 1.84- and 2.8-fold higher degradation efficiencies for Rhodamine B and Methyl Orange, respectively, compared to pristine BT. This enhancement is attributed to the interfacial charge transfer between BT and MS, which suppresses electron-hole recombination. In parallel, BT/CuO nanocomposites demonstrated multifunctional remediation under ultrasonication, effectively degrading Rhodamine B (98.4%), Methyl Orange (65.3%), and the antibiotic Ofloxacin (83.0%) within 120 min. Moreover, BT/CuO achieved 99.0% inactivation of *Escherichia coli*, highlighting its antibacterial potential. Both systems exhibited strong stability and recyclability across successive cycles. Mechanistic investigations confirm that interfacial heterojunctions, coupled with the piezoelectric field, facilitate efficient charge separation and the generation of reactive oxygen species, driving pollutant degradation.

This study highlights the promise of BaTiO₃-based heterostructure nanocomposites as efficient, stable, and versatile piezocatalysts for simultaneous removal of organic dyes, pharmaceutical residues, and microbial contaminants. The findings provide valuable insights into the rational design of multifunctional nanomaterials for wastewater treatment and environmental sustainability.

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Keywords: BaTiO₃, MoS₂, CuO, ultrasound, piezocatalysis, emerging pollutants

Synergistic Spin Polarization and Catalytic Enhancement in Transition Metal Oxide Under Magnetic Bias

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Spin-polarized catalysis has emerged as a transformative approach in heterogeneous catalysis by leveraging the spin degree of freedom of electrons to control reaction pathways and improve efficiency. In this context, transition metal oxides (TMOs) like titanium dioxide (TiO₂) offer a promising strategy to induce spin polarization and tailor the catalytic properties of this wide-bandgap semiconductor. Additionally, we explore the spin-dependent catalytic behavior of Co/N co-doped TiO₂, focusing on its impact on redox reactions such as the oxygen evolution reaction (OER). Density functional theory (DFT) calculations and experimental evidence suggest that Co/N incorporation introduces localized magnetic moments and modifies the electronic band structure, thereby generating spin-polarized states near the Fermi level. These states enhance the adsorption and activation of spin-sensitive reactants, such as OH⁻ and H⁺, facilitating selective reaction kinetics.

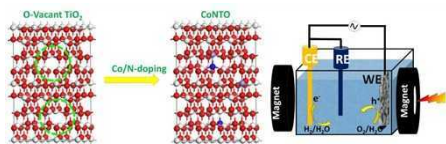


Figure 15: Structural representation of Oxygen vacancy in TiO₂ and Co/N co-doped TiO₂ with schematic representation of magneto-photo-electrocatalysis using CoNTO.

Furthermore, the synergy between the d-orbital electrons of Co and the TiO₂ lattice leads to a modulation in surface charge distribution, resulting in improved charge carrier separation and suppressed recombination. Our find-

ings demonstrate that Co/N-doped TiO₂ is a viable platform for spin-polarized catalysis under an external magnetic field, opening new pathways for designing next-generation energy conversion and environmental remediation catalysts with enhanced activity and selectivity.

Keywords:

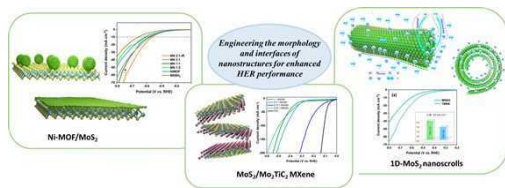
Tailoring 2D nanostructures: Strategies for enhanced electrocatalytic hydrogen production

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Escalating climate crisis and environmental damage caused by fossil fuel dependence surge the need for sustainable energy solutions. Electrocatalytic Hydrogen Evolution Reactions (HER) through water splitting present a compelling alternative, generating H₂ fuel with minimal environmental footprint. The combination of diverse surface properties, unique electronic configurations, and exceptional electrical conductivity makes 2D nanomaterials and their heterostructures particularly attractive candidates for electrocatalytic HER. In recent years, there has been a surge in research exploring metal-free 2D materials, TMDs like MoS₂, and MXenes for their application in HER[1]. Engineering of morphology and interfaces has shown significant impact in fine-tuning the catalytic properties of these materials. Linking NiMOF directly to covalently functionalized defect-rich MoS₂ nanosheets through aminophenyl linkages preserves their substantial surface area and active sites for hydrogen atom adsorption during electrocatalysis, resulting in superior hydrogen production compared to solely functionalized MoS₂ nanosheets[2]. Furthermore, inducing a reversible morphology transition from nanosheets to nanoscrolls via non-covalent interactions between MoS₂ nanosheets and phenothiazine-based organic dye demonstrates a lower overpotential, with a Tafel slope of 141 mV dec⁻¹[3].



Interestingly, the controlled growth of MoS₂ over Mo₂TiC₂ MXene yielded 48 mL of H₂ h⁻¹ cm⁻² of the loaded catalyst with a low Tafel slope of 62 mV dec⁻¹ (comparable to Pt/C with 38 mV dec⁻¹ under similar conditions) and good stability. Hence, targeted manipulation of morphology or interfaces emerges as a potent strategy for unlocking the full potential of electrocatalysts to enhance their HER performance.

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Keywords: Hydrogen production, MoS₂ hybrids, Water splitting, Electrocatalysts

UV absorption and photocatalytic properties of graphitic-carbon coated 8 mole% yttria-stabilized zirconia nanoplatelets

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Nanoparticles (NPs) of 8 mole% yttria-stabilized zirconia (8YSZ) in the form of thin platelets were synthesized by a simple chemical process. The process facilitated the growth of a thin layer of graphitic carbon on the surface of the NPs. The structural properties of the samples were studied using X-ray diffraction, high-resolution transmission electron microscopy, and Raman analysis. The optical properties were analyzed using UV-visible spectroscopy and photoluminescence studies. The graphitic-carbon-coated 8YSZ NPs exhibited excellent UV absorption properties, making them suitable for

the photocatalytic mineralization of pollutants. A detailed analysis of the photocatalytic performance of the samples was carried out using various organic dyes.

Keywords: Yttria-stabilized zirconia; Graphitic-carbon; UV absorption; Photocatalysis.

Next-Generation Semiconductor Heterostructures in Solar Fuel Production: Unveiling Trends and Underlying Mechanisms

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Photocatalytic water splitting (PWS) is a solar-driven approach to hydrogen generation from water.[1] Despite its considerable potential, the widespread application of PEC water splitting remains hindered by limitations such as low efficiency, which arises from charge carrier recombination, and sluggish reaction kinetics. The integration of cocatalyst decoration with complementary enhancement strategies has shown promise in overcoming these challenges, offering improved efficiency and stability. A promising class of next-generation photocatalysts, conjugated polymer nanostructures (CPNs), exhibit a distinctive capacity to hybridize with other nanomaterials to form heterostructures.[2,3] Notably, femtosecond transient absorption spectroscopy has revealed that the incorporation of metal oxide and polymer nanostructures substantially enhances the separation and transfer of photoinduced charge carriers.[3] For instance, embedding polypyrrole (PPy) nanofibers within Bi₂WO₆ has been shown to markedly increase conductivity and catalytic performance, while maintaining activity through multiple operational cycles. In another example, the integration of Cu₂SnS₃ quantum dots with BiOX forms an interfacial Bi-S chemical bond, which acts as a charge migration centre, creating an internal electric field at the interface that can effectively enhance photocatalytic H₂ evolution.[4] Very recently, atomic-scale interface engineering and built-in electric fields at S-scheme

Bi₂WO₆/ZnIn₂S₄ heterojunctions have demonstrated further advances for photocatalytic hydrogen evolution.[5] Furthermore, an indigenous prototype device incorporating a photocatalyst layer within a photochemical reactor has been developed, underscoring practical advancements in this field. A deeper understanding of the photoelectrochemical behavior of emerging carbon-based nanostructures, along with elucidation of their underlying mechanisms and associated challenges, holds significant potential for scaling up solar fuel production technologies.

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Keywords: Conjugated polymer nanostructures, Heterostructures, Surface engineering, S-scheme heterojunction, Photocatalytic water splitting.

Investigation of Hydrogen Evolution Reaction in Two-Dimensional Transition Metal Dichalcogenides Through Experimental, Theoretical DFT and Machine Learning Approach

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Two-Dimensional (2D) materials are class of layered materials (graphene, black phosphorous, h-BN, TMDs, MXene, etc.), have been widely studied for various applications due to interesting structural, physical and chemical properties. TMDs have the general formula MX₂ (where M = transition metal and X = chalcogen S, Se, Te) and exhibit electrocatalyst and photocatalyst behaviour for hydrogen evolution in water splitting. The current work discusses hydrogen evolution reaction (HER) of synthesized MoS₂, WS₂ samples by both wet-chemical and CVD methods. In addition, sample structural characterization of PXRD, morphological studies of SEM and TEM are reported. Electrochemical studies of linear sweep voltammetry, cyclic voltammetry and Tafel slope are measured and show an overpotential 260 mV at a current density 10 mA cm⁻¹[1]. Further theoretical DFT simulation carried out for structural, electronic and catalytic properties. Particularly, DFT focuses on hydrogen adsorption ΔG calculation for single (exclusively 2H and 1T) phase and mixed phase (combination of 2H and 1T). To improve the catalytic efficiency of HER of TMD, we propose the screening of process parameters by machine learning model[2]. Overall, these findings address combinatory studies of experimental, theoretical and ML about TMDs for HER applications, making it suitable for energy production.

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Keywords: 2D, TMD, DFT, ML.

Development and Characterization of Y-rich Zr–2.5Nb Alloys for Hydrogen Gettering Applications

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Zirconium alloys are prone to hydrogen embrittlement due to hydride formation under service conditions. Yttrium, with its strong affinity for hydrogen, offers a potential solution through gettering [1]. In this study, Y-rich Zr–2.5Nb alloys containing 50–70 wt% Y were developed and evaluated for their microstructural characteristics, mechanical properties, and hydrogen absorption behavior.

The alloys were prepared by arc melting and characterized using scanning electron microscopy, energy-dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD). A eutectic-like microstructure was observed, consisting of alternating Y-rich and Zr-rich regions. The 50Y alloy exhibited prominent dendritic features, while finer structures were seen at higher Y contents. Phase analysis confirmed the presence of α -Zr, β -Zr, and α -Y phases. Precipitates within Zr-rich regions were notably present in the 50Y alloy. Microhardness testing revealed a decreasing trend with increasing yttrium content. Hydrogen charging experiments were conducted to evaluate the alloys' getter performance. Interestingly, no hydride formation was observed at the SEM scale in any of the alloys, indicating effective hydrogen absorption and suppression of hydride precipitation.

To assess deformation behavior, one composition was subjected to room temperature rolling followed by recrystallization. In addition, a Y-rich alloy (50Y) was successfully welded with Zr–2.5Nb, enabling a bonded configuration for future H-gettering studies. Overall, the results establish Y-rich Zr–Nb alloys as promising candidates for hydride mitigation in zirconium-based systems.

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Keywords: Yttrium, Hydrogen gettering, Zr–Nb alloys, Hydride embrittlement.

Field driven orbital Hall conductivity in time reversal symmetry broken Weyl semimetals

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We present the theoretical study of orbital Hall conductivity in three-dimensional Weyl semimetals with broken time reversal symmetry. By employing the quantum kinetic approach, we explore the role of the Fermi surface and the Fermi sea contributions to the total orbital Hall conductivity. Our findings demonstrate that the dynamics of the field-driven orbital Hall response to an oscillating electric field depend on the blend of interband and intraband components of the orbital Hall current and the density matrix. We observe that the orbital Hall conductivity can be tuned with the Weyl nodes separation, Fermi energy, and applied frequency. Here, the intraband part contributes more around zero Fermi energy to the net orbital Hall response, while the interband part dominates over the intraband part as the Fermi energy increases. We support our findings by providing numerical estimation and experimental significance in the advancement of orbitronics devices.

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Keywords: Quantum materials, Orbital Hall effect, Quantum kinetic approach, Weyl semimetal.

Improved Tribo-performance of MoS₂ functionalized MWCNTs hybrid reinforced epoxy composites for severe erosion conditions

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Development of advanced polymer nanocomposites for severe erosion conditions is growing as a major thrust for structural elements in aircraft, marine and wind turbine blades. A novel hybrid nanofiller of molybdenum disulphide (MoS₂) functionalized MWCNTs have been synthesized by hydrothermal techniques.

Epoxy/MoS₂/MWCNTs nanocomposites with varying MoS₂/MWCNTs ratios were developed and tested for mechanical behaviour and solid particle erosion (SPE). Epoxy/MoS₂/MWCNTs nanocomposite showed low erosion rate of 471 mg/Kg and 132 mg/Kg at 15° and 90° impact angles, whereas epoxy/MWCNTs nanocomposite showed high erosion rate of 548 mg/Kg and 300 mg/Kg at 15° and 90° impact angles respectively. The erosion mechanism were analyzed using erosion efficiency parameter (η) and FE-SEM analysis.

Keywords: Nanocomposite, Molybdenum disulphide, MWCNTs, Solid particle erosion.

remained largely unexplored. In this context, we report the epitaxial heterostructure of cubic PbSe with two differently faceted orthorhombic CsPbBr₃ nanocrystals, synthesized via the classical heteronucleation approach in which chalcogenide PbSe grows on CsPbBr₃ perovskite nanostructures. Ultrafast transient absorption measurements reveal the facet-dependent charge carrier dynamics of these two differently shaped CsPbBr₃-PbSe heterostructures in comparison with pristine CsPbBr₃. As these nanostructures represent the first demonstration of epitaxial chalcogenide growth on halide perovskites, the findings are expected to open new pathways for designing next-generation heterostructures and for probing their charge carrier dynamics.

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Keywords: Epitaxial Heterostructure, Charge carrier dynamics.

Ultrafast Charge Carrier Dynamics in CsPbBr₃-PbSe Epitaxial Nanocrystal Heterostructures

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Lead halide perovskite-chalcogenide heterostructures that integrate both ionic and covalent interface bonding represent promising materials for achieving enhanced surface stability and superior photoresponsivity in emerging perovskite nanocrystals. However, despite considerable progress in the development of halide perovskite nanocrystals, their epitaxial heterostructures and the excited-state dynamics associated with appropriate chalcogenide counterparts have

Symposium: D

A Smart Clay Biosensor: Luminescent Clays for On-Site Phosphate Detection

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This research introduces a novel, cost-effective, and highly sensitive platform for the rapid detection of phosphate in aqueous environments, a critical need given the threat of eutrophication. The sensing material is a hybrid nanocomposite formed by the successful intercalation of europium(III) bipyridine complexes into the interlayer spaces of a clay mineral. This synthetic approach leverages the unique properties of both components: the high surface area and structural stability of the clay matrix and the distinct luminescent properties of the europium complex.

The intercalation of the europium(III) bipyridine complex was confirmed through a combination of techniques, including X-ray diffraction (XRD), which showed an expansion of the clay's basal spacing, and luminescence spectroscopy, which verified the complex's characteristic emission. The core mechanism for phosphate detection relies on the luminescence quenching of the europium complex. In the presence of phosphate ions, the complex's strong emission is significantly reduced, with the quenching efficiency directly proportional to the phosphate concentration.

Batch experiments were conducted to evaluate the sensor's performance. The results demonstrate an excellent selectivity for phosphate over other common anions, a rapid response time and a remarkably low detection limit, which is well below the concentration levels that trigger eutrophication. The clay-based host matrix prevents the leaching of the active europium complex, ensuring the sensor's long-term stability and reusability over multiple cycles. These findings suggest that this hybrid clay-complex material is a promising and practical tool for real-time, onsite environmental monitoring, providing a sustainable solution for effective water quality management.

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Keywords:

Rapid detection of Punica granatum juice adulteration via Eco-friendly AgNPs synthesised from Zingiber officinale

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Silver nanoparticles synthesis using the extract of the rhizome of Zingiber officinale and characterizing their properties using optical spectroscopic techniques like ultraviolet-visible, infrared, and Raman spectroscopy measurements. 0.1 mM silver nitrate solution was mixed with the extract of the rhizome of Zingiber officinale in double-distilled water and stirred continuously for thirty minutes. The resultant mixture was centrifuged, and the obtained residue was washed continuously with distilled water and dried at 60 °C in a hot air oven. The silver colloidal solution was characterised by optical spectroscopy (UV-VIS, ATR-FTIR, and Raman), X-ray (XRD), and electron microscopy (SEM) techniques. The ultraviolet-visible spectrum of the silver nanoparticles in the spectral region 400-600 nm with a peak at 433 nm due to the surface plasmon resonance band of metallic nanoparticles, which confirms the character of the materials. From the XRD pattern, the average size of the nanoparticles is estimated to be 20 nm. The ATR-FTIR and Raman measurements of the synthesised nanoparticles show that amide, carboxyl, and hydroxyl groups are responsible for reducing silver into its nano form.

Furthermore, the interaction of silver nanoparticles with the fruit juice of *Punica granatum* has also been studied. The addition of synthesised nanoparticles to fruit juice significantly increases the absorbance value of the 511 nm band of Anthocyanins. The Raman spectrum of the fruit juice shows weak bands at 632, 770, 939, 1089, 1103, 1259, and 1454 cm^{-1} corresponding to fructose and pectin. The addition of silver nanoparticles to fruit juice enhances the spectral features of fructose and pectin due to the electromagnetic field enhancement induced by the localised surface plasmon resonance in nanosized metallic materials and chemical enhancement caused by the charge interactions between the probe molecules and metal nanostructures induced by light. These findings highlight the potential application of AgNPs as optical enhancers for detecting purity and chemical adulteration in fruit juices, offering a simple and effective method for food quality analysis.

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Keywords: Silver nanoparticles (AgNPs); *Zingiber officinale*, Green synthesis, UV–Vis spectroscopy, ATR-FTIR; Raman spectroscopy, X-ray diffraction (XRD), Scanning electron microscopy (SEM), Surface plasmon resonance (SPR), Phytochemicals, *Punica granatum*, Fruit juice interaction, Localized surface plasmon resonance (LSPR), Food quality analysis.

Biodegradable Radiopaque Microbeads for Trans-Arterial Chemoembolization for Hepatocellular Carcinoma

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Hepatocellular carcinoma (HCC) is the fourth leading cause of cancer-related mortality worldwide, with transarterial chemoembolization (TACE) serving as a key therapeutic approach when curative options are not feasible. Conventional drug-eluting bead TACE (DEB-TACE) sustains local drug release but often results in permanent embolization, leading to compromised liver function upon repeated use. This study reports the development of 2,3,5-triiodobenzoic acid (TIBA)-conjugated zein-based microbeads as radiopaque embolic agents for TACE. TIBA was conjugated to zein via amide linkage, and microbeads were fabricated using a precipitation method. Fourier Transform Infrared (FTIR) spectroscopy confirmed conjugation, with the OH stretching peak at 3500 cm^{-1} and a shift of the zein amide band from 1600 cm^{-1} to 1545 cm^{-1} . Particle size analysis revealed a reduction from 562.73 ± 3.63 nm for bare zein microparticles to 450.43 ± 6.63 nm for zein-TIBA microbeads, attributed to increased hydrophobicity. The zeta potential decreased from $+14.5 \pm 0.16$ mV to $+9.28 \pm 0.19$ mV following conjugation. Importantly, zein-TIBA microbeads exhibited X-ray visibility, confirming their potential as dual-functional embolic agents with radiopacity and drug-loading capability for improved TACE applications.

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Keywords: chemoembolisation, drug eluting, microbeads, biodegradable polymers

DMSO-Free Tin Perovskites Solar Cells

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Dimethyl sulfoxide (DMSO) is a widely used solvent for processing perovskite solar cells (PSCs). Although it regulates the crystallisation dynamics, it also induces several detrimental effects, such as catalysing the deprotonation of A-site cations, promoting interfacial void formation, and facilitating iodine extraction from the perovskite film, eventually leading to device degradation. Besides, it oxidises Sn^{2+} to Sn^{4+} , which results in self p-doping, limiting the performance of tin-PSCs [?, ?]. Therefore, a DMSO-free processing route is crucial for efficient tin-PSCs. Previously, we have demonstrated an alternative solvent system, a mixture of DEF (N,N-Diethylformamide) and DMPU (N,N'-Dimethylpropyleneurea) for tin-PSC fabrication, which can completely suppress the Sn^{2+} oxidation. Recently, by using a pyridinium additive, we improved the crystallisation dynamics and achieved a PCE of 9.5%. Later, the introduction of an n-dopant, DMBI, has shown excellent improvement compared to the reference devices, demonstrating a PCE of 9.7%. Further, by employing a unique interface diffusion strategy, where bulky PEA^+ cations from the bottom interface of perovskite diffuse into the bulk during film formation, we have achieved a PCE of 10.4%. Recently, we achieved a PCE of 10.7% by substituting formamidinium with methylammonium cation, which suppresses lone-pair expression and enhances the efficiency and stability of tin-PSCs.

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Keywords: Tin perovskite, DMSO-free, Perovskite solar cells

Direct 3D-Printed Aligners: Integrating Material Science and Digital Orthodontics for Next-Generation

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The convergence of material science and digital dentistry has enabled the emergence of direct 3D-printed aligners (DPAs)—a transformative approach that bypasses conventional thermoforming and model-based workflows. This study from AIIMS, New Delhi, presents the first clinical evaluation of in-house fabricated DPAs for mild-to-moderate malocclusions using biocompatible aliphatic vinyl ester–urethane photopolymers. Comparative analysis with fixed labial appliances demonstrated equivalent post-treatment finishing standards (ABO-OGS median: DPA 11.5, FA 10.2) and shorter, though not statistically significant, treatment duration. Patients reported enhanced comfort and satisfaction, with no adverse biological responses, validating the safety and feasibility of the technology.

The success of DPAs highlights a growing need for cross-disciplinary collaboration to optimize resin chemistry, print accuracy, and post-curing environments—particularly nitrogen-rich photopolymerization systems—to achieve improved mechanical performance and clinical reliability. The AIIMS research group invites collaboration with material scientists, polymer chemists, and additive manufacturing experts to co-develop next-generation 3D printable aligner materials and scalable clinical workflows that merge biofunctionality with manufacturing precision.

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Keywords: Photopolymer Resin, Direct 3D Printing, Clear Aligner Materials, Additive Manufacturing Collaboration.

Fabrication of Gd-doped In_2S_3 thin films prepared by nebulised spray pyrolysis for photodetector applications

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Indium sulfide (In_2S_3) is an attractive semiconductor widely employed in ultraviolet (UV) photodetectors. In this study, we report the fabrication of gadolinium (Gd)-doped In_2S_3 thin films using the nebulized spray pyrolysis (NSP) technique and their use for UV detection. X-ray diffraction (XRD) analysis confirms the formation of the cubic $\beta\text{-In}_2\text{S}_3$ phase with a polycrystalline structure. Ultraviolet–visible (UV–Vis) spectroscopy reveals an enhanced UV absorption coefficient upon Gd doping. Photoluminescence (PL) spectra indicate the presence of oxygen (V_O), sulfide (V_S), and indium vacancies (V_In). X-ray photoelectron spectroscopy (XPS) further confirms the presence of In, S, and Gd, along with vacancy-related states such as V_O and V_S , sulfate ions SO_4^{2-} , hydroxyl ions ($-\text{OH}$), as well as secondary phases including $\text{Gd}_2\text{O}_2\text{S}$, $\text{Gd}_2\text{O}_2\text{S}_3$, and Gd_2O_3 . Photodetector measurements demonstrate that $\text{In}_2\text{S}_3\text{:Gd}(1\%)$ exhibits excellent performance, achieving a responsivity of 35.2×10^{-2} A/W, an external quantum efficiency (EQE) of 82.1%, and a detectivity of 33.8×10^{10} Jones. The device also shows outstanding operational stability over 25 repeated cycles and fast temporal response with rise and decay times of 0.53 s and 0.50 s, respectively.

Keywords: Gd-doped In_2S_3 , Indium sulfide thin films, pyrolysis, Rare-earth doping, Photodetectors.

clearance and short intra-periodontal retention. This research presents the development of a chlorhexidine-loaded, polymer-based electrospun scaffold engineered as a sustained-release local drug-delivery system for periodontitis. Biocompatible polymers were electrospun into nanofibrous matrices incorporating chlorhexidine digluconate, achieving high drug-entrapment efficiency and uniform fibre morphology. In vitro release studies demonstrated a controlled, prolonged elution profile suitable for maintaining therapeutic concentrations within periodontal pockets. Antimicrobial assays confirmed significant inhibition of bacteria, while cytocompatibility testing indicated favourable cellular responses. This research work highlights the potential of electrospun chlorhexidine scaffolds as an advanced adjunctive therapy capable of enhancing antimicrobial efficacy, reducing dosing frequency, and improving clinical outcomes in the management of chronic periodontitis.

Keywords: Chlorhexidine, Periodontal therapy, Electrospun scaffold, Local drug delivery.

Symposium: E

Chlorhexidine polymer-based electrospun local drug delivery scaffold for treating periodontitis

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Chlorhexidine remains one of the most effective antimicrobial agents in periodontal therapy, yet its clinical utility is limited by rapid

***Operando* probing of functional surfaces towards real-time monitoring of surface-analyte hybridization routes**

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Surface catalytic processes usually proceed via complex electron-exchange mechanisms between analyte-surface adsorbates, which eventually help identify the rate determining step (RDS) of a catalytic/sensing mechanism as well as the functionality of a material.[1] The synergistic overlap of spin-unquenched molecular orbitals and their intrinsic degeneracies explicitly influence the transient redox reactions.[1] However, such a mechanistic understanding, based primarily on experimental procedures, is largely lacking in both fields of surface science and materials chemistry. Our work address above issues employing multi- technique quasi-operando and operando spectroscopic approaches in two major class of functional materials: 2D and 3D. Quasi-operando Raman and photoluminescence (PL) spectroscopies have been applied on NO₂ chemisorbed few-layered MnPS₃ surfaces embedded with Sb single atoms (SAs).[2] A PL red shift of 0.2 eV indicated formation of shallow states closer to valence band maxima, supported by calculated Hirshfield charge transfer (NO₂ reduction) of 0.12e.[2] Under optimized conditions of humidity and electric field, the polarity responsive composition showed NH₃ generation at a rate of 4700 $\mu\text{mol g}^{-1} \text{h}^{-1}$. [2] Combined with DFT+U calculations, the possible reaction routes leading to surface hybridizations and NO₂ $\rightarrow$ NH₃ conversion was deciphered. Experimental evidence into existence of similar quasi-hybrid quantum states was investigated using an advanced approach of polarized operando Raman measurements on Au@CuO nanohybrids, under first-order perturbative conditions. Based on the significant 14–25% decrease in intensity of emitted polar signal, a real-time monitoring of surface-active species-polarity resolved degeneracy broken analyte (NO₂) hybrid states was achieved.[3] Above understanding further helped into development of strategically designed catalytic surfaces, exploring new mechanistic routes

towards NO₂ sensing and reduction reaction processes.

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Keywords: operando spectroscopy; surface-analyte hybridization; van der Waals materials; heterogeneous catalysis

Symposium: F

Laser ablation Synthesis for High Entropy Alloy Nanoparticle

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The rapid development of high-entropy alloy (HEA) nanoparticles (NPs) is transforming both fundamental materials science and applications in catalysis, energy conversion, and advanced coatings. Despite their remarkable properties, controlling phase composition, crystallinity, and elemental distribution within HEA NPs remains a significant materials challenge. This work presents a comprehensive investigation of non-equiatomic HEA NPs synthesized and structurally modulated using sequential laser-based techniques, highlighting new mechanisms in phase evolution and nanoparticle engineering.

We first demonstrate the synthesis of Al-rich non-equiatomic HEA NPs by ablating $\text{Al}_{40}(\text{SiCrMnFeNiCu})_{60}$ (at%) targets in deionized water using a nanosecond laser. The resulting NPs retained the complex composition and displayed B2-type AlFe and Cr_5Si_3 phases, mirroring the bulk alloy structure. Subsequent laser processing with a 532 nm source induces cyclic reheating, promoting compositional and structural reorganization at the nanoscale revealed the emergence of Cu-Ni nanoprecipitates.

In parallel, FeMnNiAlSiC HEA NPs were synthesized via picosecond laser ablation in burst mode and processed using nanosecond laser pulses. The initial PLAL step produced NPs with a diverse set of structural phases, including B2-type (Al-Fe and Al-Ni), γ -brass-type, Fe_5Si_3 , and BCC phases, as observed via structural analysis. Morphological analysis identified phase-dependent size and structure: larger particles were enriched in B2-type phases, while smaller NPs favored γ -brass and Fe_5Si_3 . The nanosecond laser processing drove profound morphological transitions, including the formation of hollow and core-shell-like nanoscale structures and an overall enhancement in crystallinity.

Extending this work, comparative studies on two non-equiatomic HEA systems, namely, FeMnNiAlCrSiC (HEA-Cr) and FeMnNiAlTiSiC (HEA-Ti), revealed how compositional design influences phase behavior.

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Keywords: Laser Ablation, Laser Processing, Nanoparticle, High-Entropy Alloys

Effects of doping and nanostructuring on magnetic and thermoelectric properties of multicomponent alloys

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We explored thermoelectric properties of an aluminium-copper-iron quasicrystal (QC) nanocomposite with soft tin (Sn) phase reinforcement, revealing enhanced electrical and thermal transport properties upon annealing. The ratio of electrical and thermal conductivity for annealed QC (with 20% Sn) was found to be the highest ($\sigma/\kappa \sim 4704 \text{ SK/W}$). Owing to changes in the crystallite size, magnetic anisotropy and number of moments were also refined [1,2]. At low temperatures, these QC present weak ferromagnetic interactions.

Further, research was conducted to understand how milling intensity affect the structure, morphology, magnetic, and thermoelectric properties of non-equiatomic nanostructured AlSiCrMnFeNiCu high entropy alloy (HEA) powders, which were produced by cryomilling. These powders, cryomilled at varying ball-to-powder ratios (BPR), exhibited a dual-phase structure with a dominant B2-type phase and a minor Cr_5Si_3 -type phase. An increase in BPR resulted in more refined crystallite size, grain size, and particle size, along with reduction in the phase fraction of the minor Cr_5Si_3 -type phase. Magnetic measurements at room temperature indicated that increase in BPR leads to a shift from multi-domain to single-domain behavior, thereby enhancing soft magnetic properties. Thermal variation of magnetization led to magnetic phase transitions, which also varied

with increasing BPR. Additionally, a change in charge carrier type from p-type to n-type was observed as grain size decreased. The figure of merit decreased from 2×10^{-5} for as-cast powders to the lowest value in the smallest grain-sized sample, primarily due to reduced electrical conductivity [3]. This work demonstrates the potential for developing non-equiatom, low-density QCs and HEAs with customizable functional properties, providing flexibility in material design for magneto-thermoelectric applications [4].

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Keywords: Laser Ablation, Laser Processing, Nanoparticle, High-Entropy Alloys

Materials selection and properties: Tailoring EMI shielding efficiency of polymer composites

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Electromagnetic waves within the microwave frequency spectrum (2–18 GHz) are vital for modern communication and electronic systems [1]. However, their interaction with various materials and living organisms can induce significant adverse effects. Electromagnetic interference (EMI) originating from diverse devices hampers performance and data transmission.

Furthermore, EMI presents health risks to humans owing to prolonged exposure. Metals, due to their inherently low skin depth, are traditionally utilized as effective EMI shields. However, their high density, susceptibility to corrosion, cost, and limited flexibility render them less appropriate for modern lightweight, portable, and flexible devices. Consequently, there is an increasing interest in developing lightweight, cost-efficient, and shape-adaptable porous materials as viable alternatives for EMI shielding.

Polymers and their composites are an ideal choice in this scenario. However, except for a few conducting polymers, most of them are dielectric and lack EMI shielding ability. However, these polymers, when processed with various fillers, can aid in EMI shielding. Thus, a wide variety of fillers, including conducting (carbon-based, MXenes), dielectric (perovskites, metal oxides), and magnetic fillers (spinel ferrites), are widely used [2,3,4]. In this work, the effect of various filler types on the EMI shielding efficiency will be discussed. The impact of conducting filler (graphene) addition on the percolation threshold, concentration of magnetic fillers (nickel ferrite and cobalt ferrite), on the magnetic properties, and EMI shielding efficiency will be addressed using epoxy resin as the matrix. Various loss mechanisms induced by the individual fillers will be discussed.

In addition to epoxy-based composites, porous foam structures such as PU foams are being explored lately due to their reusability as EMI shields [5]. A fourfold enhancement is obtained in the frequency range of 8.2 to 12.4 GHz (X-band) compared to pristine PU foam by decorating PU foams with conducting polymer/TiO₂/Ti₃C₂T_x composites. .

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Keywords: Electromagnetic interference shielding, loss mechanism, polymer composite

Symposium: G

Novel Processes for Development of Rare Earth Free Nanoscale Magnetic Materials with Tailored Morphologies for Permanent Magnets

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Permanent magnets are key components in many sectors viz. transport (electric vehicles), renewable energy generation (wind turbine) and energy storage (flywheel), which have immense importance in the strategic areas like space & defence for self-reliance. These magnets are largely fabricated from rare earth elements (REE) e.g. NdFeB or SmCo, which are critical resources whose production and distribution is largely controlled by China. Therefore, it is imperative to develop magnets without critical REE and hard hexaferrites like strontium hexaferrite ($\text{SrFe}_{12}\text{O}_{19}$ or SFO) are promising alternative to such magnets. However, SFO exhibits low figure of merit $(\text{BH})_{\text{max}}$ having values 40–44 kJm^{-3} compared to REE magnets having values more than 200 kJm^{-3} . On the contrary, many of the applications require $(\text{BH})_{\text{max}}$ value between 50–70 kJm^{-3} . Hence, for SFO an enhancement of 20% of $(\text{BH})_{\text{max}}$ is reasonable to replace REE magnets. The composition and morphology plays an important role in deciding the magnetic properties. Through tailoring the morphology or the composition, it is possible to modify the magnetic anisotropy and hence tune the coercivity or magnetization to improve $(\text{BH})_{\text{max}}$. Here, we present two alternate approaches that show enhanced magnetic properties through novel and scalable processes.

In the first approach, we have fabricated nanofibers of SFO in PVP polymer by electrospinning techniques followed by high temperature annealing to create anisotropic morphologies with enhanced coercivity and magnetization. The morphology was tailored by simple variation in the annealing temperature and heating rate that resulted in anisotropic chains of interconnected SFO nanoparticles (shown in Figure 1). The improvements are attributed to morphology-induced magnetic anisotropy with particle sizes below the single domain size.

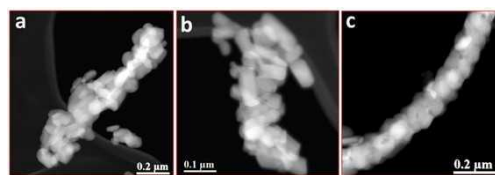


Figure 16: Scanning transmission electron microscopy (STEM) - High angle annular dark field (HAADF) imaging of the SFO nanofiber calcined at 800 °C with heating rate (a) 2 °C/min, (b) 5 °C/min, and (c) 10 °C/min.

In the second approach, the morphology and magnetic properties are tailored using triple cation substitutions (Sr by Ca and Fe by Al & Mn) in the lattice that resulted into platelet shape morphology and exhibited significant improvement of coercivity of the order of 9.13 kOe compared to 5.5 kOe for pure SFO with reasonable saturation magnetization and remanence. In conclusion, the advantages and limitations with the processes and the materials will be discussed followed by the future challenges in our approach.

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Keywords: Rare earth free permanent magnets, Morphology, Magnetic Anisotropy, Strontium Hexaferrites

Sustainable Solutions for Next-Generation Electronics: The Role of E-Waste Recycling

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The recycling of rare earth elements (REEs) from electronic waste (e-waste) and their integration into thin-film transistors (TFTs), photodetectors, and memristors offers a sustainable pathway for enhancing next-generation, cost-effective electronics. The current study targets two key objectives: first, developing advanced techniques for recovering high-purity rare earth

oxides (REOs) from e-waste; second, leveraging these reclaimed REOs as dielectric materials or alloyed semiconductors in optoelectronic devices, with a primary focus on transistors (switching device). TFTs comprise multiple layers, each utilizing distinct electronic materials, including REOs, to enhance device performance and efficiency. This approach not only promotes resource sustainability but also improves the overall efficiency of future electronic components. The development of indigenous electronic components using critical raw materials sourced from e-waste advances the country's technological self-reliance. Key materials, such as rare earth metals, will be extracted from e-waste sources, including fluorescent lamps (FLs), and LEDs. Elements such as Y, Eu, La, Tb, and Ce will be recovered through an alkali roasting process that utilizes cost-effective fluxes to break down phosphor phases into water-insoluble rare-earth hydroxides. The method of developing a solution-processed amorphous indium–zinc–tin oxide (a-IZTO) TFT using a water-based yttrium oxide (Y_2O_3) passivation layer significantly improves the stability of the IZTO TFT. Thus, many rare earth metals form strong bonds with oxygen and play a vital role as protective layers for semiconductors in electronic devices. Our approach to utilizing recovered REOs shows great potential for next-generation electronics. Ultimately, the study aims to scale these processes for industrial applications, thereby promoting sustainable electronics manufacturing.

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Keywords: Rare earth oxides; REEs; E-waste; LEDs

Effect of Carbonate Substitution on Radiation Stability of Fluorapatites

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The safe disposal of high-level nuclear waste demands host materials that can retain structural and chemical stability over geological timescales under radiation-rich conditions. Fluorapatite ($\text{Ca}_5(\text{PO}_4)_3\text{F}$), has emerged as a promising waste form, particularly for immobilizing fission products from molten salt reactors, owing to its ability to accommodate various elemental substitutions [1].

Among the various substitutions commonly found in natural fluorapatite, carbonate substitution (both A-type and B-type) is of particular interest [2]. Carbonate incorporation into the fluorapatite lattice alters the local bonding environment and introduces structural disorder, potentially affecting the material's response to radiation-induced damage. It is frequently encountered in natural settings, especially in apatites associated with carbonate-rich backfill materials, groundwater, and geochemical environments relevant to deep geological repositories. The nature and extent of anionic and cationic substitutions, particularly carbonate (CO_3^{2-}) at either the phosphate (B-type) or hydroxyl/fluoride (A-type) sites, can significantly influence the radiation response of fluorapatite. Such substitutions may induce lattice strain, affect charge compensation mechanisms, and consequently impact the material's resistance to defect formation under irradiation. While previous studies have explored the thermodynamic stability and chemical durability of carbonate-substituted apatites, limited attention has been paid to their behavior under irradiation. Understanding these effects is critical for assessing the long-term performance of fluorapatite-based waste forms, particularly in the context of self-irradiation resulting from α -decay and β – γ emissions.

In this work, electron beam irradiation is used to simulate radiation effects in both natural and synthetic fluorapatites. Natural fluorapatites having carbonate substitution sourced from West Bengal, India as well as synthetic fluorapatite powders (without any carbonate substitution) prepared by solid state reaction method were irradiated with a 10 MeV electron beam at EBC Kharghar, upto a dose of 20 MGy. FTIR spectroscopy confirms the substitution of carbonate at phosphate site in natural FAp (B-site substitution). The electronic stopping power for FAp was calculated to be $0.52135 \text{ keV}/\mu\text{m}$, indicating dominant energy dissipation via inelastic electron interactions. In contrast, the radiative stopping power ($0.09852 \text{ keV}/\mu\text{m}$), and nuclear stopping power ($2.5073 \times 10^{-5} \text{ keV}/\mu\text{m}$) had negligible contribution. FTIR and Raman spectroscopy of irradiated specimens show a shift in the P–O stretching mode indicating perturbation of the phosphate tetrahedra in both synthetic and natural fluorapatite. In case of natural fluorapatite, carbonate bands exhibited minor signs of radiation-induced alteration attributed to the lower displacement cross section of carbon. These results imply that FAP retains significant vibrational and structural stability under electron irradiation at high doses.

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Keywords: Electron irradiation, Carbonate substitution, Fluorapatite, Radiation stability

Magneto-electrodeposition of Ni-V alloy coatings for better corrosion protection

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Nickel-vanadium (Ni-V) alloy coatings of high corrosion resistance were developed using a modern approach, called magneto-electrodeposition (MED) for protection of mild

steel. Ni-V alloy coatings of varying compositions were developed using magnetic field (B) of different intensity (in terms of magnitude and direction), applied parallel to the process of conventional electroplating. The magnetic field was used as a tool to alter the crystallinity, composition, and hence corrosion resistance of alloy coatings. It was demonstrated that the corrosion resistance of Ni-V alloy coatings can be improved to many folds of its magnitude by MED method. Drastic increase in the corrosion resistance of MED coatings was found to be due to increased Ni content of the alloy coatings, affected due to higher paramagnetic property of Ni^{2+} ions. The reasons responsible for improved corrosion performance of MED (Ni-V) alloy were explained through FESEM, EDX and XRD analyses. Attempt has been made to understand changed properties of MED (Ni-V) alloy coatings in the light of magnetic field-controlled diffusion of Ni^{2+} ions, responsible for increase of its limiting current density (i_L) value. The high corrosion resistance of the MED (Ni-V) alloy coatings was explained in the light of magnetohydrodynamic (MHD) effect. The inherent limitations of the bath associated with regular type of codeposition, which impeded the development of Ni rich alloy coatings has been successfully alleviated using MED method. The experimental study has been with greater insight of both conventional electrodeposition and magneto-electrodeposition, and results are discussed.

Keywords: Ni-V alloy, Magneto-electrodeposition, Corrosion study.

Effect of Ion Irradiation on the Corrosion Resistance Behaviour of SS 304L

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The recovery of U and Pu through the PUREX route uses nitric acid as the processing medium. The reprocessing media contain highly radioactive fission products and emit radiation such as α , β and γ . This radiation can

alter the surface properties, further enhancing the material degradation in an aggressive nitric acid medium. However, mostly reported results for neutron irradiation are available in the literature. As the effects of ion irradiation/implantation to simulate the effect of irradiation on structural materials have not yet been determined, they are the subject of the present investigation.

In this study, protons of different energies (2 MeV and 3 MeV) were implanted on AISI SS304L with coarse-grained (CG) and ultrafine-grained (UFG) microstructures (90% severely plastically deformed at cryo-rolling temperature, $\text{LN}_2 \sim 77 \text{ K}$) separately, at a dose rate/fluence of 10^{16} protons/ m^2/s . The surface morphology, phases, and oxide characteristics were characterized using X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Laser Raman Spectroscopy (LRS). Electrochemical corrosion tests were performed in 11.5 M nitric acid to evaluate corrosion resistance in simulated PUREX reprocessing conditions.

XRD characterisation confirmed no phase changes for either energy level. Peak positions indicated CG austenite and UFG martensite microstructures. SEM images revealed hydrogen bubble formation, with higher bubble density in the 3 MeV irradiated specimens for both CG and UFG conditions. Potentiodynamic polarization tests showed improved corrosion resistance after 2 MeV irradiation, while 3 MeV irradiation resulted in degradation compared with the as-received CG and UFG specimens. These results provide improved understanding of the corrosion behaviour of 304L stainless steel, a key structural material in spent nuclear fuel reprocessing plants.

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Keywords: Stainless Steel, Proton Irradiation, PUREX, Nitric Acid, Corrosion

Controlled Bi-directional Threshold Switching Behaviours for Random Number Generation Applications

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Power-efficient, nanoscale two-terminal memristors with threshold switching (TS) behavior are essential for next-generation non-von Neumann computing systems. In this work, we demonstrate TS behavior in 30 keV Cu-ion implanted TiO_x memristors using conductive atomic force microscopy. Ion implantation at fluences of 10^{16} – 10^{17} ions cm^{-2} increases the oxygen vacancy concentration, enabling bi-directional TS behaviour in nanoscale devices. Higher fluences further promote the formation of a TiO_x –(Cu-O) mixed phase within the implanted region. Based on detailed XPS analysis and local I–V characteristics, we propose an n–n heterojunction model between TiO_x and Cu–O phases to qualitatively explain the significant enhancement in switching performance. Devices implanted at 1×10^{17} ions cm^{-2} exhibit low threshold voltages ($\pm 2.25 \text{ V}$), demonstrating their potential for energy-efficient in-memory computing. Additionally, key switching parameters of these devices show excellent performance in chi-square tests, indicating their suitability as a reliable source of randomness for Random Number Generation (RNG). The combination of a simple device structure and low power consumption makes these TS memristors a promising candidate for addressing the challenges of complex circuit design and high power demands in RNG applications.

Keywords: Ion implantation, oxide mixed phase, threshold switching, and random number generation.

Particle-to-wave-like crossover in thermal transport of materials: A Wigner formulation approach

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The work done in the past century discussed two distinct microscopic mechanisms for heat transport in solids: the particle-like propagation of phonon modes in simple crystals, and wave-like tunneling between pairs of vibrational eigenstates in glasses. The recently introduced Wigner formulation [1] for thermal transport in solids encompasses the emergence and coexistence of the particle-like propagation of phonon wavepackets discussed by Peierls for crystals [2], and the wave-like interband conduction mechanisms discussed by Allen and Feldman for harmonic glasses [3]. The Wigner formulation has shown that particle-like and wave-like heat-conduction mechanisms have a comparable strength when the phonon interband spacings become comparable to the linewidths, the so-called “complex crystal” regime, typical of materials with ultralow or glasslike conductivity. Thus, the Wigner formulation will accurately describe thermal transport in complex crystals and disordered materials. We applied the Wigner formulation to complex rare-earth and alkaline-earth pyrochlores – promising thermal barrier coating materials for turbine blades, power production plants, and nuclear industries [4], such as $\text{La}_2\text{Hf}_2\text{O}_7$, SrZrO_3 , and CaZrO_3 , and discuss the fundamental physics underlying the emergence and coexistence of particle-like and wave-like heat-transport mechanisms. We further extended this and developed a theoretical/computational framework that enables us to accurately predict the macroscopic thermal conductivity of compositionally disordered solids from first principles. Importantly, we show how the Wigner transport equation correctly describes the thermodynamic limit of a compositionally disordered crystal, while the Boltzmann transport equation does not [5].

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Keywords: Thermal transport, Wigner Formulation, Disordered solids, Phonon

Molecular Dynamics Simulation for Predicting the Physical Properties of Cured Hydroxy-Terminated Polybutadiene (HTPB) / Toluene Diisocyanate (TDI) System

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Composite solid propellants (CSP) play an important role in the development of launch vehicles and missile technology. CSPs are multi-component systems, which brings complexity and uncertainty in their property predictions and characterization, further leading to complex quality control checks[1]. Strategizing a suitable combined Molecular Dynamics (MD) simulation and experimental methodology will bring down the number of trials for characterization and quality controlling of various components in the solid propellants, such as hydroxyl-terminated polybutadiene (HTPB), oxidizer, etc. Further, this understanding and the developed models may help to predict the aging of CSP and develop new compositions in advance [2-4]. Seeking to parameterize models for simulating the deflagration of HTPB, we employed full atomistic molecular dynamics (FA-MD) methods for estimating transport and thermophysical properties of HTPB. Estimates for densities, enthalpies of vaporization, and self-diffusion coefficients were derived from simulations of hydroxyl-terminated 6-ethenonyl-2,8,12,16-octadecatetraene (EODT, $\text{C}_{20}\text{H}_{32}$) oligomer systems. The potential to employ the

self-diffusion coefficient predictions as a basis for parameterizing a theorized framework for modeling condensed-phase chemical kinetics is discussed [5]. In addition, we coupled Coarse-Grained MD (CG-MD) and Full Atomistic MD (FA-MD) to estimate the viscosity build-up for the curing mechanism of HTPB with TDI using the Green-Kubo formalism. The enthalpy of formation and viscosity of HTPB estimates at 298 K were also observed to be in reasonable agreement with a recently published aggregation of such values. Heat capacity estimates were in reasonable agreement with reported measured values. The viscosity build-up observed during the curing process between HTPB and TDI is comparable for FA-MD and CG-MD simulations. The theoretically predicted mechanical properties of the cured HTPB/TDI matrix are being evaluated for CSP applications.

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Keywords: Molecular simulations, Propellant; Viscosity, Mechanical Properties

Computational Insights into Biomarker Adsorption on Functionalized $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes for Neurodegenerative Disease Sensing

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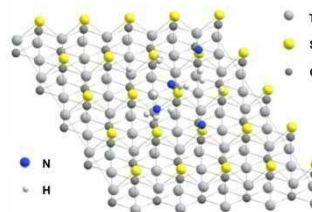
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Two-dimensional MXenes, particularly $\text{Ti}_3\text{C}_2\text{T}_x$ monolayers with tunable surface terminations, have emerged as promising candidates for biosensing applications due to their high surface reactivity, metallic conductivity, and modifiable electronic properties. Their potential for detecting biomarkers associated with neurodegenerative diseases is of growing interest, particularly for point-of-care diagnostics.

In this study, we use first-principles density functional theory (DFT) to explore the interaction mechanisms between surface-functionalized $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes (with $-\text{S}$, $-\text{O}$, $-\text{OH}$, etc.) and neurodegenerative disease-relevant biomarkers, such as ammonia (NH_3), hydrogen sulfide (H_2S), and related small volatile molecules. We focus on evaluating adsorption energies, charge transfer, work function modulation, and electronic structure changes that are key to sensor functionality. We have here calculated for NH_3 adsorption on $\text{Ti}_3\text{C}_2\text{S}$, showing strong adsorption energy and notable shifts in work function and density of states. These results indicate high sensitivity and selective interaction, essential for effective electrochemical detection. The surface sulfur termination plays a critical role in enhancing sensor response. Computational studies on additional biomarkers and alternative surface terminations (e.g., $\text{Ti}_3\text{C}_2\text{O}$, $\text{Ti}_3\text{C}_2(\text{OH})_2$) are in progress to establish a broader understanding of sensor-analyte interactions.

Our findings demonstrate that surface terminations significantly influence sensor selectivity and electronic responsiveness, offering a tunable platform for biomarker detection. This work contributes to the rational design of MXene-based biosensing layers and lays the groundwork for their integration into future neurodegenerative disease diagnostics.[1,2]



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Keywords: MXenes, Gas sensing, Hydrogen sulfide (H₂S) detection, Electrochemical biosensors

Harnessing Ferroelectricity for Multifunctional 2D Materials

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The rapid advancement of artificial intelligence (AI) and the Internet of Things (IoT) has intensified the demand for faster, miniaturized, and energy-efficient technologies, placing new challenges on materials design. Two-dimensional (2D) materials, with their diverse ferroic and spintronic functionalities, have emerged as promising candidates for multifunctional applications. Central to this progress is ferroelectricity, whose coupling with other degrees of freedom can unlock novel device concepts. Using density functional theory (DFT) calculations, we investigate two representative classes of 2D ferroelectrics: multiferroic AlXY

(X = S, Se; Y = Cl, Br, I) monolayers and sliding ferroelectric ZrX₂ (X = Cl, Br, I) bilayers. The AlXY monolayers exhibit robust in-plane ferroelectric polarization (148–177 pC/m) originating from Al displacements driven by a soft phonon mode. Their ferroelectricity couples strongly with ferroelasticity, enabling 90° polarization switching, reversible strain up to 45.1%, and tunable anisotropic mechanical and piezoelectric properties. Complementarily, ZrX₂ bilayers reveal sliding ferroelectricity with low out-of-plane polarization (0.24–0.5 pC/m) and small energy barriers (11–18.8 meV/f.u), suitable for low-power operation. Incorporating spin-orbit coupling, sliding ferroelectric switching induces a layer-polarized spin Hall effect, offering reversible control of spin transport. These results highlight ferroelectricity as a unifying principle driving coupled ferroelastic and spintronic phenomena in 2D materials, establishing AlXY and ZrX₂ as model platforms for multifunctional nanoelectronic, piezotronic, and spintronic applications.

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Keywords: Ferroelectricity, 2D Materials.

Posters

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Optoelectronic properties of ZnO/NiO based Heterostructures

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Zinc Oxide (ZnO) has emerged as one of the most promising wide-bandgap semiconductors due to its low cost, environmental stability, and versatile applications in optoelectronic devices, sensors, transparent conductors, and biomedical technologies. Its relatively high exciton binding energy of 60 meV makes it an ideal candidate for exploring interlayer excitonic interactions in nanostructured heterostructures. In this study, we focus on the synthesis and investigation of ZnO/NiO-based heterostructures fabricated using the RF sputtering technique. NiO, selected for its nearly identical bandgap and excellent chemical stability, serves as an effective partner material to tailor and enhance the optoelectronic properties of ZnO for device-grade applications. The fabricated heterostructures were systematically subjected to post-deposition processes, including thermal annealing and ion implantation with selected ions, in order to induce controlled modifications in their crystallinity, defect states, and carrier dynamics. Both pristine and ion-implanted samples were characterized through a combination of techniques such as Field-Emission Scanning Electron Microscopy (FESEM), UV-Visible spectroscopy, Raman spectroscopy, Photoluminescence (PL), and Atomic Force Microscopy (AFM). These methods enabled a detailed understanding of the correlation between structural changes, defect-

mediated optical transitions, and variations in the excitonic dynamics. The study further analyzes how the optical response and third-order non-linear optical (NLO) behavior of the ZnO/NiO heterostructures evolve after ion implantation. The observed improvements in photoresponse and tunable NLO activity highlight the potential of these heterostructures in advanced optoelectronic devices, particularly those reliant on p-n junction architectures, optical limiters, and photonic switching applications.

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Keywords: Exciton binding energy, Photoluminescence, Non-linear optical properties

Rabi splitting mediated dual electromagnetically induced transparency in a metamaterial

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Equal contribution

Electromagnetically Induced Transparency (EIT) and strong coupling are pivotal phenomena in light-matter interactions with profound implications for quantum and material sciences. EIT, resulting from destructive interference in three-level quantum systems, creates a transparency window within an absorption spectrum [1] and is classically emulated in metamaterials via bright-dark-mode interference. This enables applications such as slow-light devices, sensors, and cloaking technologies. Strong coupling, achieved when the interaction strength between a quantum emitter and an electromagnetic field surpasses system losses, leads to hybridized states (Rabi splitting), facilitating coherent energy exchange and insights into coupling mechanisms [2]. This study combines these phenomena using terahertz metamaterials to achieve tunable transitions between single and dual EIT states through strong coupling. This integration enhances the tunability of metamaterial-based devices and deepens our understanding of EIT and strong coupling, bridging classical and quantum perspectives for future applications.

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Keywords: Terahertz Metamaterials; Strong Coupling; Phonon-Polariton; Electromagnetically Induced Transparency

In recent years, resistive random-access memory (ReRAM) devices have emerged as a prominent subject of research within the field of emerging non-volatile memory technologies, particularly due to their potential applications in high-density storage and in-memory computing. We report controllable resistive switching (RS) properties of gallium oxide (GaO_x)-based devices with an $\text{Ag}/\text{GaO}_x/\text{p}^{++}\text{-Si}$ configuration, fabricated using rf magnetron sputtering. To tailor the RS behavior, the influence of two key factors, namely the growth angle and the thickness of the oxide layer, was systematically investigated. The results reveal that GaO_x -based devices annealed at 850°C for 4 hours exhibit bipolar resistive switching behavior with a significantly higher ON/OFF ratio and improved endurance compared to on-axis grown films. In contrast, multibit operation is observed in both as-grown and annealed samples. Furthermore, the devices demonstrate neuromorphic functionalities such as spike-amplitude-dependent plasticity (SADP), spike-rate-dependent plasticity (SRDP), and paired-pulse facilitation (PPF), indicating their suitability for synaptic learning and memory applications. The observed RS characteristics and tunability of the switching mechanism in both as-grown and annealed films are attributed to stoichiometric modifications in the GaO_x layers. Overall, these findings represent a significant step toward optimizing the performance of gallium oxide-based RS devices, highlighting their potential for implementation in cross-bar array architectures of ReRAM as well as next-generation memory and neuromorphic computing applications.

Keywords: Resistive switching, ReRAM, multibit operation, neuromorphic computing

Influence of thermal annealing on the resistive switching and neuromorphic behaviour of GaO_x -based ReRAM devices

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Study of Charge-transfer(C-T) Electroluminescence in TAPC: TmPyPB Bulk-hetero junction OLEDs

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In recent years, Organic light-emitting diodes (OLEDs) using the intermolecular charge transfer complexes have gained significant attention due to their broad white emission without utilizing multiple emitting layers. Among these, a donor-acceptor complex, like an exciplex or an electropex, is interesting due to

its colour tunability and simple device architecture. TAPC (4,4-cyclohexylidenebis [N, N-bis(4-methylphenyl) aniline]) and TmPyPB (1,3,5-tris(3-pyridyl-3-phenyl) benzene) are widely used as standard hole transporting layer (HTL) and Electron transporting Layer (ETL) in OLED devices, respectively, where their frontier orbital energies help to form C-T complex [1]. In this work, we fabricated bulk-heterojunction (BHJ) OLEDs by co-evaporation of TAPC and TmPyPB in a 1:1 ratio to generate the maximum chances of interaction between acceptor and donor complexes. The device stack comprises ITO anode / HIL / TAPC: TmPyPB BHJ emissive layer / EIL / Al cathode. This design greatly encourages the formation of exciplex and electropex in the BHJ region, leading to a broadband electroluminescent (EL) spectrum. Spectral characterization revealed that the EL spectrum covers almost the entire visible spectrum region, from approximately 400 to 700 nm. The EL-spectrum comprises two distinct areas: high energy emission at 425 nm, the same as photo luminance (PL), and a dominant low energy peak at 595 nm. The 595 nm is absent in the pristine film (TAPC and TmPyPB) and their 1:1 mixture. It was found that the 595 nm peaks result from the field-assisted charge recombination at the TAPC/TmPyPB interface. These findings provide a new insight into the study of charge transfer complexes like exciplex and electropex, and their origin in OLED devices. By directly comparing the EL of BHJ OLED devices and PL of their respective film, we can find out the contribution of each charge transfer complex present in emission, and these BHJ act as a model to study the field-assisted CT recombination. From a practical perspective, our result unveils that a simple BHJ device can produce a broad EL spectrum from 400 nm to 700 nm without introducing a dopant. These established a new approach to develop full-colour tunable OLEDs for the next generation.

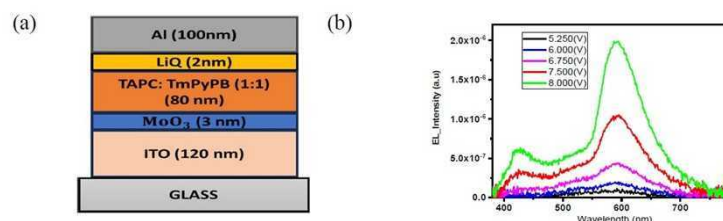


Figure 17: a: Device schematic (ITO/HIL/TAPC: TmPyPB BHJ/EIL/Al) and b: EL spectrum

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Keywords: Bulk heterojunction, Exciplex, Electropex, Charge-transfer emission.

Oxygen-Vacancy-Mediated Z-Scheme Charge Transfer in Mixed-Phase TiO₂@B-Doped g-C₃N₄ Heterojunction for Photocatalytic Degradation of Antibiotics

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In the area of visible-light-driven catalysis, there is a growing interest in designing and developing extremely durable catalysts for both energy generation and environmental mitigation. In this study, a succession of hierarchical mesoporous mixed-phase TiO₂ is fabricated on the surface of B-doped g-C₃N₄ (BCN). Several analytical methods were employed to investigate the physicochemical properties of the as-synthesized materials, including their morphology, optical and electrical characteristics, chemical environment, and crystallinity. According to PXRD and HRTEM data, the best photocatalyst (TBCN-8) mimicked P25 by forming mixed-phase TiO₂ (rutile and anatase) on the BCN surface. The catalytic activity of the as-synthesized materials was evaluated for the degradation of Ciprofloxacin (87% of a 20 ppm CIP solution) under visible-light illumination, which was significantly higher than the neat

components. A reduced electron-hole recombination rate of TBCN-8 was suggested by its larger photocurrent, smaller impedance arc, and lower PL intensity, which clarify the material's optimal catalytic activity. These results confirm the facile creation of a mixed-phase mesoporous TiO₂/BCN heterostructure and its visible-light-driven catalytic activity, governed by synergistic Z-scheme and p-n heterojunction charge-transfer mechanisms.

Keywords: Z-scheme; mixed-phase TiO₂; B-doped g-C₃N₄; ciprofloxacin (CIP).

Plasmonic Electromagnetic Damping by Hofmeister Series: Does It Follow the Electrochemical Order?

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Noble metal nanoparticles, especially gold nanoparticles, are prime model systems for probing ion-surface interactions due to their distinctive localised surface plasmon resonance (LSPR) properties. [1] This work investigates how selected Hofmeister series ions, especially Cl⁻, NO₃⁻, Li⁺, and Mg²⁺, affect plasmonic electromagnetic damping [2,3] of citrate-stabilised gold nanoparticles, and whether these damping trends align with electrochemical ion ordering. [?, ?] We have synthesised 10 nm AuNPs ($\lambda_{\text{max}} \approx 523$ nm) via the Frens citrate reduction method and drop-cast them onto graphite carbon electrodes to form plasmonic microelectrodes. Incremental volumes (25–200 μL) of 1.0 M NaCl, NaNO₃, LiCl, and 0.1 M MgCl₂ were added to a pH 7.4 phosphate buffer. LSPR evolution was monitored via UV-vis spectroscopy, DLS, and zeta potential, while cyclic voltammetry (CV) assessed electrochemical behaviour. UV-vis spectra revealed ion-specific redshifts and full-width-at-half-maximum (FWHM) broadening, significantly enhanced plasmonic damping due to ion adsorption. Cl⁻ and Mg²⁺ induced the largest λ_{max} shifts (up to +20 nm) and strongest broadening, consistent with high charge density and strong surface affinity. Damping constants (Γ) were extracted by Lorentzian peak fitting, and adsorption was modelled via the

Langmuir isotherm, yielding surface coverage (θ), binding constants (K), and binding energies. CV confirmed these optical trends: both anodic ($E_{\text{pa}}, I_{\text{pa}}$) and cathodic ($E_{\text{pc}}, I_{\text{pc}}$) peaks shifted systematically with ion concentration. Cl⁻ and Mg²⁺ exhibited pronounced peak potential shifts and increased current, consistent with strong adsorption. Scan rate studies revealed an adsorption-controlled redox process, especially for multivalent ions. So, the surface coverage was calculated from the CV data as,

$$\theta = \frac{Q}{nFA}$$

A unified correlation was established using the derived equation as,

$$\Gamma = \theta \cdot K \cdot \left(\frac{nF(I_{\text{pa}} + I_{\text{pc}})}{A 2|E|^2} \right)$$

where $|E|^2$ is the plasmonic near-field enhancement (from FEM or simulation). This expression shows that Γ scales with adsorption extent (θ), binding affinity (K), and electrochemical current, integrating LSPR damping with redox behaviour under the influence of the local plasmonic field $|E|^2$. The ion-specific behaviour was ranked as: Cl⁻ > Mg²⁺ > Li⁺ > NO₃⁻. The Cl⁻-exhibited the highest plasmonic damping and binding affinity due to strong specific adsorption and moderate hydration. Mg²⁺, despite strong hydration, caused significant damping via electrostatic binding in the Stern layer. Li⁺ showed moderate damping due to its small size, but a weaker interaction than Mg²⁺. NO₃⁻, a chaotropic ion with low surface affinity, caused minimal damping and electrochemical shifts. Overall, damping trends partially matched classical electrochemical order, with deviations due to ion-specific adsorption, hydration, dielectric changes, and Stern layer effects. This study links plasmonic and electrochemical behaviour, highlighting damping constants as a unified metric for designing ionic-specific plasmonic-electrochemical hybrid sensors.

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Keywords: Gold Nanoparticles, LSPR, Hofmeister Series, Plasmonic Damping

Solvent dependent crystal packing of a F-appended Schiff Base: Non-Linear Optical property and selective cation detection

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Engineering of crystalline compounds remain a challenging task; because crystal packing at molecular level plays significant role in potential applications.[1] Keeping in mind this idea, a F-appended Schiff Base 1,2-bis(2-fluorobenzylidene)hydrazine has been synthesized and characterized with SXRD, PXRD, TGA and spectroscopic techniques. The structural architecture showed variance of molecular packing with changing solvent system. Interestingly, the fluorinated Schiff base 1,2-bis(2-fluorobenzylidene)hydrazine molecule exhibited excellent fluorescence activity and acts as a great potential for fluorescence sensing due to presence of electronegative atoms as well as nitrogen binding sites.[2] From all other metals the compound selectively shows turn off behaviour with Fe^{3+} and turn on behaviour with Al^{3+} with limit of detection ranging in micromolar range. The compound also shows Aggregation Caused Quenching (ACQ) with addition of water to it.[3] In addition to this, non-linear optical behaviour exhibition has been due to its crystal packing. Hence, this organic compound can be utilized as a functional multifunctional material.

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Keywords: fluorescence sensing, Nonlinear optics, Aggregation caused quenching

Large Area Film of Highly Crystalline, Cleavable, and Transferable Semi-Conducting 2D-Imine Covalent Organic Framework on Dielectric Glass Substrate

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Two-dimensional imine-based covalent organic frameworks (2D COFs) are an emerging class of crystalline, porous, and -conjugated materials with immense potential in thin-film electronics, and optoelectronics. Their modular molecular design, tunable electronic structure, and structural robustness make them promising candidates for integration into functional nanodevices. In our work, we report a scalable and reproducible method for fabricating uniform, crystalline 2D imine-COF thin films via a quasi-equilibrium Schiff base condensation between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA). This approach enables the formation of large-area films (up to 2 cm) on dielectric substrates with controllable thickness and high uniformity. Controlled sonication-assisted exfoliation yielded thin and ultra-thin freestanding films with few-layer thickness while preserving structural integrity. Comprehensive characterization using SEM, TEM, and AFM confirmed the layered, highly crystalline morphology, whereas FTIR and XPS analysis verified the imine linkages in the COF structure. Thermal and mechanical stability of COF film were validated by

TGA and nanoindentation measurements. Optical absorption and dark-field scattering studies revealed a semiconducting band gap consistent with DFT-based band structure and density of states calculations, which indicate delocalized electronic states favorable for charge transport. To probe the intrinsic electrical properties, the COF thin films were integrated into vertical Ag/COF/Glass device architectures, fabricated by thermal evaporation of silver electrodes atop the COF surface. The I-V characteristics, measured under ambient conditions, exhibited semiconducting behaviour with low current density and a gradual increase in conductivity with applied bias. This field-assisted transport is attributed to hopping or tunnelling mechanisms, limited by high injection barriers at the electrode-COF interface. Overall, these results underscore the role of molecular design and interfacial engineering in modulating charge transport across COF-based thin films. The demonstrated scalability, robustness, and voltage-responsive behaviour highlight the promise of 2D imine-COFs as functional materials for next-generation optoelectronic and energy devices.

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Keywords: organic; Thin film; Charge transport; Optoelectronic materials

Defect-Rich Wide-Bandgap Li_2ZrO_3 Engineered for Multiple Functionalities through a Cation Doping Scheme

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Due to its exceptional thermal and chemical stability—arising from the strong covalent character of the Zr–O bonds— Li_2ZrO_3 (LZO) can accommodate up to 10 mol% Li deficiency.¹ This feature makes LZO an attractive platform for designing defect-engineered luminescent materials through appropriate cation-doping strategies.² In this work, we explore defect-driven optical

behavior and cation-induced electronic structure modulation by introducing $\text{Tb}^{4+}/\text{Eu}^{3+}$ dopants to enrich the optical landscape of LZO. $\text{Li}_2\text{Zr}_{1-x}\text{M}_x\text{O}_3$ ($\text{M} = \text{Eu}, \text{Tb}$; $x = 0.00, 0.05, 0.10$) samples were synthesized via a ceramic route involving high-temperature solid-state reactions. Crystal and chemical structure analyses were conducted using powder X-ray diffraction and Raman spectroscopy. By combining absorption/emission spectroscopy, electron paramagnetic resonance (EPR), and X-ray photoelectron spectroscopy (XPS), we mapped the defect-related electronic states and demonstrated redistribution of energy levels in Eu^{3+} - and Tb^{4+} -doped samples. Notably, Tb^{4+} incorporation introduced an intense yellow coloration and reduced the optical bandgap from 5.45 to 2.46 eV, along with intrinsic defect-related luminescence; the 10 mol% Tb-doped sample showed remarkable photocatalytic activity, efficiently degrading crystal violet (CV) under visible light. The reactive oxygen species involved in the photocatalytic process were determined. With Eu^{3+} doping, excitation-dependent tunable emissions (in red, blue, and white regions) were achieved. Furthermore, Li^+ in Eu- and Tb-doped Li_2ZrO_3 samples could be exchanged with protons, causing partial reduction of $\text{Tb}^{4+} \rightarrow \text{Tb}^{3+}$. These findings establish that defect-rich Li_2ZrO_3 can be engineered as a versatile, multifunctional optical material via an appropriate cation-doping scheme.

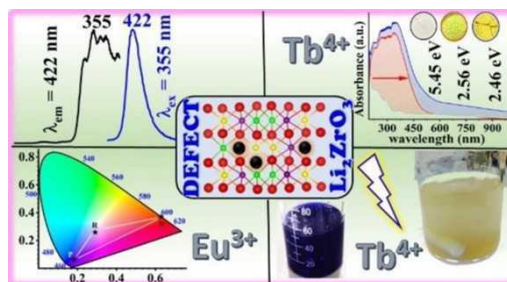


Figure 18: Pictorial representation of the key features of Li_2ZrO_3 before and after the incorporation of $\text{Tb}^{4+}/\text{Eu}^{3+}$ ions.

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Keywords: defect engineering, electron paramagnetic resonance (EPR)

Effect of Na Doping on the Power Conversion Efficiency of $\text{Cu}_2\text{ZnSnS}_4$ Solar Cells

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$\text{Cu}_2\text{ZnSnS}_4$ (CZTS) is a promising absorber material in thin film photovoltaic technology. CZTS based solar cells have their own limitations like structural disorders and Cu–Zn anti-site defects which lead to lower power conversion efficiency (PCE) than their counterparts. Alkali metal doping can enhance the PCE of CZTS solar cells at a greater extent. Sodium or potassium is introduced in CZTS for improving the PCE by enhancing crystallinity and grain size of the absorber layer [1–3]. In the present study Na has incorporated into the CZTS by evaporating NaF powder in such a way that 10 nm NaF layer is uniformly deposited using thermal evaporation method. For studying the effect of Na doping in photovoltaic characteristics of the device, solar cells (SLG/Cr/Mo/CZTS/CdS/i-ZnO/ZnO:Al/In) are fabricated with and without NaF layer and denoted as N-CZTS and P-CZTS respectively. The structural, morphological, optical and electrical properties of the CZTS absorber layer and the I–V characteristics of the fabricated cells are studied. N-CZTS cell has a PCE of $0.87^{+0.22\%}_{-0.30\%}$ and P-CZTS cell has a PCE of $1.14^{+0.26\%}_{-0.21\%}$, which was different than as expected. Similar reports suggest that the decrease in PCE on Na-doping can be due to higher doping concentration and thus significant increase in the bandgap of the CZTS layer [4]. However, this study leads to a better understanding of optimum Na concentration for achieving higher PCE by tailoring the bandgap and improving the microstructure of the CZTS absorber layer.

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Keywords: $\text{Cu}_2\text{ZnSnS}_4$, Solar cells, Alkali doping, Defects

2D MoS_2 Self-Powered Photodetector with Broadband Photodetection and Polarization Sensitivity

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Self-powered photodetector has caught significant attention in various applications such as light sensing, medical and wearable technologies due to the elimination of any external power for driving it. However, most of the study on photodetectors covers the device performance with variation in the wavelength and intensity of the light but exploration of the states of polarisation detection, an inherent property of light still remains in its infancy [1]. In this study, a plasma-based method known as magnetron sputtering, is used to synthesise a vertically aligned 2D MoS_2 nanomaterial. The deposition parameters are tuned to grow the 2D MoS_2 vertically, and a non-destructive nitrogen doping process via plasma is employed to create a p–n homojunction [2]. The optical properties, surface morphology and electrical properties has been studied thoroughly to understand the effect of nitrogen plasma on the as-synthesised vertically aligned MoS_2 . To study the polarisation sensitivity of the as-synthesised nanomaterials, various characterisations like angle resolved Raman spectroscopy, polarised absorption spectroscopy and Mueller Matrix ellipsometry are used. A homojunction device is fabricated successfully for broadband self-powered photodetection with polarisation sensitivity. The fabricated device has self-powered detection capability covering a broad spectral response from

360 nm to 1300 nm. Light polarisation sensitivity is studied using a polariser with 520 nm and 630 nm LEDs, and it shows a dichroic ratio of around 1.8. This work shows the practicality of the development of a polarisation sensitive photodetector using the specific orientation of 2D MoS₂ nanomaterials. Spectral response at 1300 nm also makes a broader prospects for its application in the field of NIR imaging.

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Keywords: Photodetection, polarisation, MoS₂

EDTA-assisted defect modification of scheelite-type NaEu(WO₄)₂ functional material for optoelectronic application and a prototype fabrication of red LED

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A scheelite-type sodium europium double tungstate (NaEu(WO₄)₂) has been synthesized using a facile hydrothermal method with EDTA as a chelating agent, followed by calcination, and has been explored as a new generation of functional materials for optoelectronic applications. Herein, we have observed a significant dependence of functionality on micro-strain and oxygen vacancies (V_O), related to structural distortions that have been analysed by powder X-ray diffraction, Rietveld refinement, Fourier-transform infrared, and Raman spectroscopic techniques. The variation in EDTA concentration has played a pivotal role in the morphological evolution of stone-like, rugby-like, and dough-like structures, as observed by field-emission scanning electron microscopy. Lower EDTA concentration corresponds to a greater presence of V_O, as corroborated by XPS measurements, and further analysed through the O–W–O bond-angle deformation in the WO₄ tetrahedral framework and

micro-strain. Optical properties have been assessed through UV–Vis absorption and photoluminescence spectroscopies. The dough-like morphology and less-deformed NaEu(WO₄)₂ material exhibit red emission at 615 nm with colour coordinate (0.666, 0.334), equivalent to the NTSC standard coordinate, and 96% colour purity, owing to the ⁵D₀–⁷F₂ electric-dipole transition of Eu³⁺ ions under 393 nm excitation, making it a viable choice for optoelectronic applications. Furthermore, we have fabricated a prototype red LED device using the improved NaEu(WO₄)₂ material for industrial phosphor-converted LEDs.

Keywords: Scheelite-type material, luminescence, phosphor converted LED

Effect of Post Annealing on Zinc Phthalocyanine Film Grown by Close Space Sublimation Method

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In recent years, Organic material-based solar cells have been promising for energy harvesting due to their advantages over silicon-based solar cells. Their low fabrication cost, flexibility, environmentally friendly, and non-toxic nature make them ideal for large-scale fabrication. Close space sublimation (CSS) is a novel technique for solar cell fabrication in which the target substrate is kept very close to the source, and fast sublimation of the material is done to get the desired film thickness in a short time. It lets us deposit thin films within seconds with much better material utilization. Zinc Phthalocyanine is a well-known donor material used in organic solar cell. Our previous work has shown that thin film of planner molecule like ZnPc, grown by CSS method, is amorphous in nature due to high rate of deposition. So, in this work we fabricated thin films of ZnPc, using CSS method and study the effect of post annealing on it. We Compared optical, morphological and structural properties of ZnPc films before and after annealing. This study will help to optimize the CSS technique and can be utilized to efficiently fabricate the solar cell device in a short time and improve the device's fabrication cost for future industrial applications

Keywords: Close space sublimation, organic solar cell, zinc phthalocyanine

MoS₂/VO₂ Based Heterostructure Device for Highly Responsive Infrared Photodetection

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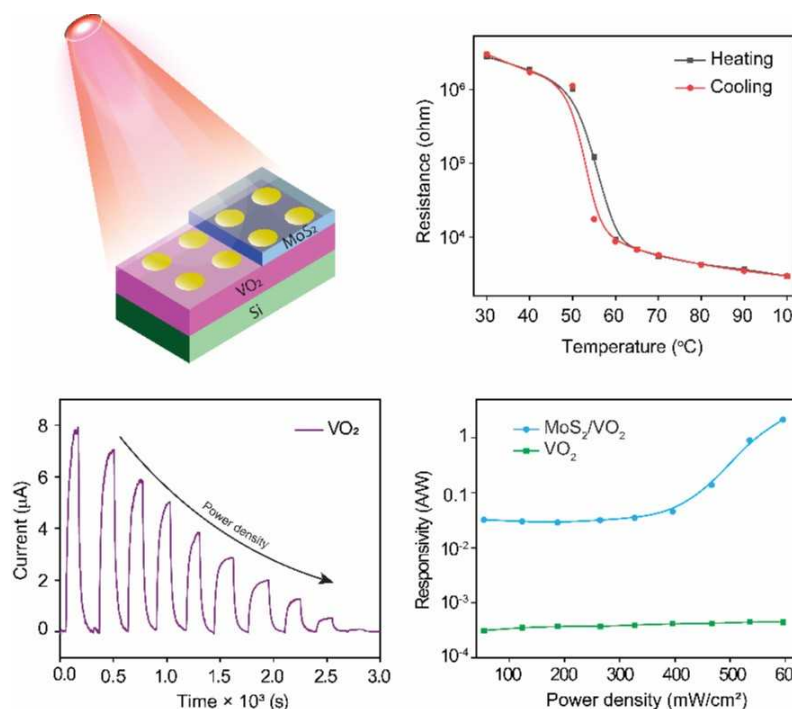
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Vanadium oxide (VO₂) has aroused researchers' curiosity among transition Metal Oxides because of its unique semiconductor-to-metal phase transition (SMT).[1] It undergoes a structural transformation from semiconductor monoclinic phase (low temperature) to metallic rutile phase (high temperature) at transition temperature $T_c \sim 340$ K exhibiting ultra-fast, fully reversible, first-order phase transition accompanied by a notable change in electronic and optical properties.[2] Transition Metal Dichalcogenides (TMDs) have also been considerably explored due to their distinctive electronic and mechanical properties. Attributed to the outstanding properties of 2D layered materials and transition Metal Oxides, these materials are well known to give ultrafast, self-biased, and broadband photodetection.[3] In this work, we deposited VO₂ film on SiO₂ substrates by using Pulsed Laser Deposition (PLD). MoS₂ film was deposited on VO₂ film using PLD to form MoS₂/VO₂ heterostructure. In short, the PLD with 248 nm KrF Excimer laser with energy 200 mJ was used to ablate the target. A repetition rate of 5 Hz was maintained with a consistent energy density of 1.5 J/cm².

For the MoS₂/VO₂ device, the responsivity was found to be 0.83 A/W as compared to 4.42×10^{-4} A/W for the VO₂ device, respectively, at 595.83 mW/cm² power density using a 1550 nm laser. Moreover, the device showed 4 orders of enhancement in responsivity and a 42-fold increase in sensitivity compared to the VO₂ device. The device exhibited excellent figures of merit in comparison with the linear VO₂ device. Clearly, the MoS₂/VO₂ device shows higher photodetection and hence gives better performance than the VO₂ device. These results indicate the potential of the MoS₂/VO₂ device for near-infrared optoelectronic applications.



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Keywords: transition metal, rutile phase, photodetection

Dopant induced room temperature phase transition in vanadium dioxide thin films

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An ever-increasing energy demand due to rapid urbanization has led to a continuous need for innovative, sustainable, and energy-efficient smart building designs. Windows constitute about $\sim 50\%$ of the total heat loss from a typical household. In this regard, regular window

designs could be improved to not only have adequate visible transparency but also modulate IR radiation based on the requirement. The improved smart window design could incorporate either electrochromic or thermochromic coatings, which change their optical behavior in response to external stimuli. Whereas electrochromic coatings require electrical power to function and thus are not suitable for energy-efficient smart windows, thermochromic coatings can alter their optical properties solely based on external/internal temperature. One of the promising materials that display thermochromism is vanadium dioxide (VO_2), which undergoes a structural phase transition (SPT) from monoclinic to rutile crystal structure at 341 K (68°C). This structural transition is coupled with a semiconductor-to-metal transition (SMT), which switches the optical behavior of this material from an IR-transparent state to an IR-reflecting state. However, the phase transition temperature (T_c) for pure VO_2 is slightly on the higher side and needs to be brought down near room temperature for its commercial applicability. One of the strategies to reduce T_c utilizes the lattice-straining method, wherein the material is strained, causing its transition to occur earlier or later depending on the type of strain. Whereas mechanical straining requires epitaxial thin-film growth and has thickness dependence, chemical straining uses dopant atoms to strain the host lattice and is thickness independent. In this work, unstrained and chemically strained VO_2 thin films are deposited on soda-lime glass (SLG) substrates using compound ceramic targets in an RF magnetron sputtering system. Four different dopants, each with varying ionic sizes and concentrations (W^{6+} , Mo^{6+} , Nb^{5+} , and Ta^{5+}), were incorporated to modify the switching behavior and transition temperature (T_c) of the VO_2 thin films. The chemically strained thin films were found to have their T_c in the range of 175 K to 334 K, depending on dopant type and concentration. Moreover, chemically strained VO_2 shows switching characteristics with $T_c = 310 \pm 7$ K, while also maintaining adequate luminous transmittance of 34.50% and a high infrared switching efficiency of 40.93% at $\lambda = 2500$ nm. Furthermore, the role of microstructure (crystallite size, stoichiometry, etc.) in altering the phase transition behavior has been studied. The obtained experimental results could help establish VO_2 as a potential next-generation material for various energy-efficient device applications.

Keywords: Chemical straining, vanadium dioxide, thermochromic, smart windows

Studies of Nickel doped Copper Oxide nanosheets for optoelectronic device applications.

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Ni-doped CuO nanosheets were synthesized by the hydrothermal method. We systematically investigated structural, optical, and electrical properties of Ni-doped CuO for device applications. The XRD pattern confirmed the monoclinic structure of the synthesized material. The study of films morphology by SEM showed that the obtained films have a nanoflakes structure. The BET result shows that specific surface area increases with Ni doping from 5.66 to 8.34 m²/g. The DLS result indicates that the particle distribution falls within the 1 to 20 nm. The FTIR shows the variation in Copper and oxygen bonding with nickel doping. The electrical properties were studied on single-layer FTO—CuO(nanoflakes)—Al device structure. The impedance studies show the device may be modelled as a parallel RC electrical circuit. The details of device applications will be presented in the conference.

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Keywords: CuO, contact resistance, monoclinic, nanoflakes

Phonons and Structural Phase Transition Study of Hybrid Organic-Inorganic Perovskite-based Molecular Ferroelectrics

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Hybrid organic-inorganic perovskite (HOIP) based molecular ferroelectrics hold great promise in photovoltaic and optoelectronic applications which combine the best from both materials offering a new way of tailoring the band structure.^{1,2,3} The understanding of electron-phonon coupling is essential for their performance in optoelectronic applications as variety of interactions and structural disorder, which may significantly affect the material's characteristics.⁴ Thus, it is crucial to study the thermodynamic structure-property relationship to get important insights towards improving their functionality. In this work, we carried out the temperature-dependent Raman scattering studies of single crystal 2-(ammoniomethyl pyridinium) SbI₅ (2-AMP-SbI₅) and hexane-1,6-diammonium pentaiodobismuth (HDA-BiI₅) HOIP in the temperature ranges 200 °C to -195 °C to study possible structural phase transition, electron-phonon interaction and structural changes during the transition. The analysis of temperature-dependent Raman data reveals anomalous changes of Raman shift and line width confirming the ferro to paraelectric transition due to structural phase transitions. In particular, the phase transition in the above molecular based HOIPs is associated with orientational changes of the organic cations produced by rotation of the ammonium heads and/or the pyridinium rings and tilting of BiI₆ octahedra and the changes of dynamics of hexane-1,6-diammonium cations is clearly established from our Raman analysis. We also discuss the nature of these transitions in terms of their activation energy and change in molecular orientations.

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Keywords: ferroelectrics, phonon, optoelectronics

Hierarchically Structured Co_{1-x}Ni_xO/Laser-induced Porous Graphene Nanohybrids for Photocatalytic Dye Degradation

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The rising demand for clean water and environmental remediation has driven the development of low-cost materials for pollutant removal. In this study, we report a sustainable, scalable approach for synthesizing Co_{1-x}Ni_xO/laser-induced porous graphene (CoNiO/PG) nanohybrids using industrial waste-derived metal precursors and a laser-induced photothermal reduction route for graphene integration. The nanohybrids feature CoNiO nanoflakes uniformly anchored onto a porous graphene framework, resulting in enhanced interfacial contact and synergistic charge transfer. Under UV-visible light irradiation, the CoNiO/PG nanohybrids demonstrate outstanding photocatalytic activity, achieving 94% degradation of 5 ppm methylene blue (MB) within 120 minutes, significantly outperforming porous graphene alone. Kinetic analysis reveals pseudo-first-order behavior with the highest rate constant ($k = 0.049 \text{ min}^{-1}$) observed at 1 ppm MB. The enhanced performance is attributed to the combined effects of improved light absorption (bandgap of 1.38 eV), efficient electron-hole separation, and accelerated generation of reactive oxygen species ($\bullet\text{OH}$, O_2^-). The porous graphene facilitates charge mobility and minimizes recombination, while CoNiO provides high

surface area and catalytic active sites. This work highlights a sustainable strategy for converting industrial waste into high-performance nanohybrids and demonstrates the potential of CoNiO/PG as a promising candidate for scalable environmental remediation applications.

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Keywords: pollutant, nanohybrids, graphene

Effect of reduced graphene oxide on solution combustion synthesized chromium oxide towards ethanol sensing

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Chromium oxide (Cr_2O_3) is a p-type transition metal oxide known for its chemical stability, semiconducting properties, and catalytic activity, which make it a promising material for gas sensing applications [1]. Cr_2O_3 has been investigated for sensing various gases such as H_2 , NH_3 , ethanol, etc., and its performance has been enhanced by incorporation of noble metals and carbonaceous materials like CNTs and graphene [2].

Graphene, a monolayer of carbon atoms tightly packed into a two-dimensional (2D) honeycomb lattice, is a basic building block for graphitic materials of all other dimensionalities [3]. Since its discovery by Novoselov and Geim, graphene has been widely used in fields such as photocatalysts, supercapacitors, gas sensors, and electronic devices due to its high specific surface area and high carrier mobility at room temperature [3]. A potentially cost-effective method for mass-producing graphene is to first produce chemically modified graphene, such as graphite oxide and graphene oxide (GO), and then reduce it to obtain reduced graphene oxide (rGO), an alternative to pristine graphene [4].

In view of developing sensors operating at lower temperatures, composites of $\text{rGO-Cr}_2\text{O}_3$ are considered in this study. Nanopowders of chromium oxide were synthesized by solution combustion synthesis with a crystallite size of ~ 42 nm. Highly conducting rGO was obtained from the reduction of graphene oxide (GO, prepared by Hummer's method) using hydrazine hydrate [4,5]. The composition and morphology of these materials were characterized by XRD, FTIR, Raman, FE-SEM, BET, and two-probe resistivity measurements carried out in a home-built apparatus. Cr_2O_3 and $\text{rGO-Cr}_2\text{O}_3$ composites were explored for ethanol sensing in an in-house designed test chamber in a concentration range between 10 ppm and 100 ppm. A decrease in response time, recovery time, and operating temperature was observed for the composites compared to pure Cr_2O_3 sensors. The addition of rGO provides a conductive network that facilitates efficient electron transfer between Cr_2O_3 nanoparticles, enhancing sensor response with faster recovery times. Furthermore, the high surface area of rGO offers more active sites for ethanol adsorption, increasing the sensor's sensitivity.

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Keywords: $\text{rGO-Cr}_2\text{O}_3$ composite; solution combustion synthesis; ethanol sensing.

Formulating Iodine-integrated SmTaO₄ for Efficient Visible-Light-Driven Degradation of Fluorene: A Synergistic Rare-Earth–Halogen Approach

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An effective partition of photogenerated charge carriers is a prerequisite for solar photocatalysis with an exalted efficacy. To serve our pollutant photodegradation purpose, iodine-incorporated bimetallic oxyhalide semiconducting nanotriangles were synthesized following a simple one-step solvothermal approach. The synthesized catalyst containing Sm and Ta as metals was analyzed using XRD, SEM, XPS, Raman, FTIR, TEM, etc. Our study's assortment of performance interpretations mutually unravels the potential of I@SmTaO₄ in the solar-light-propelled degradation of persistent organic pollutants. With the aid of advanced characterization techniques like EPR and PAS, the initiation of oxygen vacancies in the metal oxyhalide matrix was confirmed. This provided evidence that the generation of sufficient hydroxyl radicals and holes boosted its overall catalytic function and degradation of our model pollutant, fluorene.

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Keywords: Photocatalytic degradation; Fukui function; charge carrier dynamics.

Energy-Efficient Organic Bilayer Crossbar Memristor with Tunable Switching

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Memristors integrate computing and storage in a single device, addressing the inherent constraints of the Von Neumann architecture. They have recently attracted considerable attention due to their capability for in-memory computing [1]. Among them, organic memristors are emerging as strong contenders for next-generation flexible memory devices owing to their lightweight, flexibility, and structural tunability [2]. However, despite extensive investigations, achieving organic memristors with desirable characteristics such as low operating voltage, high ON/OFF ratio, long-term data retention, and mechanical flexibility remains challenging [3]. In this work, a high-performance flexible organic bilayer crossbar memristor and write-once-read-many (WORM) memory are fabricated using the small molecule 6,13-bis(triisopropylsilylethynyl)pentacene (TP) and the conjugated polymer poly(3-hexylthiophene-2,5-diyl) (P3HT) as active material at different blend ratios. The device exhibited memristive behaviour with a data retention of 10⁵ s, a high ON/OFF ratio (>10³), and lower power consumption (<360 μW) at a blending ratio of TP:P3HT = 3:1. Conversely, a 1:1 blend ratio demonstrated WORM memory. Structural characterization of the film was carried out using atomic force microscopy and Raman spectroscopy. Interfacial dipole modulation is identified as the underlying resistive switching mechanism. The switching mechanism is further supported by conduction mechanism analysis and temperature-dependent studies.

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Keywords: Organic memristor; Write-Once-Read-Many memory; Flexible device; Interfacial dipole modulation

Tunable plasmonic response in Ag nanoparticle doped ZrN thin films

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Metal nanostructures such as Au and Ag nanoparticles (NPs) exhibit fascinating optical phenomena called localized surface plasmon resonances (LSPRs). While tuning plasmonic excitation in the visible spectrum can be effectively achieved by varying NP size, shape, or surroundings, the carrier density remains fixed, thus limiting LSPR modulation. By varying the surroundings of these NPs, wide tunability can be achieved. Recent reports have shown that semiconductors and transparent conducting oxides (TCOs) have been used as the surrounding medium for these nanoparticles. However, due to restrictions in bandgap tunability in semiconductors and lower carrier density in TCOs, transition metal nitrides (TMNs) have been explored. TMNs exhibit high electrical conductivity, tunable carrier density, and plasmonic response in the near-infrared, visible, and UV regimes. In this work, we synthesized ZrN nanocomposites with varying Ag atomic concentration to utilize the wide tunability in carrier density of ZrN combined with the LSPR modulation of Ag NPs. From the SEM images of the samples shown in Fig. 1, the formation of Ag NPs can be clearly observed for Ag 40% and 80%. The increasing Ag content results in the formation of NPs with different sizes, which causes a redshift in the LSPR bands, as shown in Fig. 1(c). The samples were also annealed to study the effect on the LSPR band. Further optical characterization will be presented in the poster.

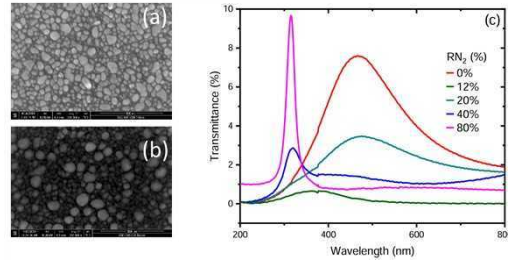


Figure 20: FE-SEM images of ZrN thin films with Ag doping concentrations of (a) 40% and (b) 80%. (c) Transmittance spectra of ZrN samples with Ag concentrations of 0, 12, 20, 40, and 80%.

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Keywords: Transition metal nitrides; nanoparticles; LSPR; plasmonics.

Synthesis and Photoluminescence Properties of $\text{KPbFe}_{2-x}(\text{PO}_4)_3 \cdot x\text{Nd}^{3+}$, $x = 0.01, 0.05$ and 0.1 Doped Phosphors for NIR-Emission

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Neodymium (Nd^{3+}) doped $\text{KPbFe}_{2-x}\text{REE}(\text{PO}_4)_3$ langbeinite phosphate phosphors, where $x = 0.01, 0.05$ and 0.1 were synthesized by solution method. The synthesized phosphors were characterized by various techniques such as XRD, FTIR, SEM-EDAX, UV-DRS and spectrofluorometry studies. From XRD analysis, the absence of any secondary phases confirmed the phase purity of all three Nd^{3+} doped materials, which are crystallize in cubic structure with $P2_13$ space group. Rietveld refinement authenticates the phase purity with low chi-square values. The lattice parameters of $x = 0.01, 0.05$ and 0.1 phosphors were identified as $950.73 \text{ \AA}$, $949.57 \text{ \AA}$, and $955.08 \text{ \AA}$, respectively. FT-IR spectra of the materials showed P-O stretching

and bending vibrational bands in the 675–1242 cm^{-1} and 489–665 cm^{-1} ranges. Surface morphological studies indicate that the particles are highly agglomerated in $x = 0.1$ phase compared to the other two phases and the presence of all the elements were confirmed by EDX analysis. Photoluminescence property of the materials was investigated by fixing the excitation wavelength in NIR region at 808 nm and observed the emissions at 874 nm ($^4F_{3/2} \rightarrow ^4I_{9/2}$), 1059 nm ($^4F_{3/2} \rightarrow ^4I_{11/2}$), 1329 nm ($^4F_{3/2} \rightarrow ^4I_{13/2}$) for $x = 0.01, 0.05$ and 0.1 , respectively. The emission wavelength falls at the NIR region and the most intense peak registered at 1059 nm. The Blasse and Dexter models reveal that the energy transfer mechanism for concentration quenching is due to the nearest neighbour ions of the host material. Since the NIR light-emitting diodes (LEDs) mostly emits at 850 - 1500 nm (NIR), the synthesized Nd^{3+} doped phosphate phosphors could be useful for NIR emitting NIR LEDs, photonic devices, and bio imaging applications as their emission wavelengths are lying in this region.

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Keywords: Rare earth doping; Langbeinite; Inorganic Phosphors; NIR-Emission

2D SnS_2 thin film-based Pyrophototronic Photodetector

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Photodetection is a field of study that utilizes light to access various technological advancements. In this domain, the photovoltaic effect is mostly used to generate an electrical signal when exposed to light energy [1]. Recently, researchers combined the photovoltaic effect with the pyroelectric effect to develop a new phenomenon, known as the pyro-phototronic effect [2]. This term was first proposed by Z. Wang et al. in 2015 [3]. Pyro-phototronic photodetectors have been known to demonstrate substantial enhancement in photoresponsivity, detectivity, and response time of the device by several folds [4], [5]. We aim to fabricate an SnS_2 2D layered material-based photodetector, exhibiting enhanced attributes. SnS_2 , being a Transition Metal Dichalcogenide (TMD), is known to evince intrinsic defects like vacancies, grain boundaries, substitutional impurities, etc [6]. These defects can lead to an enhancement in the performance of the device fabricated from the 2D material. To mitigate the challenge of the limited thickness of the film (μm), we plan to implement the plasma-based magnetron sputtering technique for depositing a thin film in the nm range with excellent uniformity and high stability [7]. This work will provide a pathway for designing a novel device with futuristic applicability in optoelectronics and sensing with enhanced performance parameters.

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Keywords: photodetection, grain boundaries

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Keywords: Additive engineering; stabilization; black-phase of FAPbI₃

Stabilization of the black-phase of FAPbI₃ perovskite by multi-dentate chelating agents

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Perovskite solar cells (PSCs) using Formamidinium lead Iodide (FAPbI₃) have the potential to achieve maximum power conversion efficiency (PCE), due to its inherent bandgap of 1.48 eV for the α -phase, which is closest to the Shockley-Queisser limit (1.34 eV) for a single-junction solar cell. However, the black-phase (photoactive α -phase) of FAPbI₃ quickly transitions to the yellow δ -phase, which is undesirable for photovoltaic applications in ambient atmospheres (exposure to oxygen and moisture). This instability of the α -phase limits the use of FAPbI₃ in various optoelectronic applications. To improve the stability of the black phase of FAPbI₃ perovskite while maintaining its inherent bandgap, we adopted an additive engineering approach. We studied the effect of multi-dentate chelating agents on the FAPbI₃ perovskite films and found that these additives help increase grain size, extend the average excited-state lifetime, and enable the additive-treated film to stay in the black phase for more than 72 hours in ambient atmosphere, whereas the untreated film transitions to the yellow phase within 30 minutes of exposure.

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Sustainable and Self-Powered NiO/TiO₂ p–n Heterojunction for High-Performance UV Sensing

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This work presents the synthesis and fabrication of a sustainable, low-cost, self-powered TiO₂ nanoflakes-based UV sensor. Single-crystal TiO₂ nanoflakes were synthesized using a simple hydrothermal method. Subsequently, a p–n junction of NiO/TiO₂ was fabricated via the hydrothermal process. Both materials possess wide band gaps with strong optical responsivity in the UV region. Under UV illumination, an electric field is generated at the p–n junction due to efficient charge separation, producing a significant measurable current. The n-type anatase TiO₂ nanoflakes exhibit good response and recovery times ($\sim$ ms) with only a very small applied bias (0.001 V), whereas the p–n heterojunction NiO/TiO₂ shows significantly faster response and recovery times ($\sim$ ms) even without an applied bias and under very low UV intensity. This UV sensor, synthesized via a facile and low-cost method, demonstrates excellent response and recovery times, high selectivity towards the UV region at low intensities, and strong potential for applications in environmental UV monitoring, wearable electronics, and optoelectronic devices. The stability, efficiency,

and environmental friendliness of the UV-active material open a sustainable pathway for high-performance UV sensing technology.

Keywords: UV sensor, p-n heterojunction, TiO₂ nanoflakes, NiO.

Terahertz Spectroscopy for Probing Intrinsic Optical Properties of Covalent Organic Frameworks

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Terahertz (THz) spectroscopy is emerging as a unique probe for understanding the intrinsic optical properties of reticular materials such as covalent organic frameworks (COFs). These crystalline, porous, and modular materials provide a versatile platform to engineer optical and electronic functionalities through rational molecular design [1,2]. While most THz studies of extended frameworks have concentrated on photoexcited carrier mobility using optical-pump-probe methods—as recently demonstrated for COF thin films—intrinsic charge transport, dielectric response, and low-energy excitations in COFs remain largely unexplored [3]. In this work, we present a THz spectroscopic study of crystalline COFs alongside their amorphous counterparts and molecular analogues, enabling direct evaluation of how framework order and rigidity govern their THz response. Our results reveal that crystalline frameworks exhibit enhanced THz transparency and optical conductivity, which we attribute to suppressed low-energy vibrational modes, whereas molecular analogues display pronounced absorption. These insights underscore the importance of structural rigidity and long-range order in dictating the optical response of COFs. Overall, this study highlights the potential of COFs as highly tunable platforms for next-generation photonic, electronic,

and quantum technologies, while also establishing THz spectroscopy as a powerful tool for probing their fundamental structure-property relationships [4].

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Keywords: Covalent Organic Frameworks (COFs), Terahertz (THz) Spectroscopy, Reticular Materials, Optoelectronic Materials

Optimization of Metal nitride – based memristor for resistive switching and neuromorphic application through reactive sputtering technique

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In the era of artificial intelligence (AI) and advanced computing systems, conventional semiconductor devices based on the von-Neumann architecture is experiencing limitations such as low processing speed, separate memory and computation units, limited scalability, and high-power consumption, making them inadequate for current computing demands. The two-terminal based memristive devices surpass these challenges through their in-memory computing abilities and high-scalable device structure. While oxide-based memristors have been extensively studied, nitride-based systems remain relatively unexplored despite their potential for stable and scalable neuromorphic platforms. Here, we present a systematic study of sputter-grown TiN-based memristive devices with the structure Ag/TiN/p⁺⁺-Si, fabricated under varying growth conditions (growth angle, N₂ flow rate, and substrate temperature). The devices exhibit stable bipolar resistive switching with a reasonable ON/OFF ratio and clear negative differential resistance (NDR) during the RESET process. Growth angle-mediated (0° to 80°) changes in morphology and stoichiometry influence the forming voltage, while growth temperature (RT to 750 °C) alters crystallinity, thereby modulating SET/RESET dynamics. Optimized growth parameters yield reproducible switching and enable the emulation of essential synaptic functions such as potentiation/depression, spike amplitude-dependent plasticity, paired-pulse facilitation/depression, etc. These findings underscore the promise of TiN-based memristors as an alternative to oxides for energy-efficient in-memory and neuromorphic computing applications.

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Keywords: Resistive switching (RS), Titanium Nitride, Negative differential resistance (NDR), Electronic synapse.

Tuning nonlinear optical response of MoS₂ monolayer by plasmonic effect with gold nanoparticles of different shapes

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2D materials provide precise control over light-matter interaction due to increased surface area, making them potential candidates for optical and nonlinear optical applications. Monolayer MoS₂ has recently been identified as a highly promising NLO candidate due to its large second-order susceptibility value ($\chi^{(2)}$) [1]. In this work, large-area continuous monolayers of MoS₂ were grown on sapphire substrates by chemical vapor deposition (CVD) technique and decorated with gold nanoparticles of three different shapes. Metal nanoparticles create localized surface plasmon resonance (LSPR) effects when the surface electrons interact with light, leading to strong field enhancement and nonlinear optical responses [2]. The presence of excitons significantly affects the absorption and emission characteristics of MoS₂, along with modifying their binding energies, valley polarization, photoconductivity, etc.

To understand the change in nonlinearity upon plasmonic effects on the MoS₂ monolayers, the gold-decorated monolayers were compared with bare monolayers. MoS₂ monolayers showed saturable absorption (SA), while adding Au nanorods increased the SA behavior. The SA behavior seemed to reduce, giving way to reverse saturable absorption (RSA) response when the Au nanorod was replaced by Au octopods [3]. On changing the particle to Au nanotriangles, switching to RSA is observed.

Numerical simulations were performed to understand the strength of the electric field due to various shapes of gold particles and to analyze these results.

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Keywords: MoS₂ monolayer, LSPR, Switchable NLO

Printed Ti₃C₂T_x MXene–High Entropy Oxide Hybrid Sensor for Selective Detection of Ammonia and VOCs

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This study explored the synthesis of Ti₃C₂T_x MXene nanolaminates prepared by etching Ti₃AlC₂ MAX phase using LiF and H₂SO₄, where the MAX phase was synthesized by mechanically mixing Ti, Al, and C powders in a 3:1.1:2 ratio, followed by pelletizing and high-temperature sintering. The resulting MXene was characterized using FTIR to detect surface terminations (–O, –OH, –F) and FESEM for morphology, Raman spectroscopy to analyze defect density, and XRD to confirm phase structure. Subsequently, solution combustion-processed high entropy oxide powder was combined with Ti₃C₂T_x to formulate a screen-printable ink for sensor fabrication. The

impact of Ti₃C₂T_x on the sensing behavior of metal oxide sensors was investigated, and the fabricated sensors were tested against analyte gases such as ammonia and other volatile organic compounds including ethanol, methanol, acetone, and formaldehyde. It was found that Ti₃C₂T_x addition influenced gas response and offered tunable sensing characteristics due to its conductive and layered nature. These findings support the development of high-performance gas sensors based on MXene–high entropy oxide hybrids and could enable early detection of toxic or flammable gases in industrial safety systems.

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Keywords: MXene, high entropy oxide, hybrid, gas sensor, ammonia detection.

A Comprehensive Comparison On Photodegradation In Tertbutyl Carbazole Based TADF Materials For Efficient Designing

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Thermally activated delayed fluorescent (TADF) materials offer a perfect blend of higher efficiency and lower cost devices. One of the most important parameters for a TADF based organic light-emitting diode (OLED) is the stability of the compound. Although high external quantum efficiency (EQE) values are most desired, however, for practical application, a long lifetime is necessary. Thus, it is necessary to enlighten the photodegradation pattern in various TADF molecules [1-3]. Here, via in-material chemistry, we investigate the photodegradation of several monosubstituted and disubstituted tertbutyl carbazole-based TADF emitters. The photodegradation was carried out under different conditions and with non-doped as well doped

conditions. The systematic photodegradation study reveals that ortho-linkage [4] effectively improves stability. Moreover, the host material interacts differently with the isomeric TADF materials, this gives ample opportunity to tune the photostability by using appropriate host material. Interestingly enough, the steric exclusion and favorable ortho linkage can act synergistically, absence of any one factor leads to loss of photostability, which is portrayed in terms of a molecular logic gate in D-A-D type TADF emitters. We believe, analyzing the photostability of these TADF emitters will equip us with in-depth knowledge of TADF molecules. The better understanding obtained from our work will disclose the role of heteroatoms, donor type, donor position, acceptor nature, as well as the role of host materials. This knowledge will help to formulate the strategy in designing other stable TADF molecules with high life-span in future.

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Keywords: TADF, photodegradation,

Single crystals of tri-allylthiourea cadmium chloride (ATCC) were successfully grown by the slow evaporation solution technique and subjected to detailed optical, dielectric, nonlinear, and ferroelectric studies. To study the surface morphology of the grown crystals of ATCC, the scanning electron microscopy (SEM) images were recorded at magnification factors of 1500, 5000, and 10000 under an operating voltage of 20 kV. UV–Vis absorption analysis confirmed a wide transparency window in the visible region with a sharp absorption edge corresponding to an optical bandgap of 3.6 eV. The melting point of ATCC is at 113.36 °C and the onset decomposition temperature is at 228 °C. Nonlinear optical characterization using the single-beam Z-scan technique (532 nm, pulse width 4999.99 ps) revealed a two-photon absorption coefficient (β) of 10×10^{-12} m/W and a three-photon absorption coefficient of 4499×10^{-12} m³/W². Dielectric studies in the frequency range 100 Hz–1 MHz and temperature range 303–373 K were performed. The piezoelectric charge coefficient was measured, and the hysteresis loop of the ATCC crystal was traced using a PE loop tracer, with loop parameters such as remnant polarization (P_r) and coercive field (E_c) determined.

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Keywords: NLO; ATCC; Z Scan.

Third-Order Nonlinear Optical, Thermal, Dielectric and Ferroelectric Characteristics of Tri-allylthiourea Cadmium Chloride Single Crystals

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Metal oxide microflower-based optoelectronic memristor for in-sensor computing applications

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Neuromorphic optoelectronic systems, inspired by the working principles of the human brain, are emerging as promising candidates to overcome the limitations of conventional von Neumann computing. In this context, optoelectronic synaptic devices that emulate biological synapses by modulating synaptic weights through light illumination offer a pathway to develop efficient optoelectronic platforms for in-sensor computing applications[1]. The integration of nanostructured materials in these systems is of particular importance, although rarely explored, due to their high surface-to-volume ratio, enhanced light-structure interactions, and photo-carrier trapping.

Herein, TiO₂ microflowers are synthesized using a simple, cost-effective hydrothermal method with varying Ti precursor concentration. The higher concentration of Ti precursor leads to the formation of a mixed phase, whereas the lower concentration yields a purely rutile phase. The mixed phase (TiO_x), containing a higher density of defects as revealed by photoluminescence spectroscopy, exhibits threshold analog-type switching and distinct synaptic behavior under dark, white-light, and UV illumination. The volatile nature of the device is beneficial for emulating synaptic functions with short-term dynamics, and when coupled with its strong photoresponse (from Figure), it becomes well-suited for in-sensor computing applications.

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Keywords: TiO₂, Hydrothermal Method, In-sensor, Neuromorphic Computing.

Versatile Metal Phthalocyanine-based Memristive Nanowire Network

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Organic memristors with tunable resistive switching (RS) characteristics are widely recognized as promising candidates for next-generation brain-inspired neuromorphic computing, owing to their ability to emulate the adaptive and reconfigurable nature of biological synapses [1]. In this study, we demonstrate a self-assembled organic nanowire network memristor constructed from copper(II) hexadecafluoro-phthalocyanine (F16CuPc), which presents an exceptionally versatile switching response, encompassing digital, multilevel, and analog modes. The mode of RS operation is effectively tuned through modulation of the compliance current (I_{CC}), highlighting the intrinsic adaptability of the device. Detailed current-voltage and impedance spectroscopy analyses reveal that the underlying transition in RS behavior arises from a conduction mechanism shift, evolving from trap-limited space charge-limited conduction (SCLC) at low I_{CC} to trap-free SCLC at higher I_{CC} . Specifically, under low I_{CC} conditions, the transport is dominated by Ag⁺ cation migration and subsequent redox-assisted interactions involving Ag-F and Ag- π inter-wire linkages, which favor abrupt, digital-like switching events. In contrast, when higher levels of charge injection are permitted under increased I_{CC} , the device favors intra-wire transport processes facilitated by strong π - π intermolecular interactions within the F16CuPc nanowires, leading to gradual and analog-like switching transitions.

To the best of our knowledge, this is the first experimental demonstration of the coexistence of digital, multilevel, and analog RS modes within a single organic memristive platform, all

realized through controlled tuning of operational parameters. The unique capability originates from the *in-situ* physical vapor transport-grown self-assembly of the nanowire network morphology [2], which ensures injection-dependent pathways for both inter-wire and intra-wire charge transport. This controlled growth strategy represents a significant advancement over conventional thin-film organic memristors, where structural disorder often limits switching versatility. Thus, our findings not only introduce a new paradigm for organic memristors but also open new pathways for multifunctional smart electronics that bridge memory, logic, and neuromorphic computing within a single device architecture.

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Keywords: Metal phthalocyanine, molecular memristor, digital switching, multi-bit, artificial synapse

Multiplexed On-Site Detection of Heavy Metal Ions in Water Using an IoT-Enabled Metal Chalcogenide Platform

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In recent years, rapid industrial growth and increased human activity have led to the release of numerous harmful compounds, such as heavy metal ions (HMIs), into water resources [1]. Consequently, water contamination by HMIs is associated with severe health risks such as kidney and neurological disorders, respiratory and cardiovascular diseases, and cancer [2]. Even at ultra-trace levels, their toxicity presents serious ecological and public health concerns, highlighting the urgent need for innovative, cost-effective,

on-site detection platforms to aid risk assessment and ensure regulatory compliance [3]. In this work, we developed a portable, nanostructured metal chalcogenide-based colorimetric sensor for the selective and simultaneous detection of Co^{2+} , Hg^{2+} , and Cr^{3+} ions. This versatile platform further reduces analytical complexity by eliminating tedious sample pre-processing steps and the need for sophisticated colorimetric probes, thereby facilitating sensitive detection on unmodified hydrophobic surfaces. The sensor achieves detection limits of 1 nM for Co^{2+} , 10 nM for Hg^{2+} , and 1000 nM for Cr^{3+} with high selectivity, repeatability, reusability, and operational simplicity. The performance is validated using real water samples collected from various lakes in Hyderabad, India, as well as tap water. A regression-based machine learning model processes the RGB signals to extract sensing features, thereby enhancing HMI classification with high accuracy. Integration with an IoT-enabled framework further enables quantification of multiplexed HMIs and supports robust remote monitoring. Overall, the study establishes metal chalcogenide nanostructures as a promising component for advanced water quality assessment, driving smarter monitoring strategies and supporting universal access to safe water.

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Keywords: Heavy metal ions; Metal Chalcogenides; portable device; IoT-enabled.

Controlled hydrothermal synthesis of La-doped CdTe nanomaterial for enhanced optoelectronic applications

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The hydrothermal synthesis approach for producing La-doped CdTe nanoparticles has been successfully carried out. Four samples have been prepared amongst which, one is undoped CdTe and other three samples are La-doped CdTe with increasing La content. Cubic phase of CdTe was established by X-ray diffraction (XRD). Peak shift towards higher theta angle has been observed due to the La incorporation in the CdTe crystal lattice. Raman spectroscopy gave important information about the vibrational modes of CdTe, and transmission electron microscopy (TEM) confirmed the CdTe phase and showed values for interplanar spacing. The X-ray photoelectron spectroscopy (XPS) inferred the electrical structure and surface composition. Increased La concentration was shown to decrease the bandgap in the 2.3-3.5 eV range using UV-Vis spectroscopy. An improved current response and significant variations in the material's rise and decay intervals under illumination were found by the photo response analysis. The photocurrent also gave good results in responsivity (R), detectivity (D) and also the I-T curves measured the rise and decay times. The nonlinear optical studies revealed significant values of the nonlinear absorption coefficient and nonlinear refractive index, indicating their potential utility in various advanced optical applications.

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Keywords: hydrothermal, detectivity

Negative differential resistance in reduced graphene oxide wrapped silicon nanorods: effect of illumination

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Miniaturization in microelectronic technology is the demand of the era for faster data communication between the transistors in a chip, which is achieved through ultra large-scale integration (ULSI), resulting in tremendous Joule heating. As a consequence, the temperature of a chip may reach the inversion temperature of doped silicon, leading the silicon (Si) microelectronic industry to stagnancy unless photonic communication replaces the conventional electronic one. Bulk Si, the most popular material in semiconductor microelectronic and photovoltaic applications, is a poor light emitter due to its indirect band gap. This limitation can be overcome in the nanodimensional regime. Silicon nanostructures (SiNS) show efficient photoluminescence (PL) despite the indirect nature of the bulk band structure, primarily due to the quantum confinement effect that relaxes the k -selection rule and enables pseudo-direct radiative recombination of photogenerated electron-hole pairs.

However, efficient electroluminescence (EL) from a SiNS-based device has yet to be achieved, mostly due to the formation of an unfavourable nonstoichiometric oxide (SiO_x) layer around the nanocrystalline core. This high-band-gap oxide hampers charge-carrier injection into the core and extraction of photogenerated carriers in EL, photovoltaic, or photosensing devices. Additionally, this oxide shell contains a high density of defects or traps, especially at the core-oxide interface. These traps play a crucial role in charge conduction through trapping/detrapping processes and act as efficient non-radiative recombination centres.

One plausible strategy to prevent the growth of this inevitable oxide around freshly prepared SiNS is to wrap the quantum structures with a transparent, thin, and conducting film such as graphene or reduced graphene oxide (RGO).

In this work, we explore the effect of illumination on charge transport through an amine-functionalized RGO-capped nanocrystalline Si layer containing Si nanorods (SiNRs), prepared by electrochemical etching of a p-type electropolished bulk Si substrate. SiNRs are visible in a 3D topographic atomic force microscopy (AFM) image. RGO is prepared via a modified Hummers' method and characterized using FTIR spectroscopy. Metallic contact to the SiNR layer is established through Al deposition using thermal evaporation. A schematic cross-sectional FESEM image shows a distinct RGO-enriched SiNR layer between the p-Si substrate and the Al metal pad.

I–V measurements are performed between two top Al contacts in dark and under illumination. The measurements are repeated after adding RGO drop-by-drop onto the SiNR layer. A salient feature in the I–V characteristics is the presence of negative differential resistance (NDR) for a particular sweep direction near ~ 8 V, similar to a tunnel diode, as previously reported for bare SiNRs [?]. The peak dark current in the NDR region increases eight-fold with the addition of RGO. Under illumination, the peak photocurrent increases by nearly twenty times for the same visible-light intensity. The observed optically enhanced NDR effect in RGO-wrapped SiNRs highlights their potential as active composite materials for oscillator and amplifier applications.

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Keywords: silicon nanorods, illumination, electroluminescence, PL

Tunable Photocatalytic and Luminescent Properties of CVD-Grown Boron Carbon Nitride Thin Films

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Hexagonal boron nitride (h-BN), although structurally analogous to graphene, exhibits fundamentally distinct electronic and chemical behavior due to the electronegativity asymmetry between boron and nitrogen atoms, which drives π -electron localization on nitrogen and yields a wide band gap (>5 eV). Extending the B–C–N compositional space enables electronic tunability spanning insulators, semiconductors, and conductors, with BCN alloys identified as promising wide-bandgap systems devoid of critical-metal dependence. We report a chemical vapor deposition (CVD) pathway for the synthesis of compositionally tunable BCN thin films. Precise control over the BN/CN flux ratio and growth kinetics enables phase-demixed BCN domains with adjustable optical gaps. Microstructural and spectroscopic analyses confirm the realization of a sp^2 -hybridized BN–CN conjugated phase, in contrast to conventional BN–graphene phase separation. This structural motif underpins continuous modulation of band-edge states, fluorescence response, and photocatalytic activity. Complementary density functional theory (DFT) calculations, employing the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE), GGA-PBE functional in VASP, confirm band-edge modulation driven by local bonding environments and validate photocatalytic activity. This synergistic experimental–theoretical framework establishes a scalable route for BCN heterostructures, advancing their application potential in wide-bandgap optoelectronics and photocatalysis.

Keywords: Exciton binding energy; Photoluminescence; Non-linear optical properties

Symposium: B

Angle-dependent growth of 2D MoS₂ monolayer, bilayer by chemical vapor deposition method

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2D Molybdenum disulfide (MoS₂) has gained significant scientific interest owing to its notable electronic and optoelectronic properties. Growing large areas and high-quality monolayer MoS₂ flakes and continuous MoS₂ monolayer films remains challenging. Here, we report the chemical vapor deposition (CVD) growth of few-layer, bilayer flakes and a continuous monolayer of MoS₂ on a Si/SiO₂ substrate by mounting the substrate at different inclinations. The morphologies and number of layers change as the substrate is placed at specific angles (90°, 60°, and 30°), respectively. This method facilitates a new pathway for the growth of the MoS₂ monolayer.

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Keywords: angles, growth, MoS₂, monolayer

Investigation of spin-wave dynamics in Co₂Fe_{0.4}Mn_{0.6}Si Heusler alloy by using Ferromagnetic Resonance technique

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Heusler alloys are intermetallic compounds that have special magnetic and electric properties. This makes them good candidates for use in spintronics applications. CFMS (Co₂Fe_{0.4}Mn_{0.6}Si), a specific type of half-metallic quaternary Heusler alloy, exhibits

nearly 100% spin polarization at the Fermi level. It possesses high magnetic moments, low magnetic damping, and robust ferromagnetism, which makes it promising for spintronics devices like magneto resistive devices. Its potential applications include magnetic data storage, spin-based logic devices, and advanced sensing technologies in material science and spintronics [1]. Thin films of CFMS are deposited on Si/SiO₂ substrates via ultrahigh-vacuum magnetron sputtering. Structural phases of bare CFMS are analyzed by X-ray diffraction (XRD) method and their static magnetic properties are characterized by Vibrating Sample Magnetometry (VSM) attached to standard PPMS system. A custom-built ferromagnetic resonance technique is used for measuring the spin-wave dynamics between 1-20 GHz in frequency sweep method. In the flip-chip configuration, the in-plane bias magnetic field was applied i.e. sufficient to saturate the magnetic domains of the sample. Along with the external magnetic field, the rf excitation field generated by vector network analyzer is launched in coplanar wave guides. From Fig 1(a) the diffraction patterns reveal the presence of CFMS (200) and CFMS (400) peaks with comparatively lower intensities than the most intense Si (400) peak arising from the substrate. the presence of a (200) superlattice peak suggests that the chemically ordered *B2* phase and/or *L21* phase is formed [1]. From figure (b), the M-H loop shows a narrow hysteresis with low coercivity (38 Oe), remanence 160 emu/cc and saturation magnetic field around 2600 Oe. FMR spectra exhibits sharp resonance peaks which shift systematically towards higher frequency with increasing applied magnetic field. The effective saturation magnetization (Ms) was found to be 1698 emu/cc, with the linewidth of ≈ 1.1 GHz. The study highlights the suitability of the Heusler alloy for high frequency spintronics applications.

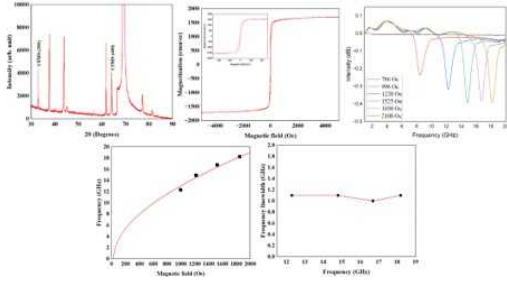


Figure 23: (a) XRD spectra for Si/ CFMS film, (b) In-plane hysteresis: PPMS data for CFMS film, (c) FMR spectra for Si/ CFMS film, (d) Frequency vs field plot for the thin film, (e) linewidth (F) vs. Frequency (F) for the thin film

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Keywords: Vibrating Sample Magnetometry (VSM), Ferromagnetic resonance (FMR), Spin polarization

Tuning magnetic anisotropy and spin states in a correlated 4d itinerant ferromagnet through the proximity of geometrically designed polar metal

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The manipulation of functional properties such as magnetism and electronic transport in complex transition metal oxides lies at the forefront of condensed matter physics and materials science. These properties are intricately governed by the underlying crystal structure and symmetry, and engineering heteroepitaxial thin films emerges as a powerful and versatile approach for precisely tuning the spin, orbital,

and lattice degrees of freedom [1]. In particular, distortions and tilts of BO_6 oxygen octahedral at epitaxial interfaces, driven by lattice mismatch or symmetry discontinuities, can profoundly influence magnetic anisotropy and electronic behavior [2]. In this work, we investigate the structural proximity effects in a heterostructures composed of a polar metal NdNiO_3 (NNO) [3] fabricated on LaAlO_3 substrate, serving as a buffer layer beneath an itinerant ferromagnetic SrRuO_3 (SRO). The trigonal distortion inherent to the (111)-oriented geometry [4], combined with the polar nature of NNO, induces significant structural modulation in the overlying SRO layer, as revealed by out-of-plane X-ray diffraction measurements. These changes are attributed to interfacial strain and octahedral distortions in the overlying SRO layer. Magnetic measurements performed by SQUID magnetometer reveal a tunable ferromagnetic transition temperature and a remarkable spin-state crossover in SRO, evolving from a high-spin to a low-spin configuration with decreasing NNO buffer layer thickness. Intermediate spin states are observed at intermediate NNO thicknesses, accompanied by a switch in magnetic anisotropy. Our findings demonstrate that geometric and interfacial design using polar metal buffer layers provides a versatile pathway to modulate spin states and magnetic anisotropy in complex oxide heterostructures.

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Keywords: structural modulation; magnetic anisotropy; proximity effect; spin-state transition

Non-trivial magnetic order in the frustrated spin-1/2 depleted-kagome antiferromagnet $\text{Cu}_7(\text{TeO}_3)_2(\text{SO}_4)_2(\text{OH})_6$

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Geometrically frustrated magnets provide a wide playground for exploring novel quantum phases of matter. The interplay of spin, lattice, and orbital degrees of freedom leads to the emergence of many fascinating phenomena at low temperatures [1,2]. Among the frustrated geometries, kagome lattice antiferromagnet (KLAF) features a very strong frustration because of its corner sharing triangular units. Herein, we report the structural and magnetic properties of $\text{Cu}_7(\text{TeO}_3)_2(\text{SO}_4)_2(\text{OH})_6$, a depleted kagome lattice compound in which 5/12 sites of kagome geometry are missing from the compound. We investigated both its structural and magnetic properties using x-ray diffraction, magnetization, heat capacity, and ^1H NMR measurements. The NMR relaxation rates ($1/T_1$ and $1/T_2$) exhibit a peak, providing evidence for a magnetic transition at $T^* \approx 4$ K. The frustration parameter $f = |\theta_{CW}|/T^* \approx 12.5$ renders the compound as a highly frustrated magnet. Furthermore, our NMR measurements reveal signatures of strong quantum fluctuations persisting even below the transition temperature, making the observed transition distinct and unusual compared to standard magnetic long-range order.

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Keywords: Quantum fluctuations, NMR relaxation, Antiferromagnetism

Investigation of Magneto-Transport Properties in Si/Ta/FeMn Heterostructures Deposited by RF Magnetron Sputtering

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Thin-film heterostructures comprising transition metal alloys have garnered substantial interest owing to their pivotal role in the advancement of spintronic devices, attributed to their distinctive magnetic and electronic functionalities. A series of Ta/FeMn heterostructures has been deposited on the (001) oriented Si, using RF magnetron sputtering under meticulously optimized deposition parameters. Structural elucidation through X-ray diffraction (XRD) analysis confirmed the oriented growth of the films, the absence of secondary phases, and characterized by well-defined diffraction peaks corresponding to the cubic phase of Ta and FeMn, signifying high crystallographic order. Atomic force microscopy (AFM) studies further corroborated the structural quality by revealing rough but smoother film surfaces, with roughness values quantified at the nanometer scale. Scanning electron microscopy (SEM) analysis confirmed the uniformity and continuity of the surface, highlighting the homogeneous film growth across the substrate. Collectively, the results from XRD, AFM, and SEM analyses underscore the high structural integrity, phase purity, and superior surface characteristics of the FeMn films, laying a robust foundation for subsequent device fabrication and exploration of their functional properties. The conventional and angular-dependent electrical and magneto transport measurements of sputter deposited Si/Ta/FeMn thin films were carried out utilizing a Physical Property Measurement System, which provides precise control of temperature and magnetic field. The data reveal a pronounced anisotropy in the magnetoresistance response, demonstrating that the electrical resistance of the films is strongly modulated by the relative alignment of the external magnetic field, film plane, and the underlying spin structure of the FeMn layer. These results suggest

that the magnetoresistive properties of FeMn-based heterostructures can be actively tuned via manipulation of the structural parameters and applied field orientation, paving the way for engineered anisotropic magnetoresistance effects suitable for next-generation spintronic devices.

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Keywords: RF Sputtering; Thin Films; Magnetoresistance; Binary Transition Metal Alloy

Insights into the Electronic Structure of Parkerite $\text{Ni}_3\text{Bi}_2\text{Se}_2$

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In pursuit of new materials exhibiting exotic quantum phenomenon, low-dimensional chalcogen compounds has gained a lot of interest. Among them are the compounds having chemical formula $\text{A}_3\text{M}_2\text{X}_2$ ($\text{A} = \text{Ni}, \text{Co}, \text{Rh}, \text{Pd}$, and Pt ; $\text{M} = \text{In}, \text{Tl}, \text{Sn}, \text{Pb}$, and Bi ; $\text{X} = \text{S}$ and Se) which shows unique physical and topological properties. For example, $\text{Rh}_3\text{Bi}_2\text{Se}_2$ exhibits superconductivity coexisting with charge density wave below 250K [1]. Kagome metals such as $\text{Ni}_3\text{In}_2\text{S}_2$ and $\text{Pd}_3\text{Bi}_2\text{S}_2$ have drawn attention owing to their remarkably high mobility, magnetoresistance, and infinite Dirac nodal lines [2, 4]. Ternary chalcogenide compound $\text{Ni}_3\text{Bi}_2\text{Se}_2$ is reported to exhibit superconductivity [5] which has prompted further investigation into its fundamental properties, leading to recent comprehensive transport measurements [6]. Despite these advancements, the electronic structure of $\text{Ni}_3\text{Bi}_2\text{Se}_2$ remains largely unexplored, that motivated us to conduct a detailed investigation of its electronic structure using laboratory- and synchrotron-based photoemission spectroscopy techniques viz. angle resolved

photoemission spectroscopy and X-ray photoemission spectroscopy. The surface morphology and crystallinity of the successfully grown single crystals was examined using the field emission scanning electron microscopy and low energy electron diffraction. In parallel, first-principles calculations are being carried out by our collaborators to support the interpretation of our experimental results. Together, these efforts aim to provide a comprehensive understanding of the fundamental electronic properties of parkerite $\text{Ni}_3\text{Bi}_2\text{Se}_2$

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Keywords: Low-dimensional, parkerite, electronic structure, photoemission spectroscopy

Engineering Magnetic Anisotropy in Co_2FeAl Thin Films Through Columnar growth on Rippled and Flat Substrates

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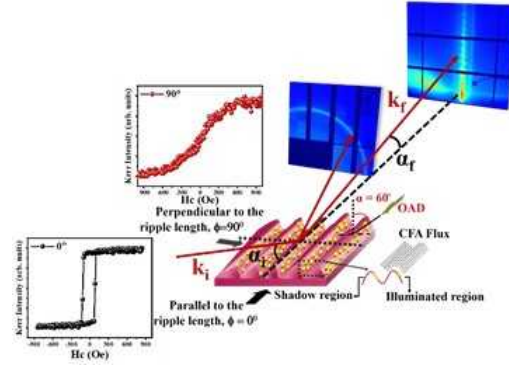


Figure 24: Schematic representation of GISAXS and GIWAXS geometry, along with MOKE loops of 50 nm CFA film deposited on rippled Si Substrates

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Keywords: Magnetic anisotropy, Oblique angle deposition, Ion beam nanopatterning, GISAXS.

Effect of thickness on Resistive Switching Characteristics of Hafnium Zirconium Oxide ($\text{Hf}_{0.75}\text{Zr}_{0.25}\text{O}_2$) thin films

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GISAXS images show vertical side streaks confirming ripple morphology, and an asymmetric scattering plume near the specular rod ($-q_y$ side), evidence of inclined columnar growth. The origin of the magnetic anisotropy is understood in terms of the two-phase magnetic response arising from the competing anisotropy components due to columns and ripple in the films. These results demonstrate that magnetic anisotropy in CFA thin films can be systematically tuned by controlling growth direction, thickness, and substrate topography, offering valuable insights for designing anisotropy-engineered spintronic architectures.

Advancements in emerging memory technologies such as RRAM, FeRAM, MRAM, and PCRAM have drawn significant attention, with RRAM standing out due to its simple metal-insulator-metal (MIM) structure and scalability. RRAM is based on resistive switching (RS), whose performance can be tailored by several parameters, deposition/annealing temperature, oxygen partial pressure, active-layer thickness, and laser fluence. Among these, the active-layer

thickness plays a crucial role. In this study, we systematically investigate the thickness-dependent RS characteristics of hafnium zirconium oxide (HZO) thin films. HZO films with thicknesses of 50, 20, 10, 5, and 3 nm were fabricated on Pt-Si substrates using the Pulsed Laser Deposition (PLD) technique, followed by thermal evaporation for the Aluminium top electrode. X-ray diffraction (XRD) and energy-dispersive X-ray spectroscopy (EDX) confirmed the structural and compositional properties, while surface morphology was studied using atomic force microscopy (AFM). To perform electrical measurements, we used a probe station to make contacts and a Keithley 2400 source meter for voltage application and current measurements. The results reveal a pronounced reduction in operating voltages as the film thickness decreases. On scaling down the thickness from 50 nm to 3 nm, the Set voltage decreases from 5 V to 0.5 V, while the Reset voltage reduces from 0.5 V to 0.05 V. We repeated the RS characteristic measurements several times to confirm repeatability. The devices exhibit stable switching over 400 cycles, a retention time of 104 seconds, and a high ON/OFF ratio of 104, which confirms their endurance, non-volatility, and reliability. These findings demonstrate that reducing the HZO film thickness is an effective way to lower operating voltages, making such devices suitable for low-power non-volatile RRAM applications.

Keywords: Resistive Switching, Endurance, Retention

Spin Hall conductivity, magnetoresistance, and nontrivial topology in BeAu

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Topological materials, characterized by various types of band crossings, provide a fertile ground for the emergence of novel topological excitations. While topological electronic excitations have been widely studied, investigations into topological phonons remain relatively limited. Exploring fermionic and bosonic topological properties within a single material opens new

avenues for advancing key concepts in condensed matter physics. In this work, we introduce BeAu as a promising candidate that hosts multiple multifold topological excitations in its electronic and phononic band spectra, each protected by specific symmetries. A detailed electronic structure analysis reveals the coexistence of three distinct topological fermions, such as Weyl, Rarita-Schwinger-Weyl, and fourfold fermions, alongside two-dimensional doubly degenerate nodal surface states. Similarly, the phonon dispersion exhibits threefold and fourfold degenerate phonons, as well as two-dimensional nodal surface states. Moreover, BeAu shows a significant spin Hall conductivity, driven by the pronounced spin Berry curvature near degenerate nodes and the spin-orbit coupling-induced band splitting in the electronic band structure. We also investigate the transverse magnetoresistance, observing intriguing behavior under varying magnetic field strengths, suggesting a potential correlation between magnetoresistance and field intensity. Our findings position this material as an exceptional platform for hosting and exploring diverse quasiparticle excitations with significant spin Hall conductivity, making it suitable for applications in spintronic devices.

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Keywords: Topological phonons, Phonon dispersion, Spin Hall conductivity

Evidence of relativistic field-derivative torque in nonlinear THz response of magnetization dynamics

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The selective addressing of spins by terahertz (THz) electromagnetic fields via Zeeman torque is, by far, one of the most successful means of controlling magnetic excitations. Here, we show that the conventional Zeeman torque on the spin is not sufficient, rather an additional relativistic field derivative torque (FDT) is essential to realize the observed magnetization dynamics. We accomplish this by exploring the ultrafast nonlinear magnetization dynamics of a ferrimagnetic garnet when excited by two co-propagating THz pulses. Having identified the Kaplan-Kittel mode at 0.48 THz, resulting from the exchange interaction between the rare-earth and transition metal sublattices, we drive this mode to a nonlinear regime. We find that the observed nonlinear trace of the magnetic response cannot be mapped to the magnetization precession induced by the Zeeman torque, while the Zeeman torque supplemented by an additional FDT follows the experimental evidences [1,2]. In addition, we have also observed signatures of FDT mediated precessional switching in the ferrimagnetic ordering.

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Keywords: Antiferromagnet; Magnon; Magnetization Dynamics; Nonlinear 2D THz-Spectroscopy.

Griffiths-like Phase, Spin-phonon coupling and large exchange bias in disordered GdSrCoMnO₆

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With exceptional structural tunability, double perovskites (DPs) serve as an excellent platform for exploring novel and diverse magnetic phenomena [1]. We report a structural, magnetic and Raman spectroscopic study on disordered GdSrCoMnO system. The substitution of Sr in place of Gd in parent compound Gd₂CoMnO₆ enhances the Curie temperature (T_c) to 153 K. Additionally, a Griffiths-like phase emerges over a wide temperature range ($T_c < T < T_{GP}$), with $T_{GP} = 245$ K, consistent with the power-law exponent $\lambda = 0.42$ [2]. Raman spectroscopy provides additional confirmation about the same through the observation of evident spin phonon coupling above T_c . Further, a robust exchange bias (379 Oe at 5 K) is observed up to 50 K indicating the possible coexistence of ferromagnetic (FM) and antiferromagnetic (AFM) phases arising from structural disorder and mixed-valence of Co and Mn ions. Our study underscores the profound impact of structural disorder on magnetic ground state, spin dynamics and lattice vibrations in GdSrCoMnO₆.

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Keywords: Double Perovskites; Griffiths-like Phase; Spin-phonon coupling; Exchange Bias

Experimental Observation and Microscopic Modeling of Skyrmion in Co/Gd Synthetic Ferrimagnetic Heterostructure

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Magnetic skyrmions offer promise for spintronic devices due to their topological protection and potential for high-speed, low-power, and high-density data transport [1,2]. Ferromagnetic skyrmions, however, face challenges such as the skyrmion Hall effect (SkHE) [2] and strong dipolar interactions that hinder the stabilization of ultra-small skyrmions. Ferrimagnets mitigate these limitations by reducing dipolar fields through weak net magnetization, enabling smaller skyrmions and higher velocities [3]. Synthetic ferrimagnets (SFiMs) further enhance skyrmion dynamics by combining interfacial spin-orbit coupling and exchange interactions to drive spin-orbit torques (SOTs). Building on these advantages, it becomes crucial to systematically explore the temperature- and field-dependent evolution of magnetization, including the labyrinth-to-skyrmion transformation, in Co/Gd-based SFiMs, a study that has so far been missing. Here, we combine experiment and theory to address this gap. Temperature-dependent magnetization measurements reveal

the interplay between antiferromagnetically coupled sublattices and their distinct thermal responses, highlighting the role of sublattice compensation in stabilizing nanoscale spin textures. Skyrmions with diameters of 140 nm are observed, confirming the suitability of SFiMs for small-sized skyrmions. To interpret these results, we employ a simplified two-layer atomistic spin model, with Co and Gd layers antiferromagnetically coupled at the interface. The simulated hysteresis closely matches experimental data, validating the framework and offering a basis for exploring rich temperature- and field-dependent phenomena in SFiM heterostructures.

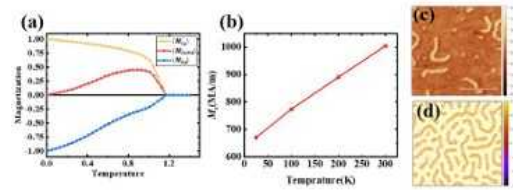


Figure 25: (a) Layer-resolved Co, Gd, and total magnetization showing the proximity effect. (b) Saturation magnetization vs. temperature. (c) MFM-image showing labyrinth-to skyrmion transition. (d) Simulated image of the same transition.

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Keywords: Synthetic ferrimagnets, Rare-Earth, Skyrmion, Spintronics

The Superconducting Diodes

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Generation of non-reciprocal response in a superconducting channel, either in a superconducting track or in a superconducting junction, is of immense technological importance. Such a non-reciprocal response in a superconducting system that is the superconducting diode effect (SDE) would pave the way to constructing two terminals, diode and rectifier-like, superconducting devices and also three terminals, gate controlled, transistor-like superconducting devices which could be backbones of fully superconducting quantum computation hardware of future. Recent theoretical and experimental advances suggest that SDE can be engineered in hybrid superconducting multilayers by breaking both time-reversal symmetry and spatial inversion symmetry. [1] This can be achieved using a combination of ferromagnetic materials and heavy metals with strong spin-orbit coupling. For instance, layering a low-temperature superconductor like Nb or NbN with a ferromagnet such as Co and a heavy metal like Pt or Ta introduces the necessary asymmetries to generate non-reciprocal superconducting transport.[2] By leveraging the intrinsic magnetization and shape anisotropy of ferromagnets, the superconducting diode effect (SDE) can be achieved without any external magnetic field known as the field-free superconducting diode effect. This breakthrough enables the design of compact, energy-efficient superconducting diodes and rectifiers. Such devices allow directional, dissipationless current flow, making them highly suitable for cryogenic environments.

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Keywords: Superconducting Diode Effect; Time reversal Symmetry; Inversion symmetry; Spin orbit coupling.

Spin Hall mediated Josephson Diode effect in Pt barrier

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Many superconducting systems that lack both time-reversal and inversion symmetry exhibit the superconducting diode effect—a non-reciprocal transport phenomenon analogous to that observed in semiconducting p-n junction diodes[1]. This effect is expected to play a critical role in the development of next-generation, low-dissipation superconducting circuits. Realizing Josephson junctions with non-reciprocal transport requires engineering supercurrent distributions that respond asymmetrically to an applied magnetic field. When the junction barrier is a material with strong spin-orbit coupling (SOC), such as Pt, the spin Hall effect can induce spin accumulation at the edges, which in turn modifies both the spatial distribution of supercurrent and the current-phase relation under applied magnetic fields.[2] In this context, we have fabricated nanoscale vertical Josephson junctions using Pt as the barrier and Nb as the superconducting electrodes. The Nb/Pt/Nb multilayers were deposited via sputtering, and the vertical Josephson nanojunctions were defined through a combination of UV photolithography and focused ion beam (FIB) milling. Magneto-transport measurements performed on these devices reveal clear signatures of non-reciprocal voltage response under reversal of the bias current, consistent with the presence of a superconducting diode effect.

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Keywords: Superconducting diode effect, Spin-orbit coupling (SOC), Current-phase relation asymmetry

Interfacial modulation of magnetic anisotropy in infinite-layer cuprate/manganite heterostructure

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Interfacial magnetic effects lie at the forefront of contemporary research, driving both fundamental discoveries and technological advancements. A particular example is the modification of magnetic anisotropy at complex oxide interface, which can result from interfacial Rashba spin-orbit coupling, strain, and orbital reconstruction [1]. Here, we demonstrate that the magnetic anisotropy of ferromagnetic $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) can be effectively modulated by forming an interface with antiferromagnetic SrCuO_2 (SCO) in LSMO/SCO heterostructure grown on SrTiO_3 (001) substrates. Static magnetization measurements revealed an in-plane magnetic anisotropy in LSMO, which becomes significantly enhanced in the LSMO/SCO, an effect absent in the control sample LSMO/STO/SCO, underscoring the critical role of the interface with SCO. This enhancement was further corroborated by Ferromagnetic resonance (FMR) spectroscopy, which revealed increased resonance fields and magnetic damping in the LSMO/SCO. The theoretical analysis based on band structure calculations excludes Rashba-type spin-orbit effects at the LSMO/SCO interface. We posit that orbital reconstruction, leading to preferential orbital occupation in LSMO at the interface, is the driving mechanism behind the observed enhancement in magnetic anisotropy in LSMO/SCO.

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Keywords: Interfacial magnetism, Ferromagnetic resonance (FMR), Magnetic damping

Quantum Phases and Altermagnetism of a Bipartite Square-lattice in an Extended Hubbard Model

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Transition metal oxides are interesting due to the intricate interplay between the charge, spin, orbital and lattice degrees of freedom. This correlation gives rise to novel and exotic electronic and magnetic ground states including colossal magnetoresistance, spin ordering, charge ordering, superconductivity and topological behavior to name a few. In this study, we investigate the coupling between spin and charge degrees of freedom in transition metal oxides by studying a bipartite lattice model consisting of two distinct sublattices, A and B. We employ an extended Hubbard model that incorporates site energy, on-site and inter site Coulomb interactions, as well as Hund's direct exchange. The model is solved using a mean-field approach to understand various electronic and magnetic ground states of the model by varying the model parameters. The phase diagram of the model obtained in various parametric planes reveal exotic phases like the charge-ordered ferromagnetic and charge-ordered antiferromagnetic phases along with non-charge ordered magnetic phases. Furthermore, spin-resolved band structure calculations display a characteristic spin-splitting in momentum space within the charge-ordered antiferromagnetic phase, reminiscent of altermagnetic behavior. The projected band structure analysis further reveal that the altermagnetism originates from the strong coupling between the charge and spin degrees of freedom of the A- and B-sites. This work thus presents a

tunable framework for engineering novel alter-magnetic materials.

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Keywords: Altermagnetism; extended Hubbard model; mean-field approach.

Quantitative Kerr microscopy in Epitaxial Fe Thin Films

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Thin film magnetism has been a pivotal area of research in the field of spintronics due to its significance and broad applicability in modern magnetic devices. The change in magnetic properties in these films due to evolution and interaction of magnetic domains is essential for understanding mechanisms responsible for governing magnetic anisotropy, domain wall motion and magnetization reversal process[1]. Understanding magnetization reversal processes in epitaxial ferromagnetic thin films is crucial for tailoring their performance in spintronic and magnetic storage applications. Kerr microscopy gives a better picture of understanding these domains, by enabling direct imaging technique and performing real time analysis of how they evolve and corresponding modifications arise. For magnetic materials exhibiting higher anisotropy, the resolution of magnetization contrast in Kerr domain images is limited, making quantitative approaches more suitable for reliable analysis. By capturing domain images with orthogonal in-plane sensitivity through different Kerr configurations simultaneously and doing calibration of Kerr contrast under same sensitivity conditions, the vector field of complete magnetization cycles along the hysteresis loop can be calculated and plotted as a coded color or

vector image[2,3]. In this work we have performed quantitative Kerr microscopy to investigate magnetic domains and magnetization reversal in Ta/Fe/MgO thin film heterostructures, exhibiting clear cubic anisotropy behaviour. By calibrating Kerr contrast to saturation states at different angles, we obtain spatially resolved magnetization maps during field-driven reversal. The measurements reveal that reversal proceeds predominantly through the nucleation and propagation of 90° domain walls, consistent with the fourfold in-plane anisotropy of the Fe surface. These results provide direct insight into the microscopic mechanisms governing magnetization reversal in epitaxial Fe films and establish Kerr microscopy as a powerful tool for correlating domain dynamics with magnetic anisotropy in epitaxial systems.

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Keywords: Anisotropy, Quantitative approach, Cubic anisotropy

Quantum dot and half-metal due to disruption by topological defects at edge of zigzag graphene nano ribbon

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Topological defects in graphene are disruptions in the regular hexagonal lattice structure of carbon atoms. These defects can arise naturally during synthesis or it can be introduced intentionally to modify graphene's characteristics. Defects of our interest occur at the junction of two graphene domains with different lattice orientations, typically composed of a series of pentagon-heptagon pairs. Electronic and magnetic properties of the Zigzag-GNRs can

be modified by introducing topological defects. We present a systematic study of the effect of topological defects on the electronic structure and transport properties of graphenic nanostructures, aimed in particular towards active device applications through tailoring of the interplay of charge and spin degrees of freedoms of the pz electrons. Topological defects, when introduced at the edges, prominent localized quantum dot states appear at the transmission gap, originating from the chopping of the edge states in that of the pristine nano-ribbon. Localized states peaked at the defects lead to non-trivial drop of transmission amplitude below Fermi energy. With clustering of defects, the width of transmission dip broadens into a wider spin resolved transmission window leading to half metallic transport. ZGNR with topological defect at edge, as can be induced simply by attaching another patch of graphene, thus result into a half metallic window followed by a spin resolved quantum dot regime as a function of gate bias. Our method is based on Green's Functions computed within the mean field approximation of the Hubbard model within a tight binding basis which we will eventually derive from first principles.

Keywords: Topological defects, Quantum Dots, Half metal, Spin Filters.

Effect of hybrid modes on the spin-torque efficiency in the FM/FiM heterostructure

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Spin-orbit torque (SOT) [1] is gaining significant attention as an efficient alternative to conventional spin transfer torque (STT) for use in spintronic devices, such as non-volatile memories and logic devices. SOT generated by the spin Hall effect (SHE) in heavy metals provides a promising route to achieve efficient electrical control of magnetization. The SOT usually has two orthogonal components, i.e., damping-like

and field-like torque. Several techniques have been developed to characterize the SOT in a typical heavy metal-ferromagnet bilayer, including harmonic Hall voltage analysis, spin-torque ferromagnetic resonance (ST-FMR) [2], and the magneto-optical Kerr effect. Among these techniques, ST-FMR is an effective and convenient method, which is therefore extensively applied for SOT characterization. In this project, we are going to study the effect of hybrid modes on the spin-torque efficiency in the heterostructure consisting of ferromagnet (FM) like CoFeB and ferrimagnet (FiM) like YIG, capped with β -W via ST-FMR [3]. The insertion of the insulating ferrimagnet YIG not only provides low-damping magnonic excitations but also enables interfacial exchange-driven magnonic spin current across metal/insulator interfaces, offering a platform for coherent information processing. In comparison to the bilayer system (CoFeB/ β -W and YIG/ β -W), the trilayer system of YIG/CoFeB/ β -W is expected to exhibit hybrid resonance spectra. When the modes approach degeneracy, the hybridization is expected to enhance the spin pumping of the system and hence alter the spin-torque efficiency, which may help engineer the spin-torque efficiency for a long-range information transfer. The results will open a pathway toward hybrid spin-orbit torque devices and energy-efficient magnonic logic using the low-power benefits of magnonics with the scalability of spintronics.

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Keywords: Spin-orbit torque, Spin-torque ferromagnetic resonance, Hybrid modes

Persistence of Incommensurate Charge Ordering in Ligand-Disordered 1T TaSeTe

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Among the transition metal dichalcogenides (TMDCs), the polytypes of tantalum diselenides (TaSe₂) provide an excellent platform for studying the coexistence of a charge density wave (CDW) and superconductivity, both stemming from electron-phonon coupling and instabilities at the Fermi surface. Here, we successfully synthesized the 1T phase in TaSeTe using the chemical vapour transport (CVT) method and investigate the properties of the CDW in the novel ligand-disordered mixed chalcogen compound 1T-TaSeTe using bulk- and surface-sensitive diffraction and spectroscopy techniques, along with transport measurements. Low-energy electron diffraction (LEED) results indicate the persistence of an incommensurate CDW (ICDW) phase with a wavevector of $q_{ICDW} \approx 0.27a^*$. Temperature dependent core-level spectra reveal the presence of non-metallic nature of Ta 4f doublet splitting below CDW transition temperature (TCDW). The extracted CDW-induced splitting closely follows the resistivity behavior and confirms the emergence of ICDW transition at around 390 K, significantly lower than that of the parent compound TaSe₂ [1]. Strong Te doping leads to a semiconductor-like behavior, lying between the metallic and Mott insulating behavior commonly observed in the 1T Ta dichalcogenides [2]. Our results demonstrate that disordered chalcogen substitution doping can modify, yet preserve, the characteristic emergent electronic properties of a transition metal dichalcogenide. Further magnetic and magneto-transport measurements of this system may prove to be of considerable interest.

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Keywords: TMDC; CDW.

Magnon mediated spin pumping by coupled ferrimagnetic garnets heterostructure

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Magnon-magnon coupling plays a pivotal role in advancing the field of magnonics by enabling the coherent interaction between spin excitations in magnetic materials. This phenomenon is particularly significant in designing energy-efficient magnonic devices for next-generation information processing [1]. In this study, we provide clear evidence of magnon-magnon coupling in an all-insulator garnet heterostructure composed of Y₃Fe₅O₁₂ (YIG) and Tm₃Fe₅O₁₂ (TmIG). The avoided crossing region between the ferromagnetic resonance (FMR) modes of YIG (n=0) and TmIG (n=0) demonstrates magnon-magnon coupling at 200 K. Notably, the mode crossing occurs at a resonance frequency of $f = 6.88$ GHz, with a minimal resonance separation corresponding to a coupling strength of 2.8 mT shown in Fig.1.

These findings not only validate the magnon-magnon coupling mechanism but also open avenues for exploring hybrid magnon physics essential for developing ultralow-power magnonic devices. We further investigate the spin pumping phenomenon in coupled YIG/TmIG bilayers with a heavy-metal layer (Pt) via the inverse spin Hall effect (ISHE). The spin pumping voltage (V_{sp}) enhancement was observed in this system in compared to their reference single layer. This highlights the crucial role of interfacial exchange coupling [2]. The magnon transmission, occurring at the FMR positions of both ferrimagnetic (FiM) layers, emphasizes the effectiveness of magnon-mediated spin transport. The combination of a magnetic insulator with low damping and a heavy-metal interface also eliminates the complexities associated with conduction electrons, providing a simplified and accurate model to study spin-charge interconversion. These results underscore the importance of magnon coupling and its role in spin pumping, offering a pathway to optimize spin transport and manipulation for spintronic applications.

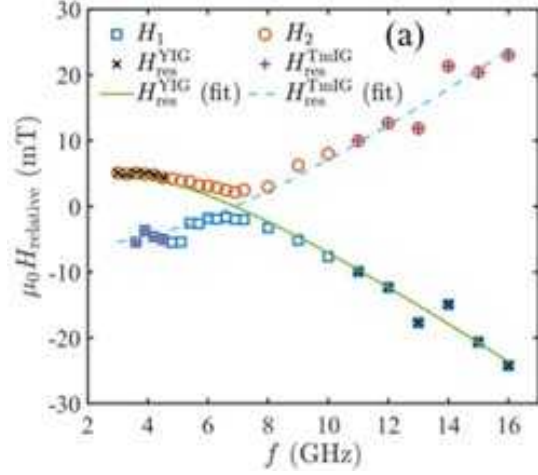


Figure 26: The full range frequency vs resonance field plot at 200 K showing avoided crossing

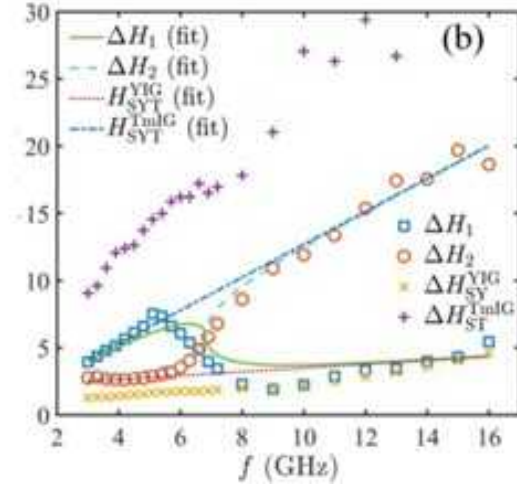


Figure 27: Linewidths of the two hybrid modes as a function of frequency

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Keywords: Magnon-magnon coupling, Ferromagnetic resonance (FMR), Inverse spin Hall effect (ISHE)

Investigation of magnetic and magneto-transport properties in non centrosymmetric antiferromagnetic semimetal GdGaSi

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In this work, we investigated the magneto-transport and magnetic properties of GdGaSi, having non-centrosymmetric tetragonal structure, with space group $I4_1md$. Our theoretical results are supported by experimental studies. First-principles calculations reveal that GdGaSi is an antiferromagnetic (AFM) semimetallic system, characterized by dominant electron-type charge carriers. In addition, the possible non-triviality of the crossing at the Fermi energy is consistent with isostructural LaPtSi-structured materials. The compound shows robust AFM ordering with a Neel temperature of 19 K, and spin-reorientation signature below TN. The semimetallic nature with positive magnetoresistance ($\approx 2\%$ at 2 K and 8 T) is observed from the magnetotransport data, having electrons as majority charge carrier, established from the Hall measurements. The strong correlation in magnetism and transport is supported by various observations, like (1) concordant transitions in $M(T)$ and $\rho(T)$ data, (2) change in the concentration and mobility of electron below TN, and (3) splitting of Kohler's plots in the two branches across the transition. Thus, our findings establish GdGaSi as a material with intertwined magnetic and transport degrees of freedom, within non-centrosymmetric lattice.

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Keywords: non-centrosymmetric, first-principles calculations, magnetotransport, spin reorientation

Synthesis and Characterisation of Single Crystals of Type-II Dirac semimetal 1T-PdSeTe

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Layered 2D transition metal dichalcogenides (TMDs) have recently emerged as an exciting class of quantum materials because of their rich electronic phases, ranging from charge density waves and superconductivity to topologically nontrivial states in conjunction with electronic nematicity [1]. Within this group, palladium-based TMDs have attracted significant attention. Recently, PdTe is reported as a type-II Dirac semimetal exhibiting unique surface states and transport behaviour [2]. And substitution of Se in place of Te enhances the superconducting transition temperature in this compound [3]. In this work, we report successful growth of single crystals of 1T-PdSeTe. This CdI₂-type layered transition metal chalcogenide are synthesized using the self-flux method. High purity Pd, Se and Te were thoroughly mixed and put together in quartz tube. The sealed quartz tube was then put in the furnace for 3 days at 800°C and then cooled to room temperature. The phase purity of the synthesized samples was examined by powder X-ray diffraction (XRD) and subsequent refinement, that confirmed the formation of a well-defined crystalline phase without detectable impurity peaks. The obtained crystals crystallize in trigonal space group $P3m1(164)$ with lattice parameter $a=b=3.91\text{\AA}$, $c=4.98\text{\AA}$, $\alpha=\beta=90$, and $\gamma=120$. To further establish crystallographic quality, single-crystal XRD measurements were performed, which verified the layered structure and provided orientation information consistent with the reported structure type. Magnetoresistance measurement as a function of temperature, magnetic field and angle led to the determination of topological

characteristics in this emergent quantum material.

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Keywords: PdSeTe, Topological materials, Nematic superconductivity, Resistivity, Magnetoresistance.

Chiral Phonon in XY type 2D layer magnet CrCl₃

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Two-dimensional van der Waals magnets CrX₃ (X = I, Br, Cl) have attracted significant interest for their tunable magnetic properties and potential applications in spintronic devices. In this study, we employ helicity-resolved Raman spectroscopy combined with first-principles calculations to investigate the chiral phonon dynamics and phase transitions in few-layer CrCl₃. Our results reveal that the degenerate E_g phonon modes exhibit distinct chiral behavior, showing a complete reversal of the incident light's helicity, while the non-degenerate A_g modes remain achiral. Angular momentum-resolved DFT calculations confirm these observations, demonstrating that the

E_g phonons possess quantized angular momentum ($l = \pm 1$) with left- and right-handed rotational vibrations. Temperature-dependent measurements uncover two critical transitions: a magnetic phase transition from paramagnetic to antiferromagnetic ordering at the Curie temperature ($T_c \approx 17$ K), evidenced by changes in phonon energy and intensity, and a structural transition from monoclinic to a mixed phase near 150 K, characterized by shifts in phonon energy and enhanced anharmonicity. These findings provide fundamental insights into the interplay between chiral phonons, magnetic exchange interactions, and lattice dynamics in 2D magnets, offering new opportunities for their application in spintronic and quantum devices.

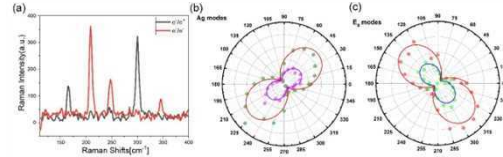


Figure 28: (a) Polarization dependent Raman for both RCP and LCP following Degree of polarization vs Raman shifts and (b-c) Raman intensity at different circular polarization angle vs Raman shifts.

Keywords: Helicity-resolved Raman spectroscopy, Structural phase transition, Magnetic phase transition

Joint Wannier Centers (JWCs) in Topological insulators and heterostructures: topological transition from the perspective of chemical bonding

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Based on generalization of geometric phases of Bloch electrons in multiple bands, we have recently proposed a scheme to obtain a spatial map of possible centers of localized orbitals constituted by the occupied states. The map is a collection of joint Wannier centers (JWC) of correlated hermaphrodite Wannier functions simultaneously contributed by electrons with their crystal momenta evolving through sets

of linearly independent directions in the BZ. In this work we present the study of topological transitions from the perspective of chemical bonding represented by the JWCs. We have explored two dimensional pristine monolayers, ribbons and hetero-structures described by the Kane-Mele model to pinpoint spatially resolved transition thresholds as function of distribution of JWCs. Evolution of JWCs has been also investigated from first principles in hydrogenated Xene and traditional bulk TI systems where emergence of inter-layer JWCs marks the onset of TI phase.

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Keywords: Topological Insulators, Kane-Mele model, Berry phase, Wannier center

Turning Superparamagnetic Nanoparticles into Ferromagnetic at Room Temperature via Molecular Functionalization for Magnetic Memory Applications

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Molecular functionalization of magnetic oxide nanoparticles can be considered an attractive approach for interfacial engineering, which can give rise to many exotic phenomena. Many reports focus on non-covalent approaches, but they can't create a robust interface. We consider

covalent surface modification of cobalt ferrite (CoFe₂O₄) nanoparticles (NPs) using a series of aryl diazonium salts to achieve a higher degree of surface functionalization and strong interfacial electronic coupling. This modification enables the formation of robust carbon-metal (C-M) covalent bonds at the nanoparticle-molecule interface, conferring chemical stability and magnetic tunability.[1,2] Notably, -electron-rich aryl compounds turn pristine superparamagnetic CoFe₂O₄ NPs into ferromagnetic at room temperature, with a marked increase in coercivity, remanent magnetization, and saturation magnetization, attributed to enhanced surface spin ordering on different sublattices and elevated effective anisotropy.[3] Zero-field-cooled and field-cooled magnetization curves demonstrate that the elevated blocking (T_b) and irreversibility (T_{irr}) temperatures, further corroborated by thermoremanent magnetization measurements, with T_b increasing from 245.9 K in pristine NPs to 336.8 K in aryl-CoFe₂O₄ NPs. Molecular-level modeling supports the origin of ferromagnetism in aryl-CoFe₂O₄ NPs. Our chemical approach allows tuning magnetic properties in pristine superparamagnetic NPs for advanced spintronic, spin-memory, and logic applications.[4]

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Keywords: Aryl diazonium; CoFe₂O₄ NPs; covalent functionalization; paramagnetic to ferromagnetic transition

Comparative Investigation of Exchange bias in $\text{Fe}_3\text{O}_4/\text{NiO}$ Core shell Structure by varying Shell thickness.

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Core shell (CS) Magnetic nanoparticles, a unique class of CS materials defined as the magnetic core encapsulated with shell that may either nonmagnetic or possess magnetic nature different from that of the core. These structural configuration enabling precise regulation of magnetic interaction, interface phenomena and surface chemistry, thereby received extensive attention across various field such as material science, physics, chemistry, bioengineering and biomedicine. we developed a $\text{Fe}_3\text{O}_4/\text{NiO}$ CS were Fe_3O_4 act as ferrimagnetic core while NiO serve as antiferromagnetic shell which creating a proper FM/AFM interface. The Fe_3O_4 core and $\text{Fe}_3\text{O}_4/\text{NiO}$ CS nanostructures were synthesized via hydrothermal method and AFM shell thickness controlled by changing Ni precursor concentration. The structural and vibrational changes of different shell thickness of $\text{Fe}_3\text{O}_4/\text{NiO}$ CS were observed through X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The elemental composition was analysed using X-ray photoelectron Spectroscopy (XPS) and the morphology and size of CS nanostructures were examined through High-Resolution Transmission Electron Microscopy (HRTEM). The magnetic properties of $\text{Fe}_3\text{O}_4/\text{NiO}$ CS nanostructures were investigated using Magnetic Property Measurement system (MPMS), focusing the changes on the magnetic saturation, remanence, coercivity and EB with systematic variation of AFM shell thickness. A non-monotonic behaviour was observed in coercivity and EB and this magnetic tunability with AFM shell thickness emphasizes the nanostructure potential for multiple applications.

Keywords: Core shell Structure, Hydrothermal Synthesis, Magnetic properties, Exchange bias.

Correlated Structural, Magnetic, and Transport Behavior in Ce_2FeAl_3

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Ce_2FeAl_3 , a composition among the Ce-Fe-Al system, is of interest for its 4f electron effects, magnetic ordering, and electron-lattice interactions. Ce_2FeAl_3 was synthesized by arc melting stoichiometric cerium, iron, and aluminum under argon, followed by annealing for homogeneity. The Energy Dispersive X-ray Spectroscopy (EDAX) analysis verified that the measured weight percentages of Ce, Fe, and Al closely match the expected stoichiometry. Powder X-ray diffraction (XRD) analysis confirmed that the sample crystallizes in cubic crystal structure, typically associated with the $Fd\bar{3}m$ space group, consistent with earlier reports [1]. Magnetization measurements as a function of temperature (M-T), carried out for zero-field-cooled (ZFC) and field-cooled (FC) sample, reveal a pronounced magnetic anomaly near 280 K, suggesting the onset of long-range magnetic ordering. The observed bifurcation between ZFC and FC curves indicates the presence of magnetic irreversibility. The M-H isotherms for Ce_2FeAl_3 indicate strong magnetic interactions at low temperatures, characterized by non-linear magnetization and weak hysteresis. The small hysteresis and unsaturated magnetization hint complex magnetic structure involving interactions between Ce 4f and Fe 3d spins [2]. The magnetization decreases with temperature, transitioning to a paramagnetic state above 280K, these features highlight the compound's complex and frustrated magnetic nature. Also, the specific heat capacity increases rapidly with temperature from near 0 K. The Cp vs T measurements indicates typical phonon contributions at low T (rapid rise) and saturation at higher T, with a possible anomaly near the peak region. The intricate coupling among structure, magnetism, and transport properties, particularly the temperature-dependent magnetic transition near 280 K, shall be explored in the backdrop of exploration in quantum materials. Neutron diffraction experiments will be crucial to unravel the correlation of magnetism

and magnetic structure.

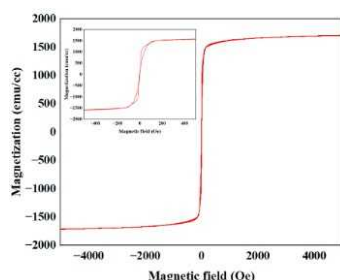


Figure 29: (a) SEM micrograph. (b) Observed and calculated (by Rietveld refinement method) profile. (c) Magnetic susceptibility versus temperature. (d) The magnetization graph at different temperatures and fields.

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Keywords: Magnetism, Heat Capacity, Neutron Diffraction

Strong Correlations in Rare-earth Intermetallic Compounds

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In rare-earth intermetallic compounds, the strong correlations between magnetic ordering and the crystal electric field (CEF) are essential to understand their many-body ground states. In such f-electron systems, CEF acts as a perturbation, lifting the degeneracy of the ground state of the magnetic element. By the virtue of its nature, the splitting of the ground state lies in the meV range, making the CEF excitations resonant to the THz range [1]. The CEF excitations at a low energy scale becomes crucial to study as it leaves its fingerprints on the exotic magnetic behavior in rare-earth orthoferrites, quantum spin liquid systems, Kondo lattices and metallic ferromagnets. Using THz time-domain spectroscopy, we have directly probed the underlying CEF states in two distinct material system: a prototype Kondo lattice system (CeAg₂Ge₂) and a metallic ferromagnet (PrSi). In CeAg₂Ge₂, we elucidate the low lying CEF state to strongly couple with the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, evidenced by a distinct blueshift in the transition frequency once the system enters the antiferromagnetic regime [2]. However, in PrSi, we identify a prominent increase in the population of the higher CEF state at the curie temperature, showcasing an intricate interplay between CEF and magnetic ordering in these strongly correlated systems [3].

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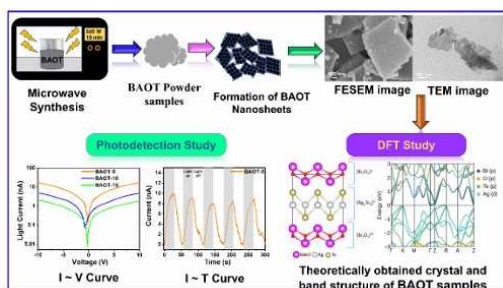
Keywords: Strongly correlated systems; CEF transitions; THz spectroscopy; Kondo lattice.

Microwave synthesis of BiAgOTe Nanosheets for Photoresponse Properties

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Metal-based oxy-chalcogenides exhibit remarkable physical and chemical properties, making them highly suitable for electronic and optoelectronic applications. In this study, bismuth silver oxytelluride (BiAgOTe) samples were synthesized using a microwave-assisted method and evaluated for their potential in photodetector applications. X-ray diffraction analysis confirmed the polycrystalline nature of the synthesized samples. Field emission scanning electron microscopy revealed nanosheet and nano walled surface morphologies across all samples, while energy-dispersive X-ray spectroscopy validated the presence and uniform distribution of constituent elements. X-ray photoelectron spectroscopy further confirmed the elemental composition and oxidation states. Optical characterization using UV-Vis spectroscopy showed bandgap values between 1.6 and 1.72 eV, confirming the semiconducting behavior of BAOT materials. Additionally, density functional theory calculations indicated low electron effective masses, pointing to high carrier mobility. The materials exhibited a clear photoresponse under both illuminated and dark conditions, and key photodetector performance parameters such as responsivity and detectivity were calculated, demonstrating the promising potential of BAOT as a viable material for next-generation photodetector technologies.



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Keywords: Bismuth silver oxytelluride; Microwave synthesis; Nanosheet; Photodetection.

Strong Correlations in Rare-earth Intermetallic Compounds

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Hexagonal boron nitride (hBN) is a highly attractive material for memristor fabrication owing to its wide bandgap, which ensures excellent insulation and enables devices with stable OFF states, which is an aspect that has remained challenging in transition metal dichalcogenide (TMD)-based memristors. To date, most hBN devices have been realized through elaborate techniques such as chemical vapor deposition (CVD), which offer limited potential for industrial scalability [1]. Liquid-phase exfoliation of hBN provides an alternative route, but devices fabricated by inkjet printing often suffer from high variability due to poor control over film quality [2]. Here, we demonstrate memristive switching in hBN devices fabricated using inks prepared by liquid-phase exfoliation and deposited via a scalable electrophoretic deposition (EPD) process. The resulting devices have been fabricated in two different architectures; a conventional crossbar geometry exhibiting stable resistive switching with an ON/OFF ratio of 10^3 ; and a non-conventional geometry employing eutectic InGa electrodes compatible with flexible electronics. In combination with the thermally stability and moisture resistant nature of hBN, our approach yields devices that

are not only robust but also compatible with large scale producibility.

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Keywords: 2D materials, Liquid phase exfoliation, Electrophoretic deposition, Resistive switching

Determination of Topological Characteristics in Single Crystals of WTe_2 by Magnetoresistance Measurements

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The topological states of quantum matter can be accessed by transport measurements, particularly through the angular dependence of magnetoresistance [1]. The discovery of extremely large magnetoresistance in semimetal tungsten ditelluride (WTe_2) is one case in example [2]. Here, we report the successful growth of high-purity WTe_2 single crystals by following the chemical vapor transport method. These single crystals exhibit extremely large magnetoresistance (23,282% at 2 K and 6.5 T). The variation of electrical resistance with B^2 dependence confirms perfectly compensated semimetallic characteristics of WTe_2 [3,4]. Resistivity measurements show no magnetic phase transition between 2-300 K. Electron-electron scattering dominates below 50 K, while electron-phonon scattering is prominent at higher temperatures. Shubnikov-de Haas oscillations were observed at low temperatures and high magnetic fields. Fast Fourier Transform (FFT) analysis of the oscillation spectrum revealed fundamental frequencies corresponding to Fermi surface

areas. A non-zero Berry phase is obtained from the Landau Fan diagram that confirms the non-trivial topological nature of WTe_2 . Furthermore, tantalum-doped WTe_2 crystals were also synthesized, with the X-ray diffraction revealing systematic peak shifts due to Ta substitution at the W site. The evolution of Berry curvature is tracked as a function of Ta doping. This work thus provides insight into the variation in topological characteristics in doped WTe_2 , paving a way for tuning its topological and transport properties.

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Keywords: topological semimetal; Magnetoresistance; Shubnikov-de Haas oscillations; Berry phase.

Emergent Non-collinear Magnetism in Cu-based Layered Hybrid Perovskites

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Transition metal based layered organic-inorganic hybrid perovskites (OIHPs) offer a versatile platform for exploring novel magnetic phenomena, enabled by their structural adaptability and tunable dimensionality [1,2]. We demonstrate a striking difference in magnetic behavior between two non centrosymmetric quasi-2D OIHPs, $(\text{C}_7\text{H}_9\text{NBr})_2\text{CuX}_4$ (where X = Cl or Br, and $\text{C}_7\text{H}_9\text{NBr} = 4$ bromobenzylammonium = A). While A_2CuCl_4 exhibits an in-plane ferromagnetic and out-of-plane antiferromagnetic-like response, its isostructural counterpart, A_2CuBr_4 , displays an opposite trend, despite both having in-plane magnetocrystalline anisotropy (MCA). Intriguingly, A_2CuBr_4 with having in-plane magnetic anisotropy exhibits magnetization behavior reminiscent of widely studied van der Waals magnets with out-of-plane anisotropy (e.g., CrI_3 , CrBr_3 , CrSiTe_3 , and CrGeTe_3). The stark contrast in magnetic response between the Cl and Br analogs is attributed to differences in their Dzyaloshinskii-Moriya interaction (DMI), and it is proposed that A_2CuCl_4 hosts a canted spin structure, while A_2CuBr_4 adopts to a transverse conical spiral arrangement. The presence of distinct non-collinear magnetism in these two OIHPs is corroborated from ac susceptibility measurements and evolution of these non-collinear ground states is depicted in their respective H-T phase diagrams. Further, a systematic evolution of magnetization has been demonstrated in these OIHPs with mixed halide

ligand composition. In essence, this study provides the microscopic origin of non-collinear magnetism and its ligand tunability in Cu based layered OIHPs.

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Keywords:

Temperature-induced spin-reorientation transition (SRT) in FeCoB/Pt multilayers with perpendicular magnetic anisotropy

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Magnetic anisotropy plays a crucial role in determining the preferred orientation of magnetization in thin films and multilayers, thereby controlling the stability of magnetic states [1]. Perpendicular magnetic anisotropy (PMA) at heavy-metal/ferromagnet interfaces arises from strong spin-orbit coupling in the heavy metal and orbital hybridization at the interface. Therefore, the study of interfaces and their correlation with magnetic properties, such as PMA, in-plane anisotropy, and SRT, is crucial. FeCoB/Pt systems are particularly noteworthy, as Pt provides a strong spin Hall effect and generates Dzyaloshinskii-Moriya interaction (DMI), making it promising for fast, low-current switching in memory applications [2]. The multilayers (MLs), [FeCoB (0.8 nm)/Pt (1.5 nm)], were deposited on Si(001)/Pt (5 nm) substrates using magnetron sputtering. A Pt buffer layer (5 nm) was introduced to prevent Si diffusion from the substrate. Multilayer's structural parameters were determined by X-ray reflectivity (XRR), while X-ray diffraction (XRD)

and magneto-optical Kerr effect (MOKE) measurements were used for structural and magnetic properties. These multilayers exhibit PMA through interfacial hybridization with Pt d-states and interface-related structural modifications. However, this PMA weakens progressively with increasing annealing temperature, around 450 °C, a spin-reorientation transition (SRT) occurs, where the magnetization switches from a perpendicular to an in-plane orientation. This transition occurs because interfacial anisotropy, which typically scales with a power of the magnetization, decreases more rapidly with increasing temperature, resulting in a reduction in effective anisotropy (K_{eff}). When the demagnetizing energy eventually exceeds K_{eff} , the system undergoes the perpendicular-to-in-plane reorientation.

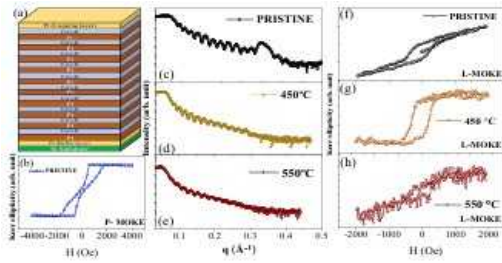


Figure 30: Fig.(a) [FeCoB/Pt]10 Multilayer structure. Fig.(b) Polar MOKE -exhibiting PMA. Fig. (c), (d) and (e) XRR, Pristine, 450°C and 550°C respectively. Fig.(f), (g) and (h) Longitudinal MOKE, Pristine, 450°C and 550°C respectively

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Keywords: FeCoB/Pt, Perpendicular Magnetic Anisotropy, Spin-reorientation transition, XRR

Optimization of Bi₂Se₃/MoSe₂ Heterostructure for a Tunable Interfacial Vibration Mode

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The integration of topological insulators (TIs) and transition metal dichalcogenides (TMDs) into van der Waals heterostructures offers a versatile platform for next-generation quantum and optoelectronic devices. A key challenge lies in controlling interfacial properties to exploit their synergistic functionalities. In this work, we optimize chemical vapor deposition (CVD) growth parameters for high-quality Bi₂Se₃ and MoSe₂, enabling the reliable fabrication of Bi₂Se₃/MoSe₂ heterostructures [1-2]. Thickness-dependent Raman spectroscopy of the individual layers confirms the expected layer-number evolution of the out-of-plane A_{1g} and in-plane E_{2g} modes in both materials. Upon forming heterostructures, we observe significant modifications in the vibrational spectra, including a pronounced softening and broadening of the Bi₂Se₃ A_{1g} mode and the MoSe₂ A_{1g} mode, indicative of interfacial charge transfer and phonon coupling. Notably, systematic variation of layer thickness allows active tuning of these interfacial vibrational modes, directly modulating the electron–phonon coupling strength at the interface. Our results pave a framework for engineering Bi₂Se₃/MoSe₂ interfaces and demonstrate thickness-mediated vibrational tuning as an effective strategy for controlling interfacial properties with implications for tunable photodetectors, sensors, and quantum technologies.

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, Fangzhu Qing, Matjaz Valant and Zhiming M. Wang. Royal Society of Chemistry.

Keywords: Synergistic effect, topological insulators, tunable photodetectors

Interface-induced spin-orbit coupling mediated weak antilocalization effect in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ thin films on (001) oriented Si substrate

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$\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) is extensively characterized by its substantial negative magnetoresistance (MR), predominantly governed by the double exchange interaction and magnetic field-induced suppression of spin-disorder scattering. However, LSMO films fabricated via pulsed plasma sputtering directly on (001)-oriented Si substrates, without buffer layer, exhibit pronounced deviations in properties. Cross-sectional transmission electron microscopy (TEM) analysis of the LSMO film revealed the presence of a distinct interfacial layer approximately 8 nm in thickness, characterized by reduced density and significantly elevated electrical resistivity relative to the overlying conductive phase. The interfacial region forms a distinct conduction channel parallel to the upper bulk regime and tunes the functional properties of LSMO. Temperature-dependent resistivity measurements reveal a metal-to-insulator transition accompanied by a low-temperature upturn in resistivity. This low-temperature resistivity upturn is predominantly governed by Kondo-like scattering arising from interfacial localized spins, rather than electron-electron interactions. Furthermore, the SOC on Mn atoms in LSMO is weak, and thus, the SOC-induced phenomena, weak antilocalization (WAL), is not observed in its bulk regime. However, SOC is enhanced at the interface, producing the WAL effect. Low-field magneto-conductivity data is fitted with the Hakimi-Larkin-Nagaoka (HLN) model, and the small negative value of the prefactor further confirms the WAL effect. One of the key attributes of WAL is positive MR,

which is observed at the low field regime, and it is suppressed by negative MR at high field. Our findings reveal dual magnetoresistance in both in-plane and out-of-plane field configurations. At 20K, the maximum positive MR is found to be $\approx 12\%$ for the in-field configuration, while it changes to $\approx 7\%$ for the out-of-plane field orientation. Similarly, the maximum negative MR is $\approx 42.5\%$ for the in-plane oriented field, which reduces to $\approx 30\%$ for the out-of-plane field geometries. Our observations provide insights into interface-induced substantial SOC for future spintronics applications.

Keywords: Spin-Orbit Coupling, Weak Antilocalisation, Magnetoresistance, Thin Film

Magnetic Hardening via Strain in Co_2FeAl Heusler Alloy Flexible Films

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Spintronics has emerged as a transformative field, driving the development of spin-based electronic devices. The rising demand for flexible and wearable technologies highlights the need for materials with high spin polarization and significant magnetostriction coefficients [1,2]. In this context, Heusler alloys, known for their high spin polarization, elevated Curie temperatures, and low magnetic damping, are promising candidates for such applications. Among these, Co-based Heusler alloys, such as Co_2FeAl (CFA), typically exhibit high Curie temperatures compared to oxide half-metals, making them promising candidates for spintronics applications at room temperature

Fig: (a) Strain dependence of squareness ratio with the magnetic field applied along the easy and hard axes. (b) with application of tensile and compressive strain of 0.12% [3]. Despite their potential, the magnetoelastic properties of Heusler alloys remain underexplored. This work addresses the gap by investigating the magneto-mechanical coupling in CFA films deposited on flexible polyimide (PI) substrates. Tensile and compressive strains, induced by substrate bending, are used to modulate the magnetic anisotropy. The angular dependence of coercivity (H_c) under tensile and compressive strains, reveals that strain along the easy or hard axes can reversibly tune M_r/M_s Fig.(a) and H_c , enabling a 90° rotation of the magnetic anisotropy Fig.16(b). Further magnetic hardening and increase in magnetization are achieved via compressible strain.

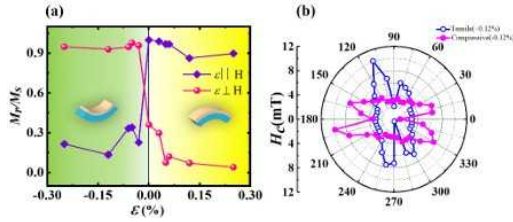


Figure 31: (a) Strain dependence of squareness ratio with the magnetic field applied along the easy and hard axes. (b) with application of tensile and compressive strain of 0.12%

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Keywords: Flexible spintronics, Magneto-elastic Coupling, Heusler alloy, Anisotropy

Evolution of electronic structure in Weyl semi-metal $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$

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Transition metal dichalcogenides such as WTe_2 and MoTe_2 , in their orthorhombic (Td) phases, have garnered attention as type-II Weyl semimetals due to their extremely large non-saturating magnetoresistance (XMR) and topological surface states. In this work, we investigate the structural evolution and transport characteristics of $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$ single crystals ($x = 0.1-0.5$), aiming to elucidate the impact of Mo doping on phase stability, magnetoresistance, and the emergence of Weyl states. Increasing Mo content induces a progressive transition from the non-centrosymmetric Td phase to the centrosymmetric monoclinic 1T phase. Notably, the $x = 0.3$ composition exhibits maximal stabilization of the Td phase, with reduced lattice distortion and improved crystallinity. Transport measurements reveal a monotonic decrease in magnetoresistance (MR) and residual resistivity ratio (RRR) with increasing Mo content, attributed to enhanced impurity scattering and increased electron-hole asymmetry. Despite the general decline in transport performance at higher Mo concentrations, the $x = 0.3$ sample stands out to retain substantial MR and displays sharp, well-defined structural and electronic features. X-ray photoelectron spectroscopy (XPS) reveals asymmetric charge redistribution between Te-Mo and Te-W bonds across all compositions. The experimental electronic band structure confirms the presence of Weyl states at Fermi level exclusively in the sample with $x = 0.3$. Our results underscore the critical role of alloy composition in governing the phase behavior, transport properties and electronic structure of $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$ making it a promising platform for exploring tunable Fermi arc states and next-generation spintronic applications.

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Keywords: Weyl semimetals; Magnetoresistance; Topological surface states; Residual resistivity ratio

Interface-induced enhanced magnetic anisotropy and observation of dual magnetoresistance in LSMO thin films on (001) Si substrate

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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 $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) films on (001) oriented silicon substrates using pulsed plasma deposition techniques. The LSMO thin films with varying thicknesses (<20 nm) demonstrate a strong magnetic anisotropy on the order of 106 erg/cm^3 , 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 $\approx 7\%$ for 12.4 nm films and $\approx 12\%$ for 20.0 nm films, while out-of-plane MR variation is limited to $\pm 0.8\%$. The in-plane MR switching field occurs at ± 0.2 kG (coercive field), whereas the out-of-plane MR switching field is much higher (up to ± 5 kG), indicating strong anisotropy modulated by interfacial exchange coupling strength. 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.

Keywords: Magnetic Anisotropy, Stoner-Wohlfarth Model, Density Functional Theory, Thin Films

Development of a Time-Resolved Magneto-Optical Kerr Effect (TR-MOKE) Setup for Probing Ultrafast Spin Dynamics in Magnetic Heterostructures

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Time-Resolved Magneto-Optical Kerr Effect (TR-MOKE) spectroscopy overcomes the limitation of temporal resolution by combining femtosecond pump-probe optics with magneto-optical detection, enabling the direct measurement of ultrafast demagnetization, damping,

spin pumping, and spin-orbit interactions. Developing a TR-MOKE platform is therefore essential to investigate non-equilibrium spin transport and interfacial exchange in complex heterostructures. Over the past three decades, TR-MOKE has progressed from the first observations of femtosecond demagnetization [1] and light-induced control of magnetic order to becoming a versatile platform for exploring diverse spin phenomena. It has been used to optically tune Ruderman-Kittel-Kasuya-Yoshida (RKKY) coupling and perpendicular magnetic anisotropy in synthetic antiferromagnets, enabling femtosecond control of interlayer exchange interactions [2]. In addition, TR-MOKE has provided all-optical access to magnetic damping and spin pumping in synthetic antiferromagnetic systems [3], revealed electrical tunability of femtosecond spin transport in graphene spin-field-effect junctions [4], and recently been extended to Altermagnets [5], where symmetry-driven spin responses go beyond the conventional ferromagnetic and antiferromagnetic framework. Together, these advances demonstrate the power of TR-MOKE in uncovering fundamental spin interactions and guiding the design of ultrafast spintronic materials. In this context, we are developing a TR-MOKE setup to provide a versatile platform for probing ultrafast spin transport, damping, and spin pumping in ferromagnet/non-magnet heterostructures. This work is important because it will enable direct exploration of femtosecond spin processes that underpin ultrafast memory, spin-orbit torque devices, and low-power spin logic technologies.

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Keywords: TR-MOKE, Ultrafast Spin Dynamics, Spin Pumping, Altermagnets.

Exploring Local Structural Distortion and Magneto electric Behavior in Skyrmion Host Cu_2OSeO_3

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Cu_2OSeO_3 (CSO) is a well-known multiferroic insulator that hosts a skyrmion lattice and helical magnetic phases below its Curie temperature ($T_c \approx 59\text{--}60\text{ K}$) [1]. Crystallizing in the chiral non-centrosymmetric cubic space group $P2_13$, CSO exhibits long-range collinear ferrimagnetic order, which is symmetry-incompatible with the reported metrically cubic structure down to 10 K [3, 4]. This naturally raises the question of whether the crystal structure undergoes a local symmetry reduction within a globally cubic structure. We investigated this paradox and find that Cu_2OSeO_3 possibly undergoes a weak structural change below T_c , as evidenced by the anomalous broadening (opposite to thermal broadening) of low-angle Bragg peaks. This is further supported by our magnetization data, which clearly demonstrates a thermal hysteresis between FCC and FCW. To probe possible local distortions directly, we performed temperature-dependent Extended X-ray Absorption Fine Structure (EXAFS) measurements at the Cu and Se K-edges. Preliminary analysis suggests local modifications in Cu–O and Se–O coordination environments across T_c . These findings support the hypothesis of local structural distortion triggered

by magnetic ordering. Additionally, CuOSeO is reported to show a magnetoelectric effect below 60 K. The ME behaviour of this compound is broadly studied in its single-crystalline form [2, 5]. However, S. Seki et al. investigated the ME behaviour in polycrystalline Cu_2OSeO_3 , which shows a dielectric anomaly near T_c in the absence of any magnetic field [6]. Interestingly, such an anomaly in temperature-dependent dielectric data is absent in the single-crystalline compound [2]. Thus, the ME property in this compound seems intriguing. More importantly, no direct evidence of ME properties in this compound has been reported to date using temperature dependent pyroelectric current measurements. Thus, we reinvestigated the ME property of polycrystalline Cu_2OSeO_3 by employing temperature-dependent dielectric and pyroelectric current measurements in the presence of magnetic fields. Temperature-dependent dielectric measurements at 50 kHz under varying magnetic fields reveal no anomaly in zero field, but pronounced dielectric features appear at 400 Oe and 600 Oe, near T_c . This field-tunable dielectric behaviour indicates a magnetoelectric (ME) response that differs from the behaviour observed in single crystals [2]. Pyroelectric current measurements (performed in zero magnetic field) did not show typical switching behaviour, while DC current data exhibit subtle anomalies that require further analysis for reliable interpretation. Thus, our study points towards the presence of hitherto undetected subtle structural changes and represents a comprehensive investigation of ME behaviour using simple dielectric and pyroelectric current measurements in polycrystalline CSO.

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Keywords: Cu_2OSeO_3 ; EXAFS; Dielectric anomaly; Magneto-structural coupling

Proton Irradiation Studies on $\text{Bi}_{1.95}\text{Sb}_{0.05}\text{Se}_3$ Topological Insulator Thin Films

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$\text{Bi}_{1.95}\text{Sb}_{0.05}\text{Se}_3$ (BSS) thin films were grown by pulsed laser deposition (PLD) and irradiated with 200 keV proton fluences of 10^{14} , 10^{15} , and 10^{16} ions cm^{-2} to study the charge compensation. SEM images in Fig.17 show that the grain size decreases with an increase in ion fluence (top left). The higher grain density indicates the increase in disorder, which is consistent with the broader peaks observed in the GI-XRD patterns at higher ion fluence. Temperature-dependent resistivity measurements reveal that insulating behavior in the pristine sample becomes more pronounced with the high ion fluence (top right). All the samples show an upturn in resistance at $T < 20$ K; however, the $R(T)$ is different for samples irradiated with the ion fluences of 10^{14} and 10^{16} ions cm^{-2} . Magneto conductance curves show weak antilocalization (WAL) in all films, i.e, pristine and proton irradiated samples (bottom left), and are fitted with the Hikami Larkin Nagaoka Equation [1]. Proton irradiated samples (10^{14} ions cm^{-2}) exhibit the highest phase coherence length of ≈ 100 nm at 4 K and decrease with an increase in ion fluence. Hall measurements show that the carrier density varies from $2 \times 10^{19} \text{ cm}^{-3}$ (pristine) to $4 \times 10^{19} \text{ cm}^{-3}$ as the ion fluence increases. These results indicate that proton irradiation yields better topological insulator properties at lower ion fluences; however, at higher ion fluences, it affects the phase coherence length and mobility due to an increase in disorder and grain boundary density.

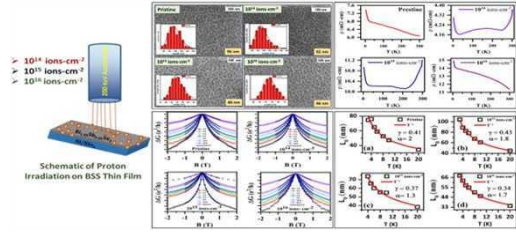


Figure 32: Effect of proton irradiation on the structural and transport properties of BSS thin films, showing reduced grain size (top left), increased resistivity (top right), presence of WAL (bottom left), and suppression of phase coherence length with increasing ion fluence (bottom right).

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Keywords: Hikami–Larkin–Nagaoka (HLN) model, phase coherence length, disorder-induced scattering

Artificial Synaptic Behaviour of Ag/Ti₃CNT_x/PMMA/ITO-Pet Nanocomposite Thin Films

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Highly power-efficient computing can be achieved via brain-inspired architectures, which mimic the structure and functions of the human brain using non-volatile memory (NVM) [1]. However, current NVM technologies face limitations in terms of device scalability, electrical performance, and operating voltage—key parameters for developing next-generation computing systems capable of transcending the constraints of Moore’s Law [2]. To address these challenges, exploring novel composite materials with finely tuned compositions is imperative. Such materials can potentially enable memristive devices engineered for ultra-low power consumption and enhanced functional performance[3]. MXenes represent an emerging class of 2D materials derived from transition metal carbides, nitrides,

or carbonitrides, generating considerable attention. Owing to their exceptional electrical conductivity, high hydrophilicity, and excellent mechanical strength, MXenes are considered highly promising candidates for advanced energy storage applications[4]. Because of its layered nanostructure, constituent elements, and terminal surface functions, Ti₃CNT_x carbonitride MXenes have appealing physicochemical features. The electrical configuration and the size of the crystalline lattice are influenced by the carbon atoms in the structure [5]. In this work, we synthesised Ti₃CNT_x MXene using a combined etching solution of hydrochloric acid (HCl) and lithium fluoride (LiF). The structural and surface morphological study revealed the crystallinity and uniformity of the material. Current-Voltage measurements of the Ag/Ti₃CNT_x/PMMA/ITO-Pet sheet device showed the synaptic properties. The device effectively replicated several synaptic learning processes present in biological neural networks, such as spike timing-dependent plasticity (STDP), short-term and long-term potentiation and depression (STP/STD, LTP/LTD), excitatory postsynaptic currents (EPSC), and paired-pulse facilitation (PPF).

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Keywords: Non-Volatile Memory, MXene, Synaptic properties, Neural networks.

Enhanced electrochemistry at $\text{Ti}_3\text{C}_2\text{T}_x$ MXene edge

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The electrochemistry at the edge of 2D materials has been a topic of immense interest in the past decade.¹ While it has been proven for 2D materials like graphene, transition metal chalcogenides, and black phosphorus, etc, the electrochemistry at the edge of newly developed MXene remains elusive.^{2,3} Herein, we conducted a comprehensive investigation of the electrochemical behavior of $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes at both basal and edge planes using various electrolytes. Our findings reveal that the electrochemical activity at the edge sites is significantly different from that at the basal planes. These insights open new avenues for employing MXenes as catalysts or catalyst supports in diverse electrochemical systems. Also, the present work highlights the importance of structural and morphological control in maximizing the functional potential of MXene-based materials.

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Keywords: MXenes, inherent electrochemistry, edge plane, basal plane

Quantitative Evaluation of Spin–Orbit Torque Efficiency in Mn_2Au Antiferromagnet-Based Heterostructures

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Antiferromagnet (AFM)/ferromagnet (FM) heterostructures have emerged as promising platforms for efficient spin–orbit torque (SOT)–driven magnetization control in next-generation spintronic devices. In these systems, AFMs with strong spin–orbit coupling (SOC) can serve as effective spin current sources, enabling the manipulation of an adjacent FM layer. Among various AFMs, Mn_2Au has drawn significant attention owing to its collinear AFM ordering, exceptionally high Néel temperature (≈ 1300 K), and strong SOC, making it a highly attractive candidate for spin Hall effect (SHE)–based spin current generation. The large SOC in Mn_2Au facilitates the generation of spin currents via the SHE, which exert torques on the FM layer and alter its magnetization dynamics. Previous studies, particularly using spin pumping, have demonstrated the remarkable efficiency of Mn_2Au in spin-to-charge conversion. Singh et al. reported a large spin Hall angle ($\theta_{SH} \approx 0.22$) and high spin Hall conductivity ($\approx 1.4610^5 (\hbar/2e)^{-1} \text{m}^{-1}$) in $\text{Mn}_2\text{Au}/\text{CoFeB}$ bilayers, along with an effective spin-mixing conductance on the order of 10^{18}m^{-2} [1]. These values are comparable to, and in some cases surpass, those observed in heavy metals such as Pt, highlighting Mn_2Au 's strong charge-to-spin conversion and spin transmission efficiency. More recently, Jena et al. employed spin pumping and inverse spin Hall effect (ISHE) measurements in $\text{Mn}_2\text{Au}/\text{Py}$ heterostructures, showing that the insertion of a Cu spacer layer significantly enhances spin transmission [2]. In this work, we present a systematic investigation of the SOT efficiency in $\text{Mn}_2\text{Au}/\text{CoFeB}$ heterostructures. By employing spin–torque ferromagnetic resonance (ST-FMR) and harmonic Hall measurements, we extract key parameters including damping-like torque efficiency, field-like torque efficiency, and spin Hall conductivity. These results provide

deeper insights into the spin current generation and torque mechanisms in Mn_2Au -based heterostructures, advancing the understanding of their potential for future spintronic applications.

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Keywords: Antiferromagnet; Spin-Orbit torque; Spin-torque ferromagnetic resonance.

Study of β -W/CoFeB Bilayer Device for Spintronic Application

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Spintronics is one of the emerging fields to replace conventional electronic devices, especially for reducing loss due to the heating effect in electron-based devices [1]. Spin-based device also increases efficiency, stability, and durability. There is a quest to find some heavy transition metal elements or compounds with a large spin-orbit coupling for spintronic devices. The β phase of W is one of the potential candidates in this regard as it provides high spin Hall angle (SHA) and large spin-orbit torque (SOT) [2]. This is the most exciting element, which has a wide application for spintronic devices due to its higher SHA (-0.5) than other elemental solids [3]. The spin-orbit torque in this system is mainly originated from the interface rather than bulk of the films, while the spin Hall effect with strong spin-orbit scattering can excite magnetic precession in an adjacent ferromagnetic film [4,5]. In fact, the flow of alternating current through a β -W/CoFeB bilayer structure

generates an oscillating transverse spin current in β -W and the resultant transfer of spin angular momentum to CoFeB induces ferromagnetic resonance dynamics. Here, we demonstrate the fabrication of the β W/CoFeB heterostructures for spintronic application and checked the structural and surface properties using Grazing Incidence X-ray Diffraction (GIXRD) and X-ray Reflectivity (XRR) measurements. Here we show the SHA and spin Hall ratio using Ferromagnetic resonance and check whether it is suitable for spintronics devices.

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Keywords: Spintronics, Spin Hall angle, Material stability.

LARGE INVERSE ORBITAL HALL EFFECT IN $\text{Cr/Pt/Co}_{40}\text{Fe}_{40}\text{B}_{20}$ THIN FILM HETEROSTRUCTURES

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The electron has both spin and orbital angular momentum. Spintronics utilizes the spin angular momentum of the electron, while the orbital counterpart has largely been overlooked due to the long-standing belief that it is quenched by the crystal field in solids. Recent

studies, however, have demonstrated the significant role of orbital angular momentum (OAM) in transport phenomena. The transverse accumulation of OAM in certain materials under an applied electric field is known as the Orbital Hall Effect (OHE), which does not require spin-orbit coupling (SOC), unlike the Spin Hall Effect (SHE)[1]. As a result, low-SOC materials (Cr, Ti, Mn, etc.) have shown large orbital Hall conductivity (OHC), even surpassing the spin Hall conductivity of many high-SOC materials (Pt, W, etc.), making them promising sources for controlling the magnetization dynamics of ferromagnets [2]. Since orbital currents cannot directly interact with magnetization, they must be converted into spin currents via the SOC of the ferromagnet itself or by using an additional conversion layer between the low-SOC material and the ferromagnet. The inverse phenomenon, the Inverse Orbital Hall Effect (IOHE), generates a transverse voltage in the low-SOC layer when orbital currents are pumped into it from the ferromagnet at ferromagnetic resonance [3]. In our study, we used Cr as the orbital current sink and $\text{Co}_{40}\text{Fe}_{40}\text{B}_{20}$ as the orbital current source, and observed a significant enhancement in the measured signal when a Pt (1.6 nm) layer was inserted in the Cr (10 nm)/ $\text{Co}_{40}\text{Fe}_{40}\text{B}_{20}$ (9 nm) bilayer. The role of Pt here is to convert the spin current from $\text{Co}_{40}\text{Fe}_{40}\text{B}_{20}$ into orbital current, and this large enhancement cannot be attributed to the inverse spin Hall effect (ISHE), as a comparatively smaller signal was observed in the Pt (6 nm)/ $\text{Co}_{40}\text{Fe}_{40}\text{B}_{20}$ (9 nm) bilayer. A systematic study of the IOHE signal with varying Cr thickness revealed a large orbital diffusion length of Cr.

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Keywords: Orbital Hall Effect, Orbital Current, Spin Current

Orbital glass behaviour and local symmetry breaking in charge-transfer insulating CoFe_2O_4

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Structural, orbital, and electronic properties of cobalt ferrite are investigated using advanced experimental methods. Synchrotron X-ray diffraction confirms phase purity and reveals a temperature-dependent superlattice reflection between $T_o \approx 200$ –100 K, indicative of short-range orbital ordering driven by cooperative Jahn-Teller distortions. The disappearance of this feature below 100 K signals orbital freezing and the formation of a glass-like orbital state. Hard X-ray photoelectron spectroscopy identifies multiplet splitting and charge-transfer satellites in the Co and Fe 2p core levels, evidencing mixed valence states and strong electron correlations. Extended X-ray absorption fine structure measurements show enhanced local disorder in Fe–O and Co–O octahedra, attributed to static, asymmetric distortions from cation redistribution and oxygen vacancies. Complementary Raman spectroscopy reveals phonon anomalies and enhanced spin phonon coupling in the same temperature window, while magnetic measurements highlight spin reorientation and exchange interaction anomalies consistent with orbital dynamics. Furthermore, room temperature resonant photoemission spectroscopy confirms strong Fe/Co 3d–O 2p hybridization. The estimated on-site Coulomb interaction energy (U) and charge-transfer energy (Δ), derived from occupied and unoccupied spectra, establish CFO as a charge-transfer insulator ($U > \Delta$). Together, these findings point to a frustrated orbital state in CFO, shaped by cooperative Jahn-Teller distortions, disrupted long-range

coherence, and orbital glass behaviour, thereby providing new insights into the interplay of orbital, spin, and lattice degrees of freedom in spinel systems.

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Keywords: Jahn-Teller distortions; orbital ordering; spin-phonon coupling; orbital glass, superlattice

Soft Magnetic Composites of Fe-Alloys and Mn-Zn Ferrite: Structural and Magnetic Properties for Advanced Electronics

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Soft magnetic composites (SMCs) have emerged as promising materials for aerospace and defence electronic applications due to their high magnetic permeability, reduced weight, thermal stability, and elevated Curie temperatures [1,2]. In this study, Fe, Fe-Ni, and Fe-Co alloy systems were integrated with Mn-Zn ferrite to develop advanced SMCs tailored for high-frequency applications. The composites were synthesized via a novel polyol-assisted method, which enabled uniform dispersion and strong interfacial coupling between the metallic and ferrite phases. Structural analysis confirmed the coexistence of a face-centered cubic (FCC)

metallic phase with the spinel ferrite structure, with grain sizes ranging from 13 to 50 nm. Magnetic properties of SMC show that the inclusion of $\text{Mn-ZnFe}_2\text{O}_4$ effectively suppressed eddy current losses while preserving high magnetic permeability. Among the investigated systems, $\text{Fe/Mn-ZnFe}_2\text{O}_4$ exhibited the highest saturation magnetization of 164 emu/g, whereas the $\text{Fe-Ni/Mn-ZnFe}_2\text{O}_4$ composite demonstrated the lowest magnetic anisotropy energy of 5.5 kJ/m³ obtained using ferromagnetic resonance. These results underscore the potential of these hybrid SMCs to deliver a tunable combination of high magnetization, low coercivity, and minimal loss, making them suitable for next-generation magnetic components in power electronics, RF/microwave devices, and electromagnetic interference (EMI) shielding applications.

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Keywords: Soft magnetic composites, Polyol synthesis, High-frequency applications, Heat loss

Quantum criticality in the Frustrated Kondo Screened Two-Impurity Model

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Recent experimental observations have shown the rare coexistence of a heavy fermionic strange metallic state with a quantum spin liquid phase in the frustrated compound $\text{Ba}_4\text{Nb}_{1-x}\text{Ru}_{3+x}\text{O}_{12}$ by tuning the Nb concentration[1]. In recent decades, spin liquids as well as strange metals have come under intensive studies as candidates for quantum matter. Spin liquids are interesting because of the absence of long-range order even down to zero temperatures and the presence of fractionalised deconfined excitations. The other exotic phase in the diagram, the strange metal, is particularly important as the parent metal of high-temperature superconductors in the cuprates, and shows

an anomalous linear temperature dependence in its resistivity. We address key questions : whether a minimal impurity model can describe the metal–insulator transition in infinite dimensions , and what fluctuations drive the system from a metallic to a ground state of spin liquid insulating phase? We propose a minimal effective impurity model comprising two localized correlated impurities, with one of them coupled to a conduction bath (c-bath) through a Kondo spin-exchange interaction and the two impurities interacting with each other through another spin-exchange coupling. We obtain the low-energy phase diagram (see Fig.19) using the recently developed unitary renormalization group (URG) method[3], and it exhibits a line of quantum critical points (QCPs) that separates two phases- one where the bath screens the impurity (KS) and another where the two impurities screen each other (IS). The low-energy effective theory for impurity model in KS phase displays local non-Fermi liquid excitations that are not adiabatically connected to the local Fermi liquid. The impurity excitations in the IS phase are instead gapped due to the absence of c-bath screening; the breakdown of Kondo screening from KS to IS is seen through the growth of spin-flip correlations between the two impurity sites accompanied by the suppression of spin-flip correlations between the impurity and the c-bath (see Fig.20). Upon mapping the local physics of the impurity model to that of the material studied above (in the limit of infinite dimensions), the gapless KS phase would describe the non-Fermi liquid phase seen in the material, while the gapped IS phase with its remnant spin-flip correlations would describe the spin-liquid phase. In this way, our model explains, from a local perspective, the coexistence of non-Fermi liquid and spin-liquid phases in a heavy fermion compound [1].

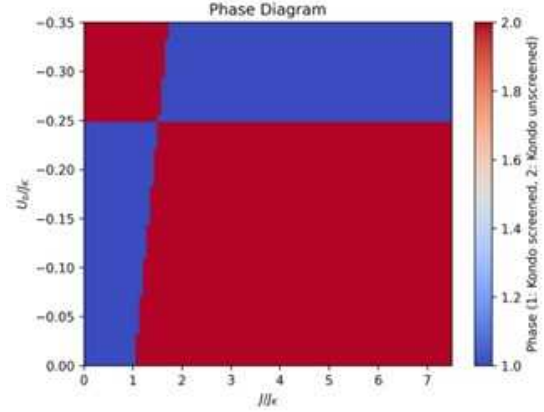


Figure 33: Phase diagram of the two-impurity model, where blue region refers kondo screened phase (KS) and red region refers the impurity screened phase (IS).

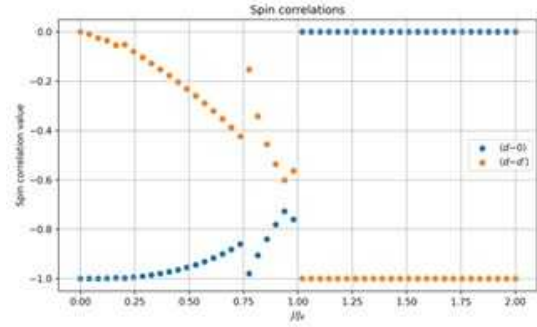


Figure 34: Spin flipping charge correlation between two impurity sites simply grows at the transition referred to by the orange curve, and impurity bath spin correlation dies, referred to by the blue curve, hinting towards the destruction of the Kondo screened phase.

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Keywords: Metal–insulator transition; Unitary renormalization group; Spin liquid ; Strange metal ; Quantum criticality.

Growth Optimization of MoS_2 and Influence of Au Plasmonic on Excitonic Luminescence

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Two-dimensional transition metal dichalcogenides (TMDs), particularly MoS_2 , exhibit strong layer-dependent optical and electronic properties, making them promising for next-generation optoelectronic and plasmonic devices. In this work, high-quality MoS_2 flakes were synthesized using atmospheric pressure chemical vapor deposition (APCVD), and growth parameters were optimized to obtain isolated triangular bilayer domains. Thin Au films of varying thicknesses (2 nm, 4 nm, 6 nm) were deposited on MoS_2 via e-beam evaporation, followed by high-temperature annealing to induce solid-state dewetting and form Au nanoparticles (AuNPs). FESEM imaging confirmed nanoparticle formation, with particle size strongly dependent on initial Au thickness. Raman spectroscopy of Au/ MoS_2 samples showed strong suppression of MoS_2 vibrational modes due to plasmonic screening and optical absorption by AuNPs. Photoluminescence (PL) measurements revealed pronounced PL quenching after Au deposition, attributed to interfacial charge transfer and the introduction of non-radiative exciton decay pathways. The study demonstrates how Au nanoparticle formation significantly modifies the optical properties of MoS_2 and highlights the role of metal-semiconductor interactions in excitonic behavior in 2D materials.

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Keywords: APCVD; Solid-state dewetting

Correlation of crystal field distribution with magnetic properties in (Ca, Ga)-substituted strontium hexaferrite

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The fascinating features of M-type hexaferrites are geometrically driven, like modifications of sublattices and evolution of microstructure. The Ca^{2+} and Ga^{3+} are completely soluble in the hexagonal crystal system of $\text{P6}_3/\text{mmc}$ space group. The incorporation of Ga^{3+} causes dilution of the superexchange interaction, apparent from the hysteresis loop. The evolution from nano to micrometer-length particles found in the magnetically diluted hexaferrite. The virgin curve of the hysteresis loop follows a different shape and path with increasing substitution percentage. The convex-concave type initial magnetization curve with higher coercivity is suspected of being due to the domain wall pinning in the substituted samples. The preferential occupation of Ga^{3+} at different crystallographically non-equivalent sites of Fe^{3+} sublattices is predicted from the sub-spectra analysis of ^{57}Fe Mössbauer spectroscopy. The magnetic ordering temperature is believed to follow the 2/3 power law with substitution. The micro-structured substituted particles are found to be magnetically multidomain. The Mössbauer spectra show preferential occupation of Ga^{3+} mainly at spin up sublattices. The neutron diffraction reveals sublattice magnetization decreases with substitution. Additionally, the possibility of off-centric displacement is investigated through dielectric properties analysis.

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Keywords: $\text{Ca}^{2+}/\text{Ga}^{3+}$ substitution, Hysteresis, Mössbauer spectroscopy, Impedance spectroscopy

Electric field driven nanoscale memory in π -bonded organic molecules and inorganic quantum dot hybrid system

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In recent years, research and development have increasingly focused on revolutionizing electronic materials to enhance operational speed, energy efficiency, and non-volatility for applications in emerging field like neuromorphic computing [1-2]. A promising direction in this field is the use of resistive switching materials, where the resistance of a material can be modulated between a high resistance state (HRS) and a low resistance state (LRS), mimicking a memory device with distinctive OFF (HRS) and ON (LRS) states [3-4]. Typically, such switching between HRS to LRS relies on the formation and rupture of conductive filaments through ion channels, triggered by electrical stimuli such as voltage, electric field, or current [5-6]. In addition to understanding these mechanisms, further miniaturization of electronic components is crucial. This project explores the possibility of resistive switching in a monolayer hybrid system comprising of π -bonded organic molecules and inorganic CdSe quantum dots (QDs), approximately 6 nm in size. The QD monolayer is assembled on top of a self-assembled monolayer (SAM) of organic molecules, forming a complete device of less than 10 nm in thickness. Experiments were conducted using a scanning tunneling microscopy (STM) setup, with the STM tip serving as the top electrode and an Au substrate as the bottom electrode. Surface topographies of

the SAM-QD layers were first recorded in constant current mode. At selected coordinates, tunneling current was measured as a function of bias voltage, followed by application of a voltage pulse, and then another set of current-voltage (I-V) measurement was measured. During this process, the STM feedback loop was disabled. It was observed that the current after the voltage pulse was significantly higher than before, indicating a transition from HRS to LRS - consistent with a conventional resistive switching behaviour. We propose that the applied voltage pulse induces a high electric field within the nanoscale device, facilitating delocalization of π -electrons from the organic molecules into the energy bands of the semiconducting quantum dots. These findings offer new insights into resistive switching mechanisms at the nanoscale.

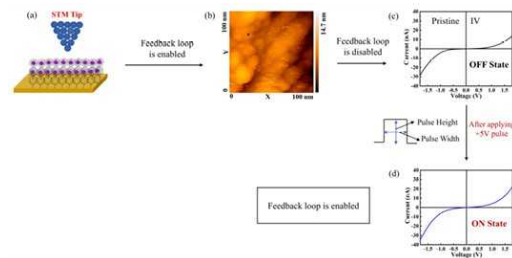


Figure 35: (a) Schematic representation of a scanning tunneling microscopy (STM) tip – hybrid system of π -bonded organic molecule and QD – Au substrate (b) Constant current topography of SAM-QD layers (c) & (d) Current-Voltage characteristics at pristine state i.e., OFF state and after application of voltage pulse of +5V i.e., ON state respectively

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Keywords: Resistive switching, Quantum dot, Electric field, π -bonded Organic molecules, Delocalization

Influence of Graphene and Antimony Underlayers on Magnetization Dynamics in FeCo Thin Films

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The magnetic properties of thin films are essential for driving advancements in spintronics, data storage, and other emerging magnetic technologies. Among these, FeCo thin films are particularly noteworthy due to their high saturation magnetization and ultra-low intrinsic Gilbert damping, making them ideal candidates for high-performance magnetic applications. One can tune the magnetic properties or make novel functionalities via interface engineering. In this context, two-dimensional (2D) materials such as graphene and antimony have garnered significant attention for their ability

to influence thin-film properties through their unique physical and electronic characteristics. These atomically thin materials offer a platform to modulate magnetic interactions at the interface, where the strength of atomic interactions both among the deposited atoms and between the film and substrate plays a critical role in determining the structural and magnetic properties of thin films. In this context, we have studied Fe₈₅Co₁₅ (FeCo) thin films deposited on graphene, antimony, an graphene/antimony bilayer substrates. The presence of these underlayers was confirmed through Raman spectroscopy. To further probe the structural and surface properties, atomic force microscopy (AFM) was employed, revealing distinct morphological variations depending on the underlayer used. These variations include differences in roughness, grain size, and surface texture, highlighting the influence of the underlayers on the growth dynamics of FeCo thin films. One key observation is the variation in coercivity among the different heterostructures. Specifically, FeCo films grown on antimony layers exhibit higher coercivity compared to those grown on graphene or graphene/antimony bilayers. Further insights were obtained through ferromagnetic resonance (FMR) studies, which revealed the presence of two-magnon scattering in the systems. An enhancement in Gilbert damping was observed in the bilayer structures compared to the reference FeCo films without underlayers. This enhancement may be attributed to spin pumping, a process where angular momentum from the precessing magnetization in FeCo is transferred to the adjacent graphene and/or antimony layers. This interaction highlights the role of 2D materials in influencing dynamic magnetic properties and demonstrates their potential in fine-tuning damping and spin-transfer effects for spintronic applications.

Keywords: 2-D materials, Magnetization dynamics, Gilbert damping, Ferromagnetic resonance

Symposium: C

Optimisation of conditions for the hydrothermal synthesis of phase-pure Zeolite-W using Kaolin for the extraction of ReO₄⁻ (surrogate for ⁹⁹TcO₄⁻)

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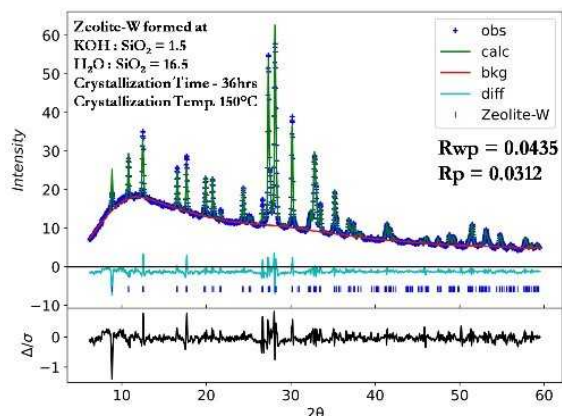


Figure 36: Figure 1. Rietveld refinement to the XRD pattern of Zeolite-W.

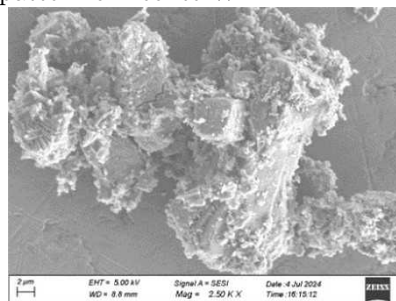


Figure 37: SEM image representing the morphology of Zeolite-W.

Technetium-99 (^{99}Tc) is an environmental hazard owing to its long half-life (2.12×10^5 years) [1]. The radioactive waste produced from the nuclear power plants significantly contains toxic ^{99}Tc , primarily as $^{99}\text{TcO}_4^-$ and thus demands extraction followed by immobilization. Zeolites with a befitting pore size and surface area are widely used as adsorbents for the extraction of such toxic anions. Owing to the cost of commercially available zeolites, we synthesized zeolite-W [$\text{K}_{5.75}\text{Al}_{5.75}\text{Si}_{10.25}\text{O}_{32}(\text{H}_2\text{O})_{7.5}$], a member of the MER zeolite framework [2], similar to the naturally occurring mineral merlinoite from an economically viable precursor, kaolin [$\text{Si}_2\text{Al}_2\text{O}_5(\text{OH})_4$, a phyllosilicate clay]. Hydrothermal synthesis route was adopted with optimization of synthesis conditions including $\text{H}_2\text{O}/\text{SiO}_2$ ratio, KOH/SiO_2 ratio, crystallization time and crystallization temperature. The crystal growth of zeolite-W was observed with a $\text{H}_2\text{O}/\text{SiO}_2 = 16.5$, $\text{KOH}/\text{SiO}_2 = 1.5$ during 36 hours of crystallization at 150°C . The Rietveld refinement of the XRD data (Figure 1) confirms the formation of phase-pure zeolite-W. FT-IR, SEM (Figure 2), BET (Table 1) and TG-DTA were carried out to gain insight into the bonding information, morphology, porosimetry and thermal stability of zeolite-W respectively. Furthermore, extraction studies of perrhenate (ReO_4^-) ions were carried out to mimic the separation behaviour of radioactive $^{99}\text{TcO}_4^-$ owing to the similar chemical properties of Re and Tc. ReO_4^- removal efficiency of $>70\%$ for zeolite-W was obtained, attributing the mechanism of extraction to sorption followed by occlusion within the pores [3].

Parameters	Values
SAM-BET ($\text{m}^2 \text{g}^{-1}$)	11.69
Total Pore Volume ($\text{cm}^3 \text{g}^{-1}$)	0.016
Average Pore Size (nm)	5.503

Table 1: Porosimetry parameters

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3. A. Maharana, A. Senapati, S. Sengupta and H. Jena, Langmuir 2024, 40, 25118–25132

Keywords: Exciton binding energy, Photoluminescence, Non-linear optical properties

SrO and Nb₂O₅ Modified Phosphate Glass Network: A Candidate Host Matrix for Radioactive waste Immobilization

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The high-level radioactive waste generated from the nuclear fuel cycle necessitates host matrices for safe storage, transportation, and final disposal through vitrification. Phosphate-based host matrices are advantageous than silicate glasses for fast reactor waste. Towards this, a new niobium oxide (Nb₂O₅) phosphate glass was researched owing to its significant favourable critical waste immobilization properties, such as the overall density and glass thermal stability. Concurrently, incorporating strontium oxide (SrO) improves the thermal stability and overall durability of the phosphate glass [1]. The present study investigates the influence of SrO on different physical and thermal properties of the pristine sodium niobium phosphate (SNP) glass. Both pristine SNP glass and 5 % SrO-containing SNP glass (Sr-SNP) are prepared by the melt quench technique and are characterized by XRD, DSC, and FTIR spectroscopy. The synthesized glasses are X-ray amorphous. From DSC thermograms (Fig.38), it is observed that the glass transition temperature (T_g) of the SrO-loaded glass is at 560 °C, representing a notable increase from the 518 °C observed for the base pristine SNP glass (40 mol% Na₂O – 20 mol% Nb₂O₅ – 40 mol% Pb₂O₅) [2]. From the FTIR spectroscopic analysis, it is observed that niobium builds 3D networks along with phosphate tetrahedra, and the addition of a strong modifier like Sr²⁺ induces rigidity to these glass networks. The most intense bands in the ranges 570 – 800 cm⁻¹ and 850 – 1250 cm⁻¹ are due to the vibrations of bonds in P-O-P bridges and the stretching vibrations of various P-ONB bonds in different Qi phosphate structural units, respectively (Fig.39). Hence, the concurrent increase in density and T_g suggests a complex yet highly beneficial synergistic effect between these network modifiers and formers, increasing overall glass durability. The linkages, such as P-O-Sr, Nb-O-Nb, and Nb-O-P, inherently create a more robust local environment that effectively compensates for any reduction in average chain length, leading to enhanced thermal stability

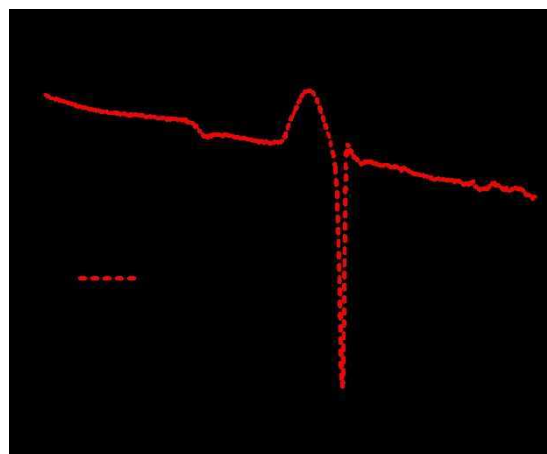


Figure 38: DSC thermograms of the glasses

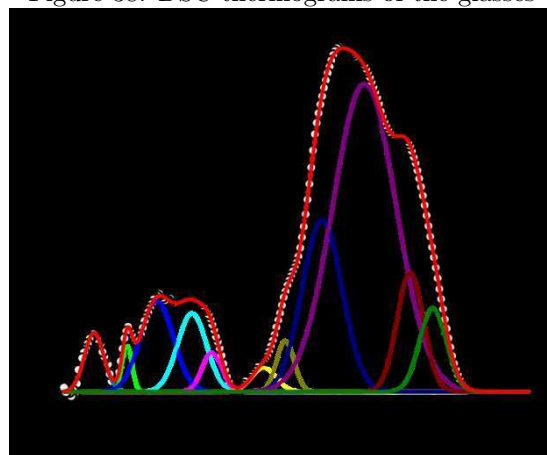


Figure 39: Deconvoluted FT-IR spectra of Sr-SNP

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Keywords: Radioactive waste, Vitrification, Phosphate glass, Thermal stability.

Spacer Cation Induced Tunable Piezoelectricity in 2D Halide Perovskite for Energy Harvesting Applications

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Ruddlesden–Popper (RP) halide perovskites represent a novel advancement in high-performance perovskite photovoltaics, offering exceptional environmental stability. The layered structure of these perovskites provides an excellent opportunity to harness their ferroelectric characteristics. However, the impact of structural and functional factors on the ferroelectric behaviour of RP perovskites remains not fully understood. Here, we observed adjustable ferroelectricity in the two-dimensional (2D) butylammonium (BA) and methylammonium (MA) RP perovskite (BA)₂(MA)_{n-1}Pb_nI_{3n+1}. The ferroelectric behaviour of the sample was systematically investigated using piezoresponse force microscopy and polarisation–electric field hysteresis measurements. The response was recorded within an active area of 4 μm × 4 μm under ±20 V applied bias, highlighting its superior ferroelectric performance among the series. We utilized Density functional theory (DFT) calculations to calculate the electronic band structure and density of states for the (BA)₂(MA)_{n-1}Pb_nI_{3n+1} series, and it reveals that (BA)₂(MA)_{n-1}Pb_nI_{3n+1} (n=1-4) exhibit a non-Centrosymmetric structure with the on-axis Pb-I bond becoming longer, typically referred to as the z-axis or [001]-direction. Furthermore, a composite of BA₂MAPb₂I₇ (n = 2) and PVDF was fabricated to inspect its potential for energy harvesting applications as a piezoelectric nanogenerator. Under an optimized applied pressure of 25 kPa, the fabricated nanogenerator device delivered instantaneous output values of 70 V and 5.1 A. The nanogenerator device also exhibited stable output performance under various mechanical stimuli—such as heel pressing, knee bending, and finger tapping—demonstrating its practical applicability for wearable energy harvesting. Our findings reveal new insights into the origin

of ferroelectricity in RP halide perovskites and provide a viable strategy to tailor their properties for next-generation optoelectronic and energy harvesting applications.

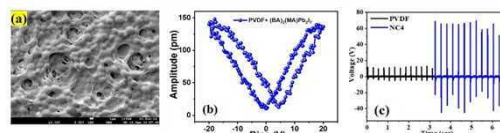


Figure 40: (a)FESEM (b)PFM amplitude and (c) generated output voltage of PVDF/BA₂MAPb₂I₇ composite film

Keywords: 2D halide perovskite; tunable piezoelectricity; spacer cation; piezoelectric nanogenerator.

Development of Supramolecular Metallogels of Chiral Bisnaphthyl Bipyridine Derivatives for Dye Degradation Application

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Small molecule-based supramolecular gels are promising materials for applications in optoelectronics, sensing, and environmental remediation. Here, we report the formation of stable organogels from two enantiomeric bisnaphthyl bipyridine diamide derivatives (S-Bpy-Nap and RBpy-Nap) in organic solvents, driven by non-covalent interactions such as hydrogen bonding, π -stacking, and metal coordination. Metallogelation studies in tetrahydrofuran (THF) with Fe²⁺, Co²⁺, Cu²⁺ and Ni²⁺ etc. revealed metal-responsive gel behavior. The gels were characterized using microscopy, UV-Vis absorption, circular dichroism (CD) spectroscopy, and rheology. UV-Vis studies confirmed selective binding of Co²⁺, Cu²⁺ and Ni²⁺ metal ions, while CD spectra showed significant red shifts upon coordination with these metal ions, indicating altered chiral supramolecular self-assembly. Additionally, Fe³⁺-coordinated S-Bpy-Nap xerogels showed photocatalytic degradation of Rhodamine B dye under blue LED (435-445 nm) light and H₂O₂, highlighting potential for environmental remediation. This work demonstrates the multifunctionality of chiral bipyridine-based gelators in both advanced materials and sustainable applications.



Figure 41: : Supramolecular metallogels of Bis-naphthyl Bipyridine Derivatives for dye degradation study

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Keywords: Radioactive waste, Vitrification, Phosphate glass, Thermal stability

Layer-Engineered Capacitive-Coupled Organic Memristor Based on PEDOT:PSS-Ion Gel Bilayers

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We report a systematic study on vertical bilayer devices composed of PEDOT:PSS (doped with DMSO and TsOH) and an ion gel (PVA/H₂SO₄/PEG), where tuning the relative layer thicknesses yields four distinct non-pinched I-V hysteresis loops: non-crossing (C1M4), positive-bias crossing, negative bias crossing, and dual-bias crossing. Structural and spectroscopic analyses confirm doping-induced modifications, while electrical measurements demonstrate reproducible endurance over 100 cycles, stable retention for 1200 s, and ON/OFF ratios ranging from 1.25 to 6. The observed switching arises from the interplay of ion migration in the gel and redox/filament processes in PEDOT:PSS,

described by a unified chemical-mathematical model where a dimensionless thickness factor (β) governs the transition between crossing behaviours. This work establishes a design strategy for tailoring hybrid organic-ionic devices and provides a foundation for fabricating organic electrochemical memtransistors with tunable memory and neuromorphic functionalities.

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Keywords: Organic Electronics; Memristors; Capacitive Coupling

Oxygen-Vacancy-Engineered LaFeO/FeOOH an S-Scheme Heterojunction for Sono-Photo-Fenton Degradation and Water Splitting

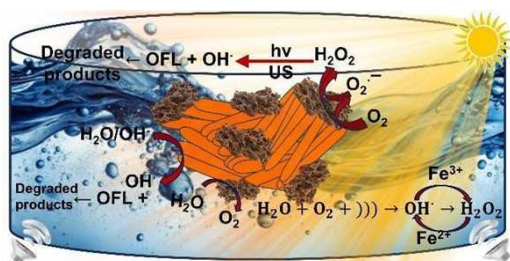
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The rising contamination of aquatic systems with pharmaceutical residues poses a serious risk to human and environmental health, necessitating the development of sustainable remediation strategies. Among various approaches, ultrasound-assisted photo-Fenton reactions have emerged as highly promising, offering eco-friendly and efficient oxidation capabilities. This study highlights the S-scheme charge transfer mechanism in a FeOOH-decorated *LaFeO*₃ heterojunction designed for the degradation of the antibiotic ofloxacin (OFL), utilizing ultrasonic irradiation in combination with simulated solar light. The heterojunction was synthesized via a simple two-step sol-gel method followed by in situ coprecipitation, resulting in

strong interfacial connectivity and a high density of oxygen vacancies (OVs). The optimized photocatalyst exhibited remarkable sono-photo-Fenton degradation efficiency (92.3%) for OFL, with an apparent rate constant (k_{app}) of 21.95 min^{-1} — 2.19 and 2.05 times greater than those of the individual components. Additionally, the catalyst achieved an impressive O_2 evolution rate of $1270 \mu\text{mol h}^{-1}$ during water splitting. The improved photocatalytic activity is attributed to enhanced charge carrier separation via a dynamic S-scheme charge transfer pathway, synergistically supported by the presence of OVs, and $\text{Fe}^{3+}/\text{Fe}^{2+}$ redox cycling. Comprehensive structural and physico-chemical characterizations—including EPR, Raman, and XPS—confirmed the successful formation of OVs and validated the S-scheme charge migration route. Radical scavenging and EPR experiments further substantiated the reactive species involved. Systematic analysis of reaction kinetics, recyclability, and structural stability revealed the catalyst's excellent durability and practical applicability. This dual-functional heterostructure serves as a promising model for next-generation AOPs, targeting environmental pollutants while concurrently enabling solar fuel production. optimized via EPD for next-generation energy storage devices.



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Keywords: Water splitting, Oxygen vacancy, S-Scheme, Sono-Photo-Fenton degradation

All-inorganic lead-free triple perovskites for two-terminal analog memristor-based artificial synapses

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Lead halide perovskites have attracted wide interest for their remarkable optoelectronic properties, such as strong light absorption and long carrier diffusion lengths. However, their instability and the toxicity of lead limit their practical applications [1]. To address these challenges, lead-free alternatives are being explored. Among them, bismuth-based halides, especially $\text{Cs}_3\text{Bi}_2\text{I}_9$, are promising due to their environmental safety, structural diversity, and excellent air and moisture stability [2]. With its zerodimensional perovskite structure, $\text{Cs}_3\text{Bi}_2\text{I}_9$ exhibits unique optical properties and potential for photovoltaic and radiation detection applications [3,4]. In this work, we synthesized $\text{Cs}_3\text{Bi}_2\text{I}_9$ perovskite material using bulk solution based technique. The structural and surface morphological study revealed the crystallinity and uniformity of the material. The optical properties of the material have also been studied viz., UV-vis, Photoluminescence. In electrical properties, Current-Voltage measurements of the $\text{Ag}/\text{Cs}_3\text{Bi}_2\text{I}_9/\text{ITO}$ device showed the synaptic properties. The device effectively replicated several synaptic learning processes present in biological neural networks, such as spike-timing-dependent plasticity (STDP), short-term potentiation and depression (STP/STD), excitatory postsynaptic currents (EPSC), Inhibitory Postsynaptic Current (IPSC), and paired-pulse facilitation (PPF).

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Keywords: Lead free halide perovskite, Synaptic learning process, IPSC, STP

Enhanced Piezoelectric Performance in Ion-exchanged Silver Niobate GlassCeramics: A Lead-Free Alternative for Energy Harvesting Applications

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This study introduces a novel synthesis strategy for silver niobate (AgNbO_3) glass-ceramics (GCs) via ion-exchange (IoX) from sodium niobate (NaNbO_3) GCs. This approach overcomes the limitations of conventional melt-quenching methods, which are constrained by silver's low solubility in glass matrices. IoX was performed by immersing heat-treated (NaNbO_3) GCs in silver nitrate solution for 5, 24, 48, and 96 hours, yielding samples labelled SAN-5, SAN-24, SAN-48, and SAN-96, respectively. The untreated (NaNbO_3) GC (SAN-0) exhibited a modest piezoelectric response, generating an average peak voltage of 2.05 V under mechanical stress. In contrast, SAN-5 showed a marked increase to 9.0 V, with output voltages further improving with longer IoX durations. The maximum response was observed for SAN-48, attributed to the formation of polar (AgNbO_3) nanocrystals within the glass matrix, as confirmed by XRD and TEM analyses. Furthermore, the ion-exchanged samples retained excellent mechanical integrity, with Vickers hardness values exceeding 7.8 GPa. These results underscore IoX as an effective route to produce lead-free (AgNbO_3) GCs with enhanced piezoelectric and mechanical properties. Such materials hold

strong promise for use in energy harvesting devices, capacitors, and sensors, offering a sustainable path toward next-generation smart energy technologies.

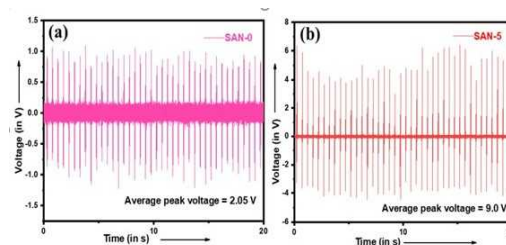


Figure 42: Output voltage of (a) SAN-0 and (b) SAN-5 glass-ceramics.

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Keywords: Glass-Ceramics; Ion-Exchange; Piezoelectric; Energy Harvesting; dielectric capacitor

Theoretical Investigation of B_2CaS as an Anode for Post Lithium Ion Batteries

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In recent years, two-dimensional (2D) materials have garnered considerable attention due to their exceptional properties and promising potential in energy storage applications. One such material, B_2C , exhibits remarkable properties, making it a strong candidate for anode materials in metal ion batteries (Ca/K-ion batteries)^{1,2}. The increasing interest in CIBs and KIBs as viable alternatives to lithium ion batteries (LIBs) is largely driven by abundance and low cost of calcium and potassium resources as compared to

those of *lithium*³. However, the search for identifying suitable electrode materials for these batteries remains a significant challenge. In this research, we utilize first-principles calculations to investigate the electronic and structural changes within B₂C during metal ion loading. With the help of the Climbing Image Nudge Elastic Band (CI-NEB) method, diffusion barriers were calculated for the migration of Ca/K ions onto B₂C⁴. A low diffusion barrier of 0.14/0.07 eV was obtained for Ca/K migration. Our findings reveal that, B₂C demonstrates promising performance, with an excellent Ca/K storage capacity. Additionally, B₂C demonstrates electronic conductivity and excellent structural stability during calcination and potassination processes. These results indicate that B₂C holds substantial potential as a high-performance anode for next-generation CIBs/KIBs, paving the way for more efficient and sustainable energy storage appliances.

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Keywords: LIBs, electronic conductivity

Structural, Morphological and Electrochemical Investigation of Mn and Mo Doped BiPO₄ for Energy Storage Applications

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Supercapacitors (SCs) have been considered as the distinct category for electrochemical energy storage systems because of their ability towards practical applications. BiPO₄ and its

solid solutions have been developed as promising electrode materials for SCs due to their intrinsic redox-active species, high crystallinity, chemical and thermal stability, abundance, and eco-friendly nature. In this research work, we have synthesized Mn and Mo substituted bismuth phosphate with the general formula Bi_{1-x}Mn_xP_{1-x}Mo_xO₄ (x = 0.01 to 0.05) by solution route and investigated the electrochemical performance. The phase purity and crystallinity of the materials were studied by X-ray Diffraction (XRD) technique and found that the x = 0.01 phase crystallize in monoclinic structure with P21/n space group. The P-O and Mo-O stretching and bending vibrational modes were observed in the range of 900–1100 cm⁻¹ and 813 cm⁻¹ respectively. Electrochemical studies were performed on the pristine Supercapacitors (SCs) have been considered as the distinct category for electrochemical energy storage systems because of their ability towards practical applications. BiPO₄ and its solid solutions have been developed as promising electrode materials for SCs due to their intrinsic redox-active species, high crystallinity, chemical and thermal stability, abundance, and eco-friendly nature. In this research work, we have synthesized Mn and Mo substituted bismuth phosphate with the general formula Bi_{1-x}Mn_xP_{1-x}Mo_xO₄ and the modified electrodes by a three-electrode system using Cyclic Voltammetry (CV), Galvanostatic Charge-Discharge (GCD), and Electrochemical Impedance Spectroscopy (EIS) measurements. The high specific capacitance, long cyclic life, and enhanced rate performance of Mn and Mo modified electrodes indicate that they can be a good sustainable and efficient electrode materials for next-generation SCs.

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Keywords: Fermi level pinning; Integer charge transfer model; Perovskite; SAM.

Turbostratic Twisted Graphene Bilayer Structures Detected in a Carbon Material Obtained from Coal and Supercapacitor Application

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Graphene has emerged as one of the most extensively studied materials in recent years. The design and synthesis of multi-layered graphene have garnered significant attention due to its suitability for various advanced applications. However, the crystal lattice, atomic configuration, and symmetry of these stacked multi-layered structures are influenced by van der Waals interactions, leading to diverse interlayer orientations. In this paper, turbostratic twisted bilayer graphene has been successfully synthesized from a coal carbon precursor and its formation and associated structural features have been thoroughly investigated. Selected Area Electron Diffraction (SAED) analysis confirmed the presence of turbostratic stacking with random orientations, resulting in twisted bilayer graphene with distinct or broad twist angles below 21° and 27°, leading to lattice misalignment. The formation of twisted bilayer graphene was further verified using high-resolution transmission electron microscopy (HR-TEM), Raman spectroscopy, and atomic force microscopy (AFM). Moreover, the as-prepared turbostratic graphene was utilized as an electrode material in a two-electrode supercapacitor configuration, delivering an impressive specific capacitance of 158 F g⁻¹ at a current density of 0.5 A g⁻¹, highlighting its potential for application in hybrid supercapacitors.

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Keywords: turbostratic graphene, twisted bilayer graphene, supercapacitor, coal.

GeSnSbTe₂: Structural Analysis and Prospects for Thermoelectric Performance Enhancement

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Thermoelectric materials are of great interest for sustainable energy conversion, as they can directly convert waste heat into electricity. Among these, chalcogenide-based systems have attracted wide attention due to their tunable band structures, strong lattice anharmonicity, and intrinsically low thermal conductivity. Within this class, GeTe is a well-known p-type thermoelectric material, crystallizing in a rhombohedral structure (R3m) at room temperature and transforming to a cubic phase (Fm-3m) at elevated temperatures. Its high hole concentration, originating from Ge vacancies, together with band convergence near the Fermi level, contributes to a large Seebeck coefficient, while alloying and multicomponent substitution are often employed to optimize carrier concentration and suppress lattice thermal conductivity. Analogous multicomponent systems such as AgSnSbTe₃ and PbSnSbTe₃ have attracted increasing attention for their ability to introduce chemical disorder and improve thermoelectric performance. In this direction, we have successfully synthesized GeSnTe by a melt-state reaction, and XRD confirmed its rhombohedral crystal structure having space group R3m, while XPS validated the phase composition. Future studies will focus on doping GeSnTe, where Ag and Cu substitution will be explored for their

potential to reduce lattice thermal conductivity, while S and Se incorporation at anionic sites will be used to enhance phonon scattering. Additionally, temperature-dependent XRD will be performed to probe phase-change characteristics, along with thermal conductivity, Seebeck coefficient, and electrical conductivity measurements to evaluate its thermoelectric performance.

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Keywords: Chalcogenide thermoelectric materials, XRD, XPS, Figure of merit

Evolution of microstructure, magnetic, and electrical properties of novel double-layered Ruddlesden-Popper Perovskite $\text{Sr}_3\text{NiNbO}_{7-\delta}$

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The evolution of microstructure, magnetic, and electrical properties of a theoretically predicted $\text{Sr}_3\text{NiNbO}_{7-\delta}$ (SNNO) perovskite synthesized by modified sol-gel technique is investigated for the first time. Rietveld refinement of the XRD pattern reveals a double-layered Ruddlesden-Popper (RP) phase with $I4/mmm$ space group of tetragonal structure. XPS analysis confirms Sr^{2+} and Nb^{5+} oxidation states, Ni exists as Ni^{2+} and Ni^{3+} , accompanied by

oxygen vacancies. A detailed analysis of thermomagnetic behavior reveals an antiferromagnetic interaction between Ni^{2+} and Ni^{3+} , with an effective magnetic moment of $3.75 \mu_B$, confirmed from the fitting of χ^{-1} vs T with the modified Curie-Weiss law. Again, the isothermal magnetization loop discloses a second-order magnetic transition using the Arrott plot for various temperatures and a weak ferromagnetic contribution in low-field regions at room temperature induced by the exchange interaction between spin-polarized magnetic ions mediated by oxygen. The frequency-dependent ac conductivity at various temperatures (50–440 °C) within the frequency range of 1 Hz to 1 MHz reveals the conduction described by two mechanisms, i.e., correlated barrier hopping (CBH) below 170 °C and nonoverlapping small polaron tunneling (NSPT) above 170 °C. Further, an increasing trend of conductivity, with the highest conductivity of $1.7 \times 10^{-4} \text{ S cm}^{-1}$ observed at 440 °C from the electrical impedance spectroscopy (EIS) method, confirms the semiconducting nature of the sample. The newly synthesized SNNO can be used to develop energy-efficient materials for applications in fuel cells and advanced electronic devices.

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Keywords: Ruddlesden-Popper perovskite, Modified Curie-Weiss law, electrical conductivity.

Next-Gen Clay Nanocomposites for Mercury Remediation

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This study explores the synthesis of novel clay-based nanocomposites for the efficient removal of mercury ions from contaminated water. We developed eight distinct composites by combining four different clay minerals (kaolinite, halloysite, sepiolite, and bentonite) with either magnesium oxide (MgO) or magnesium sulfide (MgS) nanoparticles. The composites were

subjected to thermal treatment to improve their structural stability and surface reactivity. Subsequent batch adsorption experiments demonstrated a notable increase in mercury removal efficiency for all nanocomposites compared to their unmodified clay counterparts. These results highlight the strong potential of MgO- and MgS-modified clays as highly effective and sustainable adsorbents for mercury remediation. The findings not only offer promising solutions for treating industrial effluents and purifying drinking water but also present new avenues for developing low-cost materials for a range of environmental remediation applications.

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Keywords: nanocomposites, halloysite, radiation

Transition-Metal-Incorporation in NiCo₂O₄ Spinel Framework as Superior Oxygen Evolution Catalysts

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Spinel oxides (ABO) have emerged as promising electrocatalysts for the water splitting application owing to their unique crystal structure, tunable electronic properties, and excellent stability in alkaline media. The development of efficient and stable oxygen evolution reaction (OER) electrocatalysts is essential for advancing water-splitting technologies.[1-4] In this

work, Fe incorporated NiCo₂O₄ spinel catalysts were synthesized via a hydrothermal method with different iron concentrations (Fe(x), x = 0-4 wt%). Structural and morphological analysis using XRD, Raman spectroscopy, SEM, and BET confirmed the successful formation of spinel phases with uniform Fe incorporation. Among the compositions, NiCo₂O₄-Fe1 (1% Fe) exhibited the highest surface area enabling efficient ion diffusion and enhanced electroactive site exposure. Electrochemical evaluation demonstrated that NiCo₂O₄-Fe1 delivered the best OER performance, achieving an overpotential of 282 mV at 10 mA cm² and a Tafel slope of 62.03 mV dec⁻¹, indicative of favorable reaction kinetics. The improved OER activity is attributed to the synergistic effect of Fe incorporation, which optimized the electronic structure, increased active site density, and accelerated charge-transfer kinetics. These results establish Fe-incorporated NiCo₂O₄ spinels, particularly NiCo₂O₄-Fe1, as promising non-noble-metal catalysts for efficient and durable OER applications

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Keywords: NiCo₂O₄, OER, Electrocatalyst, water splitting

A Family of Methylene Bridged Fully Functionalized Polynitroarenes and Tetrazole-based Energetic Materials

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In the last few decades, apart from having military applications, there has been a rapid increase in the use of energetic materials for various civilian applications, such as for space exploration, mining of minerals, in the construction industry, drilling oil wells, etc. To meet modern requirements, high-energy-density materials (HEDMs) not only exhibit excellent energetic performance but also demonstrate sufficient physical and thermal stability for safer handling, transportation, and use.¹⁻² To address this, the present work focuses on fine-tuning the energetic properties of the thermally and physically stable 2,4,6-trinitrobenzene-1,3-diamine/diol framework by connecting an energetic tetrazole moiety through a methylene bridge. The amino/hydroxy functionalities between the nitro groups on the benzene ring provided extensive inter- and intra-molecular hydrogen bonding interactions, contributing to improved stability, whereas the tetrazole ring increased the nitrogen percentage and energetic performance. Due to the presence of one and three labile protons in amino derivative (compounds 4) and hydroxy derivative (compounds 5), respectively, a series of mono- and tricationic salts were prepared to fine-tune the overall performances further. Among all the synthesized compounds, the tricationic energetic salt 10 ($D_v = 8135 \text{ m s}^{-1}$, $IS \approx 40 \text{ J}$) exhibited energetic performance comparable to TATB and was insensitive. All of the compounds were characterized through IR, NMR spectroscopy, differential scanning calorimetry (DSC), elemental analysis, and HRMS studies. The relationship between structure and properties was further explored using Hirshfeld surface, noncovalent interaction (NCI), LOL-, and electrostatic potential (ESP) Analysis.

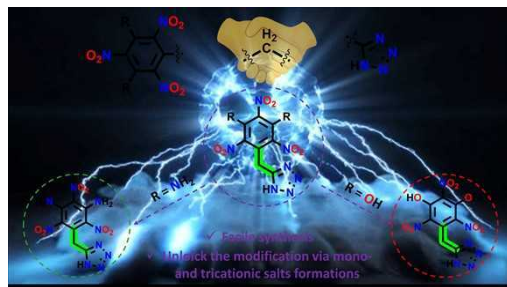


Figure 43: Strategic combination of Polynitroarene with tetrazole via a methylene bridge for Fine-tuning energetic performances.

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Keywords: Polynitroarenes; tetrazole; methylene bridge; tricationic energetic salt.

Gas Sensing by RGO Wrapped Fe_2O_3 Nanorod

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Gas sensors usage extended from household to industries, hospitals, mines etc. Out of all gas sensors metal oxide semiconductor are the widely used as they are budget friendly, environment friendly, cheap, compact, easy to operate. Fe_2O_3 are found abundantly in environment but however they are not used as gas sensors as compared to other metal oxides like TiO_2 , SnO_2 , ZnO . In this work we will show synthesis and gas sensing by Fe_2O_3 , and rGO wrapped Fe_2O_3 . First nanorod was deposited on FTO by using chemical bath deposition technique and was annealed to get the required phase. After Fe_2O_3 nanorod formation rGO was wrapped. To study the morphological and compositional characteristics FESEM, XRD, and Raman spectroscopy were done. Sensing of NO_2 , CH_4 , CO_2

were done to find selectivity. Effect of temperature and humidity on sensor had also been shown to find the suitable operating temperature at a particular humidity. Finally all the results from pristine Fe_2O_3 nanorod and rGO wrapped Fe_2O_3 nanorods were compared to find rGO wrapped Fe_2O_3 nanorods show better sensitivity than Fe_2O_3 .

Keywords: rGO wrapped Fe_2O_3 nanorod, Fe_2O_3 nanorod, operating temperature, metal oxide gas sensors, Chemical Bath Deposition

Energy-Saving Multifunctional Electrocatalyst Based on NiAl LDH MXene Heterostructure for HER, OER, and Hydrazine Oxidation Reaction

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Designing efficient and multifunctional electrocatalysts is essential for advancing low-energy hydrogen production. A hybrid catalyst composed of NiAl layered double hydroxide (LDH) anchored on $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanosheets demonstrates outstanding electrocatalytic performance for the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and hydrazine oxidation reaction (HzOR) in alkaline media. Structural and surface characterisations (XRD, SEM, TEM, and XPS) confirm a flake-like layered morphology with strong interfacial integration, promoting enhanced charge transfer, abundant active site exposure, and electronic modulation. The NiAl LDH–MXene composite exhibits low overpotentials and Tafel slopes for HER and OER, while significantly outperforming OER when HzOR is employed as the anodic process. Owing to the lower thermodynamic potential and faster kinetics of HzOR ($E = -0.33$ V vs. RHE), the overall water splitting cell voltage is reduced to below 0.21 V at 10 mA cm^{-2} which is 1.55 V lower than traditional OER—HER system using the same catalyst. This dramatic energy savings

highlights the catalytic synergy and multifunctionality of the composite electrode. The system delivers high Faradaic efficiencies of 98.9% (HzOR || HER) and 98.5% (OER || HER) for hydrogen production, indicating excellent charge utilization and selectivity. These results position MXene/NiAl-LDH as a robust, energy-efficient platform for low-voltage hydrogen production.

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Keywords: MXene, layered double hydroxide, Co-electrolysis, hydrazine oxidation, water splitting, green hydrogen

Composite Nanomaterial as Nanofillers for Enhanced Electroactive Phase of PVDF Piezoelectric Sensors Applications

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Piezoelectric nanogenerators (PENGs) have emerged as a promising technology for converting mechanical energy into electrical energy at the nanoscale, offering long-term power solutions for self-powered systems. This work investigates the design and performance of a piezoelectric nanogenerator (PENG) composed of polyvinylidene fluoride (PVDF) with added nanofillers. The piezoelectric property of PVDF can be amplified by mechanical stretching, nanofiller incorporation and electrical poling, making it an attractive choice for energy harvesting applications.¹ PENGs can be used for various applications as vibration sensors and energy harvesting for running small electronic appliances.² This study uses the addition of

Vanadium disulfide/Tungsten trioxide composite nanomaterial into a PVDF matrix for a polymer nanocomposite piezoelectric film with high -phase crystallinity. A composite material was made and incorporated into PVDF with an optimised concentration. Tungsten trioxide has already been reported as a dielectric material, can contribute to piezoelectricity, and Vanadium disulfide is highly negatively surface-charged micro-flowers, which disperse in the PVDF matrix throughout to enhance -phase. Further, a real-time prototype of area 2.72 cm² was fabricated and tested for output performance. It generates a maximum voltage output of 8.9 V at 10 M resistance, @5N, and a Power density of 10.21 μ W/cm² @1 M resistance.

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Keywords: Piezoelectricity, pressure sensors, nanocomposites

High Temperature Thermal and Melting Properties of Multivalent and Offstoichiometric Mixed Actinide Oxides

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Recycling of minor actinides (MAs), mainly americium (Am), and plutonium (Pu) from spent nuclear fuel is actively pursued for beneficial applications, e.g., ²⁴¹Am radioisotope can be used as thermoelectric generators, radioisotope heating units for space applications, and a neutron source. In the context of partition and transmutation, the recycled MAs can be transmuted into shorter-lived fission products in a fast reactor or in an accelerator-driven subcritical system [1]. The knowledge of the thermal properties of MA-bearing fuels is crucial for fuel design, performance modelling, and safety analysis. However, there are limited experimental data on MA-based nuclear fuels available in the literature, especially near the melting temperature. Acquiring such thermophysical data from Molecular Dynamics (MD) simulations can be a good alternative. The accurate evaluations of properties of MA-bearing MOX fuels using MD simulations pose several challenges due to the presence of multivalent actinides and their off-stoichiometry. Currently, for such fuels, there is no MD simulation-based modelling framework which addresses all these features. The present study develops a framework by combining the interatomic potentials of MAs in multivalent states and using it in MD simulations to generate the thermophysical properties and melting behaviour of off-stoichiometric MA-bearing nuclear fuels over a wide range of temperatures. We have generated thermal properties (thermal expansion coefficients, specific heats, and melting temperatures) of hypo-stoichiometric Pu_{1-y}Am_yO_{2-x} MOX by creating oxygen vacancies, and the charge balance is achieved by replacing Am⁴⁺ by Am³⁺ near the oxygen vacancies. A recent high-temperature X-ray diffraction data [2] suggests the partial reduction of Am⁴⁺ to Am³⁺ during heating, though Pu remained tetravalent in Pu_{1-y}Am_yO_{2-x} MOX. The MD results of lattice parameter variation as a function of temperature are found to consistently reproduce recent high-temperature X-ray diffraction data [2] with reasonable accuracy, as compared in Fig. 1. Further, data on specific heats and melting temperatures are generated where limited/no experimental data is available.

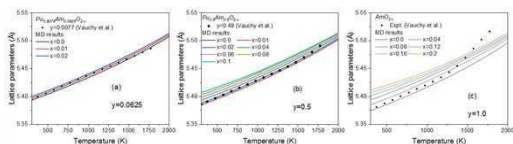


Figure 44: A comparison of MD calculated lattice parameter of $\text{Pu}_{1-y}\text{Am}_y\text{O}_{2-x}$ as function of temperature for (a) $y=0.0625$, (b) $y=0.5$ and (c) $y=1.0$, for various x values, with available experiments

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Keywords: Nuclear fuels, Minor actinides, MD simulation

Chemical Vapor Deposition of Copper Selenide (Cu_2Se) on copper foil for Supercapacitor application

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Transition metal chalcogenides have been explored for their energy storage applications. Copper being a transition metal is earth-abundant and widely used. This transition metal in the form of thin foil is directly selenized via chemical vapor deposition at relatively low temperature of 500 °C using nitrogen gas as carrier. This method does not require the use of Ar/H_2 mixture gas thus reducing the synthesis cost and being sustainable. During the selenization process thin film peeling-off issues were faced. This problem was overcome by varying the elemental Se precursor amount, reaction time and reproducibility of this process was achieved. The selenized thin layer was characterized by X-ray diffraction technique which confirmed the formation of orthorhombic Cu_2Se and the morphology of the thin films characterized by SEM revealed that it has flake-like structures. The chemical compositions of thin films were

analyzed using EDS and mixed oxidation state of copper (+1, +2) was revealed by XPS characterization and crystallinity was further confirmed by HR-TEM. The synthesized thin films were further characterized by performing electrochemical studies such as cyclic voltammetry and galvanostatic charge-discharge cycles. Reduction peaks were observed only at negative voltages and charge-discharge cycles were performed in negative voltage window of -0.05 V to -0.5 V. The thin films exhibited good cycling stability of over 500 cycles with a specific capacitance value of 110 F g^{-1} . After these electrochemical studies the thin films retained their crystallinity and peeling off from the substrate was not observed. This work reveals that transition metal chalcogenides synthesized by direct selenization onto metal foils can be used as electrode material in supercapacitor applications and this eliminates the extra step involved in preparing/coating the electrode and non-usage of binders.

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Keywords: Transition metal chalcogenides, Chemical vapor deposition, Supercapacitor

Ni Incorporation in Fe-Mn Based Prussian White to Subdue Octahedral Tilt Distortion and Jahn-Teller Distortion

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Fe-Mn-based Prussian white $\text{Na}_2\text{Fe}_{1-x}\text{Mn}_x[\text{Fe}(\text{CN})_6]$ is the most competitive cathode composition with a theoretical capacity of 170 mAh g^{-1} in sodium-ion batteries, rivalling commercially available LiFePO_4 cathodes (lithium-ion batteries). The open framework structure of Prussian blue analogues (PBAs) is analogous to that of perovskites ABX_3 . This atomic arrangement is advantageous in accommodating a larger alkali metal ion (Na) into the structure. However, when the stoichiometry of Na is closer to 2 in PBAs, the interaction between Na and the cyanide ligand grows stronger, which

leads to octahedral tilt distortion and the structure deviates from its ideal cubic structure to rhombohedral or cubic. This phenomenon can control the size of pores formed by the transition metal and cyanide ligand. Therefore, narrower pores can restrict the motion of Na⁺, causing poor electrochemical performance. The pristine Na₂Fe[Fe(CN)₆] (NFe) delivers a reversible capacity of 120 mAh g⁻¹ and capacity retention of 92% after 50 cycles at C/10. Na₂Mn[Fe(CN)₆] (NMn) delivers a reversible capacity of 119 mAh g⁻¹ and capacity retention of 56% after 50 cycles. The capacity was further improved by the Fe–Mn-based cathode Na₂Fe_{0.60}Mn_{0.40}[Fe(CN)₆] (NFeMn6040), with a reversible capacity of 137 mAh g⁻¹ and capacity retention of 77% after 50 cycles. The composition was further tuned to combat poor cyclability by incorporating Ni into the structure Na₂Fe_{0.60}Mn_{0.35}Ni_{0.05}[Fe(CN)₆] (NFeMnNi603505). This composition delivered a reversible capacity of 130 mAh g⁻¹ and capacity retention of 90% after 50 cycles at a C/10 rate. Distortion δ is calculated by the ratio of the change in the volume of the desired PBA to the volume of the undistorted cubic PBA. The XRD patterns of NFe, NMn, NFeMn6040, and NFeMnNi603505 were found to be monoclinic (P2₁/n). The respective volumes of the samples were calculated using Rietveld refinement. The volumes of NFe, NMn, NFeMn6040, and NFeMnNi603505 were 566.0 Å³, 555.2 Å³, 563.8 Å³, and 587 Å³, respectively. The distortion was calculated using the undistorted PBA with the *Fm* $\bar{3}$ space group having a volume of 1103 Å³. The distortion of NFe, NMn, NFeMn6040, and NFeMnNi603505 was found to be 0.486975, 0.496764, 0.488969, and 0.46794, respectively. The highest distortion was obtained in NMn due to octahedral tilt and Jahn–Teller distortion, which exist together and result in poor cyclability. The least distortion was obtained in NFeMnNi603505, which shows improved reversible capacity and better cyclic retention. The structure was further probed by analyzing octahedral tilt angles, water content in the lattice using TGA, morphology using SEM, and chemical surroundings using FTIR and Raman spectroscopy to probe further factors influencing the electrochemical performance.

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Keywords: perovskites, ligand, electrochemical

TiO₂ thin films grown by atomic layer deposition (ALD) for photocatalytic reduction of CO₂

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This work reports the atomic layer deposition of different thickness of TiO₂ on glass substrates. Borosilicate glass substrates (7mm thick) were taken and coated with different thickness of TiO₂ starting from 5 nm upto 50 nm. ALD coating was done with Titanium tetraisopropoxide with oxygen plasma as oxygen source at 300°C. These glass substrates were then kept inside the photocatalytic reactor for CO₂ reduction. Product formed in the reactor during regular interval of time was analysed using a gas chromatograph (GC). Concentration of product formed over time was calculated. The structural, optical and morphological properties of thin film coated by atomic layer deposition were thoroughly investigated. Scanning electron microscopy, UV- visible spectroscopy were employed to study the surface morphology and optical properties. Variation in the product generation rate by varying the thickness of TiO₂ has been analysed. 5 nm thick TiO₂ deposited by ALD has shown the higher production of CO and CH₄ after 10 hr. Similarly, TiO₂-GO coated glass substrates were also analysed for CO₂ reduction. The work demonstrated the effectiveness of artificial porosity, enhanced surface area, greater light harvesting, prevention of agglomeration of photocatalyst and minimization of materials expenses towards a more efficient photoreduction of CO₂ into useful fuels.

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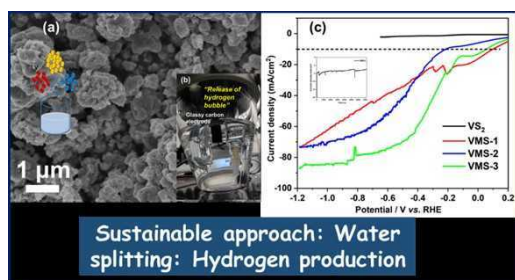
Keywords: CO₂ reduction, TiO₂, Atomic layer deposition, reduction products.

Hydrothermally Synthesized VS₂/MoS₂ Nanocomposite for Green-Hydrogen Evolution Reaction

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Hydrogen, with its high energy density, stands out as a clean, efficient, and cost-effective energy carrier. Among various production methods, electrochemical water splitting emerges as a promising, eco-friendly, and low-cost approach for sustainable hydrogen generation. Transition metal dichalcogenides (TMDs) have garnered significant attention due to their high surface-to-volume ratio and excellent mechanical stability [1]. In this study, a VS/MoS composite was synthesized via a hydrothermal route, and its nano-flower-like morphology was confirmed through field emission scanning electron microscopy (FE-SEM). High-resolution transmission electron microscopy (HRTEM) and selected area electron diffraction (SAED) patterns further validated the composite formation. While pristine VS exhibits relatively low catalytic activity for water splitting, its performance is notably enhanced upon compositing with MoS. This improvement is attributed to the increased number of exposed active sites and superior charge transfer kinetics provided by MoS [2]. Notably, the composite with higher molybdenum content demonstrated better catalytic performance, achieving an overpotential of approximately 56 mV at a current density of $-10 \text{ mA}\cdot\text{cm}^{-2}$. Furthermore, chronoamperometry measurements confirmed the long-term operational stability of the material.



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Keywords: TMDs; Hydrothermal method; Green energy; Hydrogen.

Asymmetric bridging site CoSeTe as a Co-catalyst on C,S-Doped g-CN for Superior Photocatalytic Hydrogen Generation

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The ever-increasing global energy demand necessitates a transition from conventional fossil fuels to renewable resources. Among them, solar energy is the most promising, as it is abundant and continuously replenished. A sustainable method for harnessing solar energy is photocatalytic hydrogen production, which depends solely on water and sunlight. However, practical application is limited by intrinsic drawbacks of photocatalysts, such as rapid charge recombination, poor light absorption, photocorrosion, and low solar-to-hydrogen efficiency. To overcome these challenges, we employed a visible-light-active photocatalyst, leveraging the fact that nearly 45% of the solar spectrum lies in the visible region. Graphitic carbon nitride (g-C₃N₄), a two-dimensional layered semiconductor, was chosen as the base material. To address its inherent limitations, we developed carbon and sulphur-self-doped porous g-C₃N₄ (2.75 eV), which introduces localized states (S 2p) between the conduction and valence bands, shortens diffusion lengths, enhances reactant adsorption, and extends the light absorption region. This tailored photocatalyst demonstrated a hydrogen evolution rate of 1.3 mmol/h/gcat. To further amplify activity, an asymmetric bridging site co-catalyst, CoSeTe, was introduced. Systematic optimization of loading revealed that 10 wt.% CoSeTe on C,S co-doped g-C₃N₄ achieved a remarkable hydrogen production rate of 13 mmol/h/gcat with excellent stability over five consecutive cycles. The asymmetric bridging sites in CoSeTe provide dual active centers, where Se-H and Te-H intermediates exhibit distinct bond energies, facilitating balanced hydrogen adsorption and desorption. This unique configuration accelerates surface reaction kinetics

and contributes significantly to the enhanced hydrogen evolution performance. To predict the electron transfer pathway, Ultraviolet photoelectron spectroscopy (UPS) was recorded, confirming that the work function (ϕ) of CoSeTe exceeds that of C,S co-doped g-C₃N₄, inducing upward band bending at the interface. This establishes a Schottky junction, which significantly enhances charge separation, facilitates electron transfer, and suppresses backflow of electrons. The detailed synthesis strategy, structural/electronic characterization, and mechanistic insights into charge transfer dynamics will be presented. These findings offer a pathway toward rational photocatalyst design for efficient and stable solar hydrogen production.

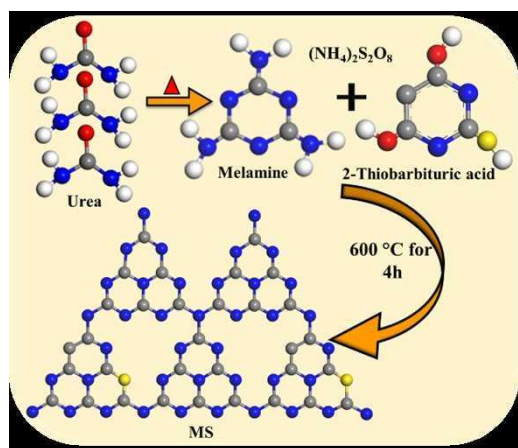


Figure 45: Schematic representation of the synthesis of C and S self-doped g-C₃N₄

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Keywords: Radioactive waste, Vitrification, Phosphate glass, Thermal stability

Sustainable Water Purification Novel Nanozirconia-Intercalated Clay composite for Fluoride Remediation

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This study presents the synthesis and characterisation of a novel zirconia-kaolinite intercalated composite (ZKIC) for the effective removal of fluoride from aqueous solutions. The composite was synthesised through a straightforward intercalation process, and its properties were extensively characterised using a suite of analytical techniques. X-ray diffraction (XRD) confirmed the successful intercalation of zirconia into the kaolinite structure, while scanning electron microscopy (SEM) and Energy-dispersive X-ray spectroscopy (EDX) provided clear evidence of morphological changes and the uniform distribution of zirconium within the matrix. Brunauer–Emmett–Teller (BET) and Dynamic Light Scattering (DLS) analyses revealed significant increases in surface area and colloidal stability, respectively, both of which are critical for enhanced adsorption performance. Batch adsorption studies were performed to optimise key parameters, including pH, contact time, and adsorbent dosage. Kinetic modelling indicated that fluoride removal follows a pseudo-first-order model. The composite demonstrated high fluoride removal efficiency in acidic environments and maintained good reusability over multiple cycles. Crucially, its practical applicability was validated using real-time contaminated groundwater samples, where it effectively reduced fluoride levels to below WHO-permissible limits. These results confirm that ZKIC is a promising, cost-effective, and highly efficient material for real-world water defluoridation applications

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Keywords: Hydrogen generation, Hydrogen evolution reaction, Water dissociation, Electrocatalysis, Water splitting.

DFT-guided graphene and graphene oxide in NiO: Engineering charge transfer process for optimized supercapacitor and electrochromic operation

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Though belonging to the same family of carbon, graphene (Gr) and graphene oxide (GO) show different mechanisms of charge transport, especially in the context of their electrochemical applications [1]. Here, the doping of Gr and GO nanoflakes, pre-optimized using density functional theory (DFT) calculations, was carried out in nanogranular NiO to design an electrochromic supercapacitor. The GO–NiO electrode shows diffusion-controlled mechanism-based charge storage properties [2], with sufficient color-modulating capability to design a color-indicative supercapacitor. The GO–NiO electrode, when realized as an asymmetric supercapacitor (GO–NiO–SCD), displays a high capacitance value of $\sim 105 \text{ mF cm}^{-2}$ with 100% capacitance retention. The color change, coherent with the (dis-)charging process, demonstrates its multifunctional applications. A prototype solid-state capacitor was able to light an LED, thereby demonstrating its on-field applicability. On the other hand, the Gr–NiO electrode demonstrated a surface-controlled charge storage mechanism, as also depicted from molecular electrostatic potential (MEP) plots of Gr and Gr–NiO. This approach suggests that Gr and GO, although belonging to the same family of carbon, can be utilized for different application purposes in electrochromic supercapacitor-based electrodes and devices [3].

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Keywords: Carbon, mechanism, Supercapacitor, Electrochromism.

Two-dimensional [Co(btbbH)₂(dpe)₂]·DMF metal–organic framework–derived low-cost nanocomposites for electrochemical nitrate reduction for ammonia production

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Excess nitrate (NO_3^-) accumulation occurs due to an imbalanced nitrogen cycle, primarily driven by artificial nitrogen fixation. In the meantime, environmental NO_3^- buildup has a substantial adverse effect on human health and the ecosystem. The electrocatalytic nitrate reduction reaction (NO_3RR), which yields value-added compounds like ammonia (NH_3), has lately attracted attention as a viable technique for environmental and energy-related concerns. The NO_3RR suits the urgent need to remove NO_3^- and create NH_3 through an alluring electrocatalytic pathway. Thus, this paper will discuss the preparation of novel 2D $[\text{Co}(\text{btbbH})_2(\text{dpe})_2]\cdot\text{DMF}$ metal–organic frameworks, which crystallize in the triclinic crystal system belonging to the $P\bar{1}$ space group using a solvothermal method. Among the nanocatalysts used, metallic cobalt nanoparticles supported on nitrogen-doped carbon (CoNPs/NC-600), as facilely prepared through the thermal decomposition of Co-MOF, have been shown to be highly efficient electrocatalysts for NH_3 production from NO_3RR . The CoNPs/NC-600 nanocomposites exhibit a maximum partial current density (PCD) of $-66.03 \text{ mA cm}^{-2}$ for NH_3 production, achieving a Faradaic efficiency (FE) of 72.25% at -0.5 V vs. RHE. Additionally, the highest yield rate for ammonia reached a noteworthy value of $30.79 \text{ mmol h}^{-2} \text{ cm}^{-2}$. Furthermore, density functional theory (DFT) calculations revealed that the Co[111] surface provides active nitrate reduction surpassing the

water dissociation over the Co_3O_4 [311] surface. Hence, this work provides a new design strategy for developing high-performance MOF-derived electrocatalysts for nitrate reduction reactions (NO_3RR) aimed at NH_3 production. Overall, this work presents a new design strategy for developing high-performance MOF-derived electrocatalysts for nitrate reduction reactions aimed at efficient NH_3 production.

Keywords: Metal-organic framework; Single crystal structure; Electrochemical NO_3RR ; Density functional theory

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NiCo LDH derived mesoporous Se doped NiCoP nanoflower architecture having regional defects for improving oxygen evolution reaction (OER)

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The rational design of efficient and stable doping with defect-engineered electrocatalysts is vital for enhancing oxygen evolution reaction through water electrolysis to address the energy crisis. In this present research, we report Se doped NiCoP mesoporous nanoflower architecture on three-dimensional nickel foam as the electrocatalyst through solvothermal followed by pyrolysis method. This optimised catalyst is derived from NiCo LDH (NCL/NF). This optimised catalyst NCP-Se/NF displayed enhanced OER activity in compared to parent NCL/NF and NCP/NF. It requires only 270 mV of overpotential to attain 10 mA/cm² current density and exhibits lowest Tafel slope of 28.17 mV dec⁻¹ with long-term durability. The improved performance of NCP-Se/NF catalyst associated to the one-pot phospho-selenisation synthesis strategy leading to create Se doping and P-vacancy in

bimetal phosphide simultaneously which induces electronic redistribution around Ni/Co sites reveal to optimizing the d-band centre subsequently provide more exposed active site, minimizes the diffusion path length and reduces the kinetic energy barrier for OER. More in CTAB integrated NCL/NF nanoflower under high temperature give mesoporous framework in NCP-Se/NF catalyst. This unique mesoporous flakes of nanoflower structure increased specific surface area with facilitates the electrolyte penetration and accelerate the formation/liberation of O₂ gas bubble. The combined strategies of element doping and vacancy engineering in this work offer valuable insights into the design of high-performance electrodes.

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Keywords: OER, Se doping, P-vacancy, mesoporous

Unravelling the Oxygen Reduction Reaction Activity under Acidic Medium Using Designed N-doped Graphene Catalyst

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In the search for low-cost, high-performance oxygen reduction reaction (ORR) catalysts for the advancement and viability of hydrogen fuel cell technology, the discovery of metal-free N-doped carbon materials has revolutionized catalysis research. In addition, later studies revealed that pyridinic-N (pyri-N) creates the O₂ adsorption site at the neighboring carbon.[1] The N-doped carbon materials have displayed ORR activity comparable to that of the state-of-the-art Pt/C catalyst under alkaline electrolyte (KOH). However, the origin of the lower ORR activity under acidic media ($\text{H}_2\text{SO}_4/\text{HClO}_4$) is still not

clarified. Studies show that bulkier counter anions and protonation of doped N are mainly responsible for the reduced activity by limiting O₂ accessibility and lowering the adsorption energy at the active sites.[2] To understand the ORR mechanism under acidic media, the development of N-doped carbon catalysts with uniform N-doping and well-defined structure is a primary requirement.[3] In the present study, a thin-layer coating of cyanuric acid (N-precursor) functionalized (hydroxyethyl)methacrylate (HEMA) polymer was achieved over graphene oxide (GO) via controlled UV polymerization. The uniformly distributed N-precursor over the GO layer was utilized for N-doping through high-temperature treatment, resulting in N-doped reduced graphene. The chemically N-doped graphene (cNrGO) obtained through the controlled coating process exhibits superior catalytic activity ($E_{onset} \approx 0.852$ V, $E_{1/2} = 0.691$ V vs. RHE) compared to the physically mixed sample (pNrGO) ($E_{onset} = 0.52$ V, $E_{1/2} = 0.31$ V vs. RHE). Furthermore, the ORR catalytic pathway was confirmed through density functional theory (DFT) calculations using the Vienna *ab initio* simulation package (VASP), illustrating the role of protonation of doped N in altering ORR activity. In addition, the effect of spin-density variation induced by N-doping was verified using electron paramagnetic resonance (EPR) studies.

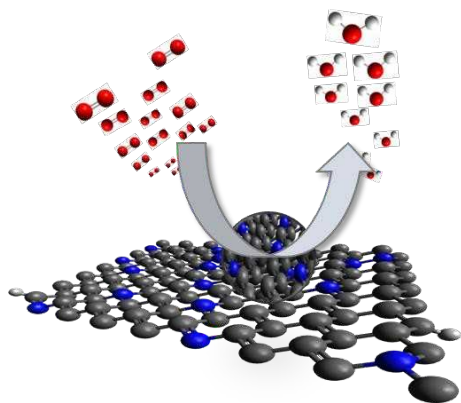


Figure 46:

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Keywords: Electrocatalysis, metal-free catalyst, N-doped graphene, ORR mechanism.

Tuning thickness of Molybdenum Nitride thin films for improved electrochemical sensing

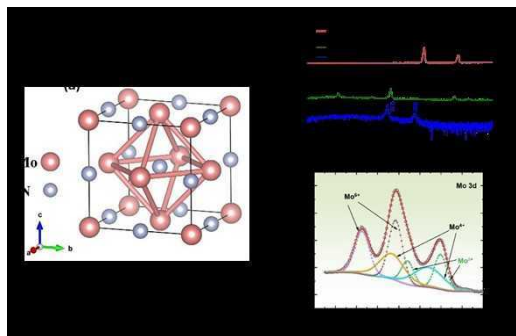
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Transition metal nitrides (TMNs), particularly molybdenum nitride (Mo₂N), have gained increasing attention due to their exceptional properties such as high electrical conductivity, chemical stability, and catalytic activity. Varying the thickness of these films can significantly affect their electrochemical performance, as not only the crystallinity but also the density of active sites is notably modified with decreasing thickness. In this study, Mo₂N thin films with varying thicknesses were synthesized via reactive DC/RF magnetron sputtering under a controlled nitrogen–argon atmosphere. The films were deposited on various substrates, including Ni foam, silicon, and fluorine-doped tin oxide (FTO). The formation of the γ -Mo₂N phase was confirmed by grazing-incidence X-ray diffraction (GI-XRD). X-ray photoelectron spectroscopy (XPS) revealed the presence of Mo in both Mo⁴⁺ and Mo⁶⁺ oxidation states, indicating minute oxygen contamination, primarily at

the surface, along with the dominant nitride phase. An additional δ^+ oxidation state was also observed in the XPS spectra, which may arise due to differences in electronegativity between the oxide and nitride species present in the films. Film thickness and density were determined using X-ray reflectivity (XRR). Preliminary electrochemical studies suggest that films with a thickness of approximately 75 nm are the most promising for the intended application.



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Keywords: Electrocatalysis, metal-free catalyst, N-doped graphene, ORR mechanism.

Polyoxometalate-loaded reduced Graphene Oxide-modified Metal Vanadate catalysts for Environmental Pollutant Remediation.

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The escalating global energy demand and increasing environmental concerns have intensified efforts toward the development of advanced photocatalysts for solar fuel production and environmental remediation. Metal vanadates, particularly silver vanadate (AV) and copper vanadate (CV), have emerged as attractive visible-light-active photocatalysts owing to their

narrow bandgap and favorable band-edge positions. Nevertheless, their practical applicability remains constrained by the rapid recombination of photogenerated charge carriers. Rational design of heterostructures by incorporating polyoxometalate (POM)-loaded reduced graphene oxide (RGO) as a co-catalyst offers a viable approach to overcome these limitations by improving charge separation and electron transfer. The present study deposited AV and CV onto POM-functionalized RGO (RPOM) via a one-pot coprecipitation route, yielding RPOM-AV and RPOM-CV nanocomposites. The electrochemical analyses revealed markedly enhanced photocurrent densities of 223.7 and 85.8 mA cm² for RPOM-AV and RPOM-CV, respectively, corresponding to 51-fold and 6-fold improvements relative to pristine counterparts. These enhancements were correlated with an increased donor density and improved interfacial charge dynamics within the heterostructure. The photocatalytic performance evaluations demonstrated that RPOM-AV achieved a 94% reduction of Cr(VI) within 60 min ($k = 0.044 \text{ min}^{-1}$), alongside 94% removal of rose bengal dye within 120 min, driven by synergistic adsorption-photocatalysis. In contrast, RPOM-CV exhibited 96% degradation of methylene blue with a rate constant of 0.011 min^{-1} . The superior activity of both systems is attributed to the establishment of an indirect Z-scheme heterojunction between metal vanadates and POM clusters, with RGO serving as an electron mediator to facilitate directional charge transfer, suppress recombination, and promote spatial separation of photogenerated carriers. It underscores their potential as advanced materials for wastewater remediation and solar energy-driven environmental applications

Keywords: Hydrogen generation, Hydrogen evolution reaction, Water dissociation, Electrocatalysis, Water splitting

Enhancing Energy Density of Tailored 2D Nb₂C MXene/CoNb₂O₆ Hybrids for Lithium-Ion Hybrid Capacitors.

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Lithium-ion hybrid capacitors (LIHCs) are rapidly gaining attention as next-generation energy storage devices, uniquely combining the high energy density of batteries with the ultra-high power capability and cycling stability of supercapacitors. However, their widespread deployment is still constrained by the challenge of developing robust anode materials that can deliver high capacity, fast kinetics, and long-term stability simultaneously. Recently, MXene-based composites have emerged as promising candidates for meeting this requirement, owing to their high electrical conductivity and adaptable surface chemistry, which make them suitable for a broad range of applications. In this work, we investigate two niobium-based materials such as 2D Nb₂C MXene and conversion-type CoNb₂O₆, as potential anodes for LIHCs. Their structural and surface properties were characterized using XRD, FESEM, XPS, and HR-TEM. While looking at electrochemical performances, Nb₂C delivers a stable specific capacity of 190 mAh/g over 100 cycles with excellent rate capability, and CoNb₂O₆ demonstrates a higher initial capacity but suffers from rapid capacity fading due to its conversion reaction mechanism, retaining only 200 mAh/g after 15 cycles at the same current density. To address this limitation, we propose a hybrid strategy by integrating CoNb₂O₆ with Nb₂C MXene to leverage the mechanical robustness and electronic conductivity of MXene for stabilizing the electrochemical behavior of CoNb₂O₆. Drawing inspiration from our previous work on Nb₂C/FeCo-LDH composites, various mass ratios of Nb₂C and CoNb₂O₆ were synthesized and studied to identify the optimal composition. The best-performing hybrid anode was further integrated with a high-surface-area porous carbon (2000 m²/g) cathode to assemble a full-cell LIHC, wherein the anode was pre-lithiated to improve initial coulombic efficiency and overall performance. The results

highlight the potential of MXene-based hybrid architectures in overcoming conversion material limitations and advancing the practical viability of next-generation LIHCs.

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Keywords: 2D Materials, MXenes, Hybrid Composites, CoNb₂O₆/Nb₂C, Lithium-ion hybrid capacitor.

Tailored Nanoparticle Organic Network Membranes for Hydrogen Generation

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Assembling metal nanoparticles (MNPs) into extended structures is an emerging area of research for designing metamaterials. Conventional strategies for MNP assembly are primarily driven by noncovalent interactions, often resulting in trade-offs between structural integrity and ease of processability.^[1] In this direction, nanoparticle organic network membranes (NONM)^[2] are developed using a unique covalent chemistry-inspired liquid-liquid (L/L) interfacial approach. The NONM fabrication has been achieved in two consecutive steps. In the first step, functionalized silver nanoparticles (AgNPs) are covalently anchored to free formyl groups of pre-mature covalent organic framework membranes (COFMs) - to suppress the agglomeration of AgNPs, and in the second step, further covalent connections are established with

dialdehydic linkers, resulting in free-standing NONMs (AgNONMs).^[3] Capitalizing on the electrocatalytic activity of AgNPs and the enhanced charge transfer, the AgNONMs pose potential as ready-to-use membrane electrodes for electrochemical hydrogen evolution reaction (HER). HER finding of AgNONMs shows a higher current density and lower overpotential compared to the pristine COFMs. Furthermore, we anticipate that our unique approach of assembling MNPs in a processable form will stimulate the creation of next-generation NON membranes tailored for electrocatalytic and optoelectronic applications.

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Keywords: Metal nanoparticles, Nanoparticle organic network, membrane electrode, Hydrogen evolution reaction.

Electrochemical Deposition of NiCo LDH on Diverse Substrates for Improved Electrocatalytic Oxygen Evolution Activity

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The global energy transition toward sustainable and low-carbon energy systems has become rapid increasing due to the finite nature of fossil fuels and their contribution to greenhouse gas emissions. Hydrogen is considered

a clean, renewable, and highly efficient energy carrier, offering great potential in achieving a low-carbon energy future. Developing efficient and durable electrocatalysts for the oxygen evolution reaction (OER) is a key step in improving electrochemical water splitting, particularly under alkaline conditions. In this study, NiCo LDH nanostructures were synthesised through an electrochemical deposition method on three different conductive substrates: nickel foam (NF), graphite sheet (GS), and carbon cloth (CC). The structural and morphological properties were analysed using XRD, XPS, FESEM and HRTEM. Electrochemical studies, including cyclic voltammetry (CV), linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), and chronopotentiometry (CP), were carried out to compare the catalytic performance of NiCo LDH on all substrates. Among the tested electrodes, NiCo LDH grown on NF exhibited the highest catalytic activity, achieving an overpotential of 260 mV at a current density of 50 mA/cm², Tafel slope of 57 mV/dec, and a double-layer capacitance (Cdl) of 2.86 mF/cm², indicating excellent charge transfer properties. Furthermore, the catalyst showed no noticeable performance degradation even after 100 CV cycles. The full-cell configuration requires an overall potential of 1.61 V to reach a current density of 10 mA/cm². This study emphasises the importance of substrate selection and surface architecture in optimizing NiCo LDH electrocatalysts for renewable energy applications.

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Keywords: Layered double hydroxides; Substrate effect; Electrodeposition.

Double-encapsulated red-emitting formamidinium lead halide perovskite nanocrystals for fluorescent sensing and lighting applications

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In recent years, metal halide perovskite nanocrystals (NCs) have offered several optoelectronic and sensing applications due to their unique photophysical properties. Formamidinium (FA) based perovskite NCs exhibit better thermal and structural stability than the corresponding volatile methylammonium (MA)-based counterpart, which quickly decomposes to release gaseous methylamine. FA-based perovskite NCs also demonstrate more fantastic responses towards different environmental stimuli, which is helpful for different sensing applications. However, FAPbI₃ NCs suffer from phase instability and degrade very fast under external stimuli. Here, we synthesised mixed halide FAPb(B/I)₃ NCs by partially replacing I-ions with Br-ions to address the key challenge of phase instability of FAPbI₃ NCs. Further, with a surface modification approach like encapsulating the NCs' surface with silica and also double-encapsulating silica-polymethyl methacrylate (PMMA) polymer, we enhanced the stability of the NCs against heat, ion migration, and UV irradiation. Such double-coated red-emitting FAPb(B/I)₃ NCs (emission peak 642 nm) were tested for temperature sensing, exhibiting a relative sensitivity (RH) of 12.5 %-K⁻¹. We also prepared fluorescent humidity sensors that revealed the lowest detection limit of 5% RH. Finally, down-converted WLEDs were fabricated using double-coated green-emitting Cs-doped FAPbBr₃ NCs and red-emitting FAPb(B/I)₃ NCs in thin-film form and embedded on a blue LED chip. These results will boost the development of high-performance sensors and lighting technologies.

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Keywords: nanocrystals, perovskite, WLED

Photolithographic patterning of metal halide perovskite nanomaterials for advanced anti-counterfeiting devices

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The rapid expansion of global markets and information technology has led to a growing demand for advanced anticounterfeiting devices to prevent forgery, currency piracy, QR-code duplication, and brand infringement. Conventional anticounterfeiting labels are often vulnerable to cloning due to inadequate security features, while many materials employed for anticounterfeiting and information encryption exhibit only limited reversibility, restricting their reuse over multiple cycles. Consequently, there is a pressing need to develop reversible and multimodal anticounterfeiting labels that integrate optical and/or physical modes, offering high reliability, reproducibility, and resistance to replication.

In recent years, metal halide perovskite nanocrystals (NCs) with an ABX₃ crystal structure have emerged as promising candidates owing to their exceptional and tunable photophysical properties, including high photoluminescence quantum yield, color tunability, narrow emission bandwidth, and defect tolerance. Despite these advantages, perovskite NCs suffer from poor environmental and chemical stability, being highly sensitive to humidity, temperature, polar solvents, halide exchange, ion migration, and prolonged ultraviolet exposure. These limitations severely hinder their commercialization in anticounterfeiting applications, particularly under conventional lithographic processing conditions involving harsh photoresists, developers, acetone, and high baking temperatures.

Here, we report a novel patterning strategy for perovskite NCs that completely avoids the use of harsh photoresists, developers, and high-temperature baking processes. We demonstrate the synthesis of a lyochromic perovskite material exhibiting highly reversible switching between luminescent and non-luminescent states. This patterning approach is employed to fabricate advanced anticounterfeiting labels and

information encryption platforms with high reproducibility, reversibility, and long-term reliability, offering a robust pathway toward secure and reusable perovskite-based anticounterfeiting technologies.

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Keywords: Metal halide perovskite; Photolithography; Anticounterfeiting; Reversibility.

Integrated SERS Detection and Photocatalytic Degradation of Microplastics: A Dual-Strategy Approach Using Ag-Cu Nanoparticles and ZnTi-Layered Double Hydroxides

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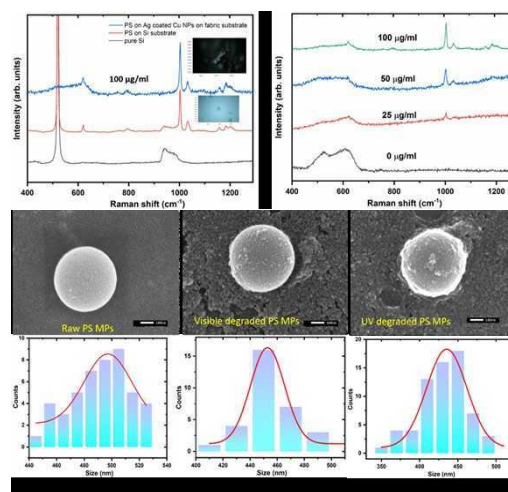
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Microplastic contamination poses a significant environmental threat, necessitating the development of advanced detection and remediation strategies. This study presents a comprehensive approach integrating sensitive detection via Surface-Enhanced Raman Spectroscopy (SERS) with photocatalytic degradation for effective microplastic management. Two SERS substrates were developed and compared: silver-coated copper nanoparticles (Ag-Cu NPs) and copper-silver-gold (Cu-Ag-Au) trimetallic nanobowl-coated cotton fabric, both evaluated for their sensitivity in detecting 10 m polystyrene (PS) microplastics. The Ag-Cu

NP substrate exhibited superior sensitivity, attributed to its enhanced hydrophobicity, which facilitates improved adsorption of PS microplastics. In addition to its high detection capability, the Ag-Cu NP substrate is cost-effective, making it a promising candidate for large-scale environmental monitoring. The SERS technique employed enables rapid, nondestructive, and highly specific identification of microplastics, addressing the urgent need for reliable and scalable detection methodologies in environmental assessment.

For remediation, zinc-titanium layered double hydroxide (ZnTi-LDH) photocatalysts were synthesized via hydrothermal methods and evaluated for microplastic degradation. The LDH exhibited a bandgap of 2.9 eV, enabling activation under both UV and visible light. Photodegradation studies using 500 nm PS microplastics at 100 ppm revealed 8.8% degradation under visible light and 12.47% under UV light over 24 hours. FESEM analysis confirmed degradation through particle size reduction and morphological changes. The mechanism likely involves reactive oxygen species attacking polymer chains, resulting in fragmentation and eventual mineralization.

The integration of sensitive SERS detection with LDH-based photocatalytic degradation offers a holistic and sustainable approach to microplastic management. Utilizing earth-abundant materials, the system enables accurate, real-time monitoring and efficient remediation, which enhances its feasibility for large-scale environmental applications. **Keywords:** Microplastics, Surface-enhanced Raman spectroscopy (SERS), Photocatalytic degradation, Layered double hydroxide, Polystyrene, Visible light photocatalysis



Keywords: Microplastics, Surface-enhanced Raman spectroscopy (SERS), Photocatalytic degradation, Layered double hydroxide, Polystyrene, Visible light photocatalysis.

Green synthesis of a magnesium single-atom catalyst from *Spinacia oleracea* chlorophyll extracts for sustainable electrocatalytic nitrate reduction to ammonia

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Ammonia is one of the most used chemical compounds, and its electrochemical synthesis is a promising alternative. Herein, we report a practically viable magnesium single-atom catalyst (MgNxC) for the promising reduction of nitrate to ammonia. The catalyst was prepared using green leaf extracts of *Spinacia oleracea* via simple one-step pyrolysis. The MgNxC catalyst, anchored on a defective graphitic matrix, exhibits the best-optimised potential of 0.58 V vs. RHE, a faradaic efficiency of $81.5 \pm 2.9\%$ and a yield rate of $392.5 \pm 41.2 \mu\text{mol h}^{-1} \text{mg}^{-1} \text{cat.}$ with excellent repeatability. DFT is employed to optimize the most stable reactive site and various reaction pathways for a favorable nitrate reduction reaction, with probable reaction intermediates were explored. Collectively, our work demonstrates a simple, cost-effective, and convenient way to synthesise SACs.

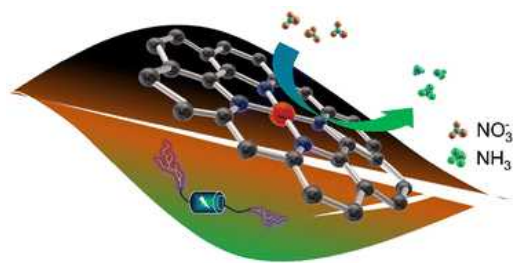


Figure 47: TOC

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Keywords: Sustainable Ammonia production; Magnesium single atom catalysts (Mg-SACs).

Graphite supported Ni-Co-P: A Promising Electrocatalyst for Hydrogen Evolution

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The increasing demand for sustainable hydrogen production has intensified research into non-precious electrocatalysts. Transition metal phosphates (TMPs) have emerged as promising candidates for electrochemical water splitting owing to their abundance of redox-active metal centers. The phosphate groups in TMPs not only enhance electrical conductivity but also provide a high density of exposed active sites and act as proton acceptors. Among them, nickel-cobalt phosphate (NiCoP) nanoparticles are particularly attractive due to their favourable electronic properties. In this work, NiCoP nanoparticles were synthesized through potentiostatic electrodeposition—a simple, binder-free, and cost-effective technique that enables the fabrication of uniform and phase-pure phosphate-based catalysts. Graphite sheets were employed as the deposition substrate because of their high conductivity and chemical robustness. By tuning the phosphorus concentration within NiCoP, we systematically evaluated its catalytic efficiency for water splitting. Structural and electronic alterations, such as the generation of lattice defects, further contributed to the creation of additional active sites, thereby improving catalytic activity. The prepared NiCoP samples were thoroughly analyzed using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), field-emission

SEM (FESEM), and high-resolution transmission electron microscopy (HRTEM) to examine their crystal structure, oxygen vacancy formation, and surface morphology. Electrochemical testing revealed that the NiCoP(1.6)/GS electrode required an overpotential of only 140 mV to achieve a current density of 50 mA cm² and lowest Tafel slope value of 81 mV/dec in 1.0 M KOH during the hydrogen evolution reaction (HER).

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Keywords: Hydrogen evolution reaction; Nickel cobalt phosphate; Graphite sheet; Electrodeposition.

Solution-Processed Cs₃Bi₂I₉-PMMA Composites for Flexible Memristive Devices

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Metal Halide Perovskites (MHP) have emerged as one of the most promising materials of modern electronics due to its excellent optoelectronic properties, e.g., high absorption coefficient, composition-tunable gaps, low exciton binding energies, facile solution processability, etc. Mixed electronic-ionic behavior of MHPs underpins its applications in the field of memristive devices and has proved its potential to emulate human synapses in neuromorphic computing systems. By contrast, polymer matrices act as a flexible, low-cost, host material for active switching elements in the field of resistive switching (RS) devices. Polymer matrices function as insulating or semi-insulating layers whose electrical and mechanical performances can be tailored through doping, functional group engineering, or incorporation of different additives.

Thus, hybrid nanocomposite functional films, utilizing the merits of both organic and inorganic phases, have shown considerable promise for advanced optoelectronic applications. In the present study, a zero-dimensional (0D), lead-free all-inorganic perovskite, Cs₃Bi₂I₉, was introduced as a functional additive into a poly (methyl methacrylate) (PMMA) host to create HP-polymer composites, and systematically investigate the effects of perovskite inclusion on the polymer host. Cs₃Bi₂I₉ was synthesized via a one-step solution process, and HP-polymer composites with varying perovskite weight% were prepared by controlled solution mixing. Structural characterization by X-ray diffraction (XRD) and optical analysis using UV-visible spectroscopy (UV-vis) and Fouriertransform infrared spectroscopy (FTIR) of the pristine HP and the HP-polymer composites, confirms successful incorporation of the additives in the polymer matrix. To evaluate device-level performance of the synthesized samples, flexible memristive devices were fabricated. Resistive switching (RS) is observed in the perovskite incorporated devices with ON/OFF ratio, switching endurance and retention, which shows systematic enhancement with increasing additive concentration. These results clarify to understand the role of Cs₃Bi₂I₉ as a functional additive in polymer matrices and demonstrate its potential to improve the performance of polymer-nanocomposite based flexible RS devices with optimized additive concentrations.

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Keywords: Halide perovskite; Polymer; Composites; Resistive switching.

Electromechanical and Computational Insights into Bent Core Liquid Crystal-Infused PVDF Composites for Improved Piezoelectric Performance

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Organic ferroelectric polymers, viz. polyvinylidene fluoride (PVDF) and its copolymers are widely explored for flexible energy applications owing to their excellent mechanical resilience and ease of processing. Augmenting their electromechanical response through molecular engineering has become a key focus in recent material design approaches. Here, we demonstrate that the infusion of a novel polar noncentrosymmetric bent-core liquid crystal (BCLC) into a semicrystalline PVDF matrix at optimised weight fraction offers an interfacial engineered approach for improved dielectric and electromechanical properties of the resultant polymer composite-based piezoelectric systems [1]. The incorporation of bentcore liquid crystals (BCLC) into the PVDF matrix resulted in a nearly three-fold enhancement in the piezoelectric output voltage compared to pristine PVDF. Furthermore, at an optimal loading of 3 wt% BCLC, the composite exhibited significant improvements in both dielectric constant and electrical conductivity, underscoring the role of BCLC infusion in tailoring the electromechanical performance of the system. To better understand the mechanisms underlying this improvement, detailed density functional theory (DFT) computations were conducted using the Gaussian-16 software package to examine the interfacial interactions and modifications in the electronic geometry of PVDF/BCLC composites. The DFT calculation indicates that the electropositive moieties present in the BCLC forms weak intermolecular hydrogen (H) bonds with the electronegative fluorinated segments of PVDF, promoting a transition from the non-polar -phase to the highly electroactive -phase

by stabilising dipole alignment within the polymer matrix. These interactions are thermodynamically feasible, as demonstrated by interaction energy analysis, and promote phase stabilisation, crucial for piezoelectric activity. Further, the electronic structure calculations show a significant reduction in the HOMO–LUMO band gap upon BCLC infusion in the PVDF matrix at an optimised weight fraction. This narrowing is attributed to enhanced charge delocalisation and stronger orbital overlap at the PVDF/BCLC interface, leading to improved polarisation and electronic coupling. Electrostatic potential maps and charge density distributions further validate these interfacial effects. Together, the computational and electromechanical insights demonstrate that BCLC-induced molecular ordering and electronic tuning play a pivotal role in optimising the piezoelectric performance of the composite. This study highlights the potential of BCLCs as functional additives in next-generation organic piezoelectric assemblies and underscores the worth of integrated computational experimental approaches in designing high-performance energy harvesting materials.

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Keywords: Polymer Composites; Bent Core Liquid Crystals; Piezoelectricity; Density Functional Theory.

Piezoelectric Mono-elemental Black Phosphorus for Pressure Sensing Applications

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The attention to two-dimensional mono-elemental structures is increasing. Even though single elemental materials, such as graphene, fail to exhibit piezoelectric behaviour because of a lack of ionic polarization, there are possible mono-elemental possibilities from the pnictogen family. [1, 2]. The exploration towards pnictogen chemistry began after the discovery

of black phosphorus. With its differently positioned P atoms, black phosphorus acquires a non-centrosymmetric puckered-orthorhombic structure, leading to intrinsic piezoelectricity. [3] aims to provide a facile synthesis and understanding of the piezoelectric characteristics of a few-layered black phosphorus. The as-synthesised black phosphorus exhibits excellent piezoelectric behaviour. In light of this, this study is extended to the fabrication of piezoelectric sensor devices, which involved the selection of appropriate substrates, binders, solvent optimizations and material loading. Furthermore, various optimisations at the device level are carried out. It was observed that the bare devices are superior in their performance and quite promising for real-time pressure sensing applications.

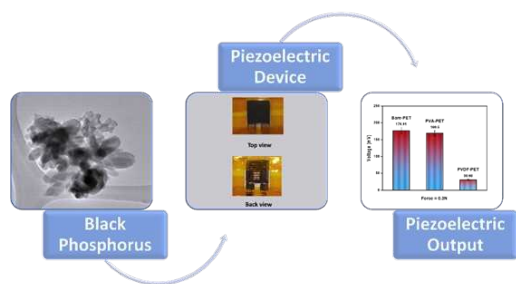


Figure 48: TOC

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may use as an active material in pressure sensing devices. Hence, this study *Chemie International Edition*, 2019. 58(23): p. 7551-7557.

Keywords: Piezoelectricity, Black phosphorus, Pressure sensors.

Harnessing Cobalt-Based Heterostructures For The Efficient Removal Of Nitrofurantoin Via Peroxymonosulfate activation

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The elimination of the antibiotic drug nitrofurantoin (NFT) from water, primarily used to treat urinary tract infections, has become a concerning topic of water sustainability, due to increase in the water contamination and antimicrobial resistance. The current work contributes to the development of CoWO₄ and Fe, W codoped Bi₂Mo₃O₁₂ heterostructures (weight ratios of 0:1, 1:0, 0.5:1, 1:1, and 1:0.5) fabricated by the hydrothermal method for the potential degradation of NFT under visible light via peroxymonosulfate (PMS) activation. The phase purity, presence of functional groups, composition, morphology, and band gap of the materials were evaluated using the powder X-ray diffraction technique (XRD), Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), high-resolution transmission electron microscopy (HRTEM) with selected area electron diffraction (SAED), and UV-Visible diffuse reflectance spectroscopy (UV-vis DRS). The formation of CoWO₄, as well as Fe, W-codoped Bi₂Mo₃O₁₂ phases, was observed in the XRD pattern. The change in the Mo-O and Bi-O stretching peaks denoted the formation of heterostructures, was noted in the FTIR spectra. The presence of Bi, Mo, Fe, Co, W, and O elements in the CoWO₄: Fe, W codoped Bi₂Mo₃O₁₂ (0.5: 1 wt%) was confirmed from the XPS analysis. The morphology of Fe, W-codoped Bi₂Mo₃O₁₂, CoWO₄, CoWO₄: Fe, W codoped Bi₂Mo₃O₁₂ (0.5: 1 wt%) exhibited as nanoplates, agglomerated nanorods, and combination of nanorods and nanosheets, respectively. The visible light-active catalyst

CoWO₄: Fe, W codoped Bi₂Mo₃O₁₂ (0.5: 1 wt%) possessed a bandgap of 1.87 eV, exhibited a highest degradation efficiency of 99.7 % towards NFT within 10 min via PMS activation. Scavenger tests revealed the participation of reactive species in the order of photogenerated holes; singlet oxygen; superoxide radicals; sulfate radicals; hydroxyl radicals, in the efficient degradation of NFT in the presence of PMS. Furthermore, LC-MS analysis corroborated the degradation intermediates of NFT. This work offers a sustainable approach towards highly effective degradation of emerging pharmaceutical contaminants such as NFT in water under visible light in a short time.

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Keywords: Nitrofurantoin, Peroxymonosulfate, CoWO₄, Bi₂Mo₃O₁₂

Role of V₂O₅ in Modifying the Sintering Kinetics and Electrical Characteristics of Lead-Free BNT-BT-KNN Ceramics

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The demand for environmentally benign piezoelectric ceramics has driven the development of lead-free alternatives to conventional lead-based materials such as Pb(Zr,Ti)O₃. Among these, Bi_{0.5}Na_{0.5}TiO₃ – BaTiO₃ – K_{0.5}Na_{0.5}NbO₃ (BNT–BT–KNN) Systems are particularly promising due to their morphotropic phase boundary (MPB) compositions, which enable enhanced electromechanical properties. However, achieving optimal densification and stable

electrical performance remains challenging because of the high volatility of alkali components and limited grain growth during sintering. In this work, we investigate the role of vanadium pentoxide (V₂O₅) as a low-level sintering aid for tailoring the structural, microstructural, and electrical characteristics of 91BNT–5BT–4KNN ceramics prepared via the conventional solid-state reaction method [1]. X-ray diffraction confirmed the formation of a pure perovskite phase with coexisting rhombohedral and tetragonal structures across all doped compositions, indicating preservation of the MPB region. Scanning electron microscopy revealed that the incorporation of 0.1 wt% V₂O₅ achieved the highest density of 5.15±0.002 g/cm³ with uniform grain growth, whereas higher dopant concentrations required elevated sintering temperatures without providing significant microstructural benefits. Dielectric measurements showed a strong frequency- and temperature-dependent response, with all compositions exhibiting peak permittivity near 400 °C [2]. The 0.1 wt% V₂O₅ composition demonstrated the best dielectric performance, attaining a maximum dielectric constant of 2945 at 1 kHz, alongside low dielectric loss values (tan δ < 1), reflecting high-quality insulating characteristics. Polarization–electric field (P–E) hysteresis loop analysis confirmed the ferroelectric behavior of all samples. Maximum polarization (P_{max}) increased with dopant concentration, reaching 9.34±0.002 μC/cm² for the 1.0 wt% composition, while remnant polarization (P_r) and coercive field (E_c) values varied systematically with V₂O₅ content. Compared with undoped and other doped lead-free systems reported in the literature, the present V₂O₅-modified ceramics exhibited superior densification, enhanced dielectric response, and improved ferroelectric polarization. The observed improvements are attributed to the fluxing action of V₂O₅, which promotes grain boundary diffusion, reduces porosity, and stabilizes the MPB region, thereby facilitating efficient domain wall motion and enhancing overall electrical performance. In summary, this study demonstrates that controlled addition of V₂O₅, particularly at 0.1 wt%, provides a simple and effective route to optimize the sintering kinetics and electrical characteristics of BNT–BT–KNN ceramics. These findings establish V₂O₅ doping as a viable strategy for advancing the functional performance of lead-free piezoelectric materials.

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3. D. Khademi, M. Zargazi, M. Chahkandi, M. Baghayeri, Environmental Research 2023, 219, 115154.

Keywords: Lead-free piezoelectric ceramics, V_2O_5 doping, BNT–BT–KNN, dielectric properties, ferroelectricity, sintering kinetics.

Enhancing the Longevity of Perovskite Solar Cells via Spacer Cation Engineering

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Organic-inorganic metal halide perovskites (OIHPs) have garnered immense interest for their exceptional power conversion efficiency (PCE) [1]. However, their susceptibility to environmental factors like moisture, oxygen, and heat hinders their commercialization. A promising strategy to improve perovskite solar cell (PSC) stability involves the creation of 2D/3D hybrid perovskites by introducing spacer cations into the 3D structure [2], [3]. This study investigates the effect of octylammonium iodide (OAI) as a spacer cation in MAPbI₃. Octylammonium Iodide incorporation targets defect passivation, aiming to mitigate defects on the surface and grain boundaries of MAPbI₃. X-ray diffraction (XRD), UV visible spectroscopy, Steady State PL, TRPL Raman spectroscopy, FTIR spectroscopy, Scanning Electron Microscopy (SEM) were employed to analyze the impact of OAI on crystal structure, Photophysical properties, chemical bonding and morphology of the perovskite film. The results suggest that mixed dimensional perovskite films are retaining their unique initial properties for a longer time than 3D perovskites.

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Keywords: Lead-free piezoelectric ceramics, V_2O_5 doping, BNT–BT–KNN, dielectric properties, ferroelectricity, sintering kinetics.

Wheat-Bran Derived Carbon Activation via Green Activation: A Structural and Electrochemical Insights of Supercapacitor Application

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The search for sustainable and high-performance electrode materials for supercapacitor applications has motivated the use of biomass precursors combined with green activation strategies. In this work, wheat bran, an abundant agro-waste, was utilized as a carbon precursor, and natural lemon extract served as a bio-based activating agent to synthesize activated carbon at varying concentrations (100%, 50%, and 33% v/v). The resulting materials, denoted as WBA0, WBA1, and WBA2, were systematically studied to correlate structural modification, surface functionality, and

electrochemical performance for electric double-layer capacitor (EDLC) applications. Structural characterization using X-ray diffraction (XRD) revealed that untreated carbon (named as WB) exhibited a broad, low-intensity hump, confirming its predominantly amorphous carbon nature with residual starch peaks around 18–19°. Upon activation, starch peaks disappeared, while the WBA's samples displayed sharper reflections at 26° (002) and 43° (100), indicating partial graphitization and improved ordering [1]. WBA1 showed the most prominent (002) peak, signifying enhanced graphitic domains induced by citric acid and flavonoids in lemon extract. Fourier Transform Infrared Spectroscopy (FTIR) analysis confirmed significant chemical modification, with the disappearance of ether and oxy-compound vibrations and the emergence of strong carbonyl (C=O) peaks around 1714 cm⁻¹ in activated samples [2]. These features indicate functionalization of carbon surfaces, beneficial for ion adsorption and electrochemical activity. Field Emission Scanning Electron Microscopy (FESEM) revealed a clear morphological transformation, i.e., pristine WB displayed dense starch granules, while activated carbons exhibited porous, interconnected architectures. WBA1, in particular, developed hierarchical porosity with larger pore interconnectivity, facilitating electrolyte accessibility and charge storage. Galvanostatic charge-discharge (GCD) testing confirmed the enhanced capacitive behavior. At the current of 0.3 mA, WBA1 delivered the maximum specific capacitance of 29.02 F.g⁻¹, corresponding to an energy density of 4.03 Wh.kg⁻¹ and a power density of 150 W.kg⁻¹. The electrochemical impedance spectroscopy (EIS) findings revealed reduced equivalent series resistance (ESR) and lower charge-transfer resistance in activated carbons compared to WB [3-4]. Collectively, the results confirm that lemon extract serves as an effective, eco-friendly activating agent. Among all samples, WBA1 (50% lemon extract) provided the most balanced performance, combining high specific capacitance, improved energy density, and reduced internal resistance. This study highlights the potential of agricultural by-products activated with natural extracts as sustainable and cost-effective electrode materials. The findings pave the way for scalable green synthesis approaches that bridge renewable resources with energy storage applications.

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Keywords: Supercapacitor; Wheat Bran; Lemon Extract; Green Synthesis.

Design and Development of High-Performance Silicon-Based n-i-p Heterojunction Photoanode for Large-Scale Photoelectrochemical Water Splitting Application

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With the rising global demand for sustainable energy, the production of green hydrogen through the photoelectrochemical (PEC) route has emerged as a highly promising solution. Heterojunction photoelectrodes are advantageous for PEC applications due to their ability to enhance light absorption, improve charge carrier generation, and facilitate efficient

charge separation and transfer while minimizing recombination losses. In this work, a high-performance silicon-based n-i-p heterojunction photoanode with an FTO/TiO₂/Si/NiO architecture has been successfully developed using earth-abundant materials, leveraging the inherent benefits of the heterostructure design. Targeting the practical application of the photoelectrodes for solar fuel production, the heterojunction was fabricated via the industry-relevant magnetron sputtering technique, ensuring scalability and uniformity. The optimized FTO/TiO₂/Si/NiO configuration achieved an impressive surface photovoltage of 600 mV and delivered a photocurrent density of approximately 0.65 mA/cm² at 1.23 VRHE under simulated solar illumination (100 mW cm²), with a low onset potential of around 0.11 VRHE, attributed to the strategic selection of materials and architectural design. The photoanode also demonstrated remarkable photochemical stability, retaining over 96% of its initial photocurrent after 10 hours of continuous operation in 1 M KOH (pH 13.5). Furthermore, the successful fabrication and demonstration of a large-area (25 cm²) photoanode validated both the performance and the scalability of the approach, reinforcing its potential for industrial-scale PEC water splitting applications.

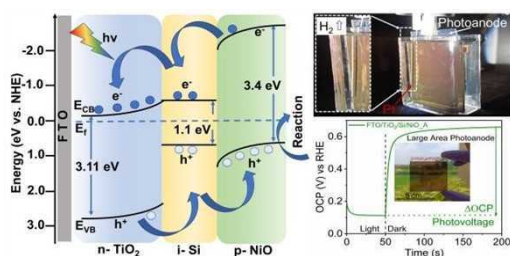


Figure 49: : n-TiO₂/i-Si/p-NiO heterojunction photoanode enabling efficient water splitting with enhanced photovoltage and visible hydrogen evolution on a large-area photoanode.

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Keywords: Photoelectrochemical water splitting, Si-based photoanode, n-i-p heterojunction, magnetron sputtering, large area device.

Enhancing charge transfer dynamics through S-scheme based WS₂/SCN photocatalyst for simultaneous O₂ reduction reaction and crystal violet degradation

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Hydrogen peroxide (H₂O₂) generation via a photocatalytic O₂ reduction reaction has been considered an economically efficient and environmentally friendly synthesis method. However, the productivity of H₂O₂ production is restricted because of sluggish reaction kinetics and fast recombination of photoinduced excitons. Therefore, a novel photocatalyst was developed for simultaneous O₂ reduction reaction and degradation of pollutant offering a promising strategy to deal both energy crisis and environmental pollution based on WS₂/ sulphur-doped g-C₃N₄ (WSCN). The two-dimensional 2D/2D WS₂/sulphur-doped g-C₃N₄ (WSCN) hybrid material was successfully fabricated to address the associated limitations through a combination of wet impregnation and calcination techniques for simultaneous H₂O₂ production and pollutant degradation. The effective anchoring of WS₂ nanoplates onto sulfur-doped g-C₃N₄ (SCN) nanosheets facilitates the effective separation of photoinduced excitons with sturdy redox properties, which is attributable to the establishment of S-scheme heterojunctions between WS₂ and SCN through WS bonding as substantiated by X-ray photoelectron spectroscopy (XPS) analysis. The WS bond at the interface acts as a bridge for effective charge segregation pathways. Among the series, the optimized 5WSCN heterojunction achieved H₂O₂ production rate of 1926.71 mol g⁻¹ h⁻¹ paired with simultaneous degradation of 95% of crystal violet (CV), wherein the CV molecules functioned as hole quencher during photocatalytic activity. The enhanced photocatalytic performance was figured out by high cathodic current

density and heightened separation of charge carriers supported by PL, EIS and transient photocurrents measurement. The S-scheme charge-transfer pathway was well validated by a radical scavenging experiment and work function was evaluated from VB-XPS analysis and in situ XPS measurement. This research offers a paradigmatic idea for constructing an S-scheme photocatalyst for simultaneous H_2O_2 generation and CV degradation.

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Keywords: Sulphur-doped $\text{g-C}_3\text{N}_4$, S-scheme heterojunction, H_2O_2 production, Crystal violet degradation.

Engineering Non-Centrosymmetric Bismuth-Based Photocatalyst and Investigation of Their Influence on Mixed Pollutant Degradation

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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 BiOBrO₃ 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 BiOBrO₃ 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 BiOBrO₃, 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 BiOBrO₃ 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 BiOBrO₃ arises from its non-centrosymmetric lattice, where the stereochemically active Br³⁺ lone pairs and the asymmetric BrO₃ 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.

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Keywords: BiOBr, BiOBrO₃, non-Centrosymmetric, mixed pollutant.

Development of MOF-Based materials from lean resources

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Metal-organic frameworks (MOFs) are crystalline coordination polymers developed from metal nodes and organic linkers, possessing exceptional porosity, tunability, and surface areas that enable high-performance gas sorption, separation, catalysis, as well as sensing. The modular chemistry allows targeted functionalization to elevate selectivity and stability for carbon dioxide (CO) capture under post-combustion conditions. The present work emphasised the development of MOF-based materials from lean resources by valorising iron-rich industrial residues (tailings, red mud, low-grade oxides) as metal precursors and employing oxo-phospho ligands/modulators, directing porous framework formation. We systematically studied and optimized the role of oxo-phospho reagent concentration, reaction temperature (mildly elevated temperatures favour ordered coordination and higher surface area), nucleation pH, and porosity for controlled reagent modulation, and to avoid extreme reagent conditions that might reduce phase purity. These trends are consistent with general MOF nucleation/growth studies and metal-oxo cluster chemistry governing node formation. CSIR-IMMT couples beneficiation and hydrometallurgical extraction of iron with downstream coordination chemistry to create value-added Fe-MOFs, thereby reducing feed-stock costs and environmental burden while enabling circular resource management. The synthesized materials are characterized by powder X-ray diffraction (PXRD), FTIR, TGA, BET surface area and porosity analysis, SEM/TEM morphology studies, and ICP/elemental analysis to confirm composition, coordination, stability, and textural properties. CO adsorption testing (adsorption isotherms at 298 K; cyclic stability) shows that appropriately modulated Fe-MOFs

derived from lean iron resources achieve competitive uptake and recyclability relative to benchmark materials — underscoring the promise of resource-efficient MOF manufacture for practical CO mitigation.

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Keywords: MOFs, combustion, hydrometallurgical

Computational Engineering of KCaX₃ (X = Cl, Br, I) Halide Perovskites: Unveiling their Potential in Energy Conversion and Optoelectronics

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Hybrid organic-inorganic perovskite (HOIP) based molecular ferroelectrics hold great promise in photovoltaic and optoelectronic applications which combine the best from both materials, offering a new way of tailoring the band structure.^{1,2,3} The understanding of electron-phonon coupling is essential for their performance in optoelectronic applications, as a variety of interactions and structural disorder,

which may significantly affect the material's characteristics.⁴ Thus, it is crucial to study the thermodynamic structure-property relationship to get important insights towards improving their functionality. In this work, we carried out the temperature-dependent Raman scattering studies of single crystal 2-(ammoniomethyl pyridinium) SbI₅ (2-AMP-SbI₅) and hexane-1,6-diammonium pentaiodobismuth (HDA-BiI₅) HOIP in the temperature ranges 200 °C to -195 °C to study possible structural phase transition, electron-phonon interaction, and structural changes during the transition. The analysis of temperature-dependent Raman data reveals anomalous changes of Raman shift and line width, confirming the ferro to paraelectric transition due to structural phase transitions. In particular, the phase transition in the above molecular-based HOIPs is associated with orientational changes of the organic cations produced by rotation of the ammonium heads and/or the pyridinium rings and tilting of BiI₆ octahedra and the changes of dynamics of hexane-1,6-diammonium cations is clearly established from our Raman analysis. We also discuss the nature of these transitions in terms of their activation energy and change in molecular orientations.

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Keywords: Single perovskites, Thermoelectric materials, Band Gap Engineering, Lead-Free Semiconductors.

Phonons and Structural Phase Transition Study of Hybrid Organic-Inorganic Perovskite-based Molecular Ferroelectrics

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Hybrid organic-inorganic perovskite (HOIP) based molecular ferroelectrics hold great promise in photovoltaic and optoelectronic applications which combine the best from both materials, offering a new way of tailoring the band structure.^{1,2,3} The understanding of electron-phonon coupling is essential for their performance in optoelectronic applications, as a variety of interactions and structural disorder, which may significantly affect the material's characteristics.⁴ Thus, it is crucial to study the thermodynamic structure-property relationship to get important insights towards improving their functionality. In this work, we carried out the temperature-dependent Raman scattering studies of single crystal 2-(ammoniomethyl pyridinium) SbI₅ (2-AMP-SbI₅) and hexane-1,6-diammonium pentaiodobismuth (HDA-BiI₅) HOIP in the temperature ranges 200 °C to -195 °C to study possible structural phase transition, electron-phonon interaction, and structural changes during the transition. The analysis of temperature-dependent Raman data reveals anomalous changes of Raman shift and line width, confirming the ferro to paraelectric transition due to structural phase transitions. In particular, the phase transition in the above molecular-based HOIPs is associated with orientational changes of the organic cations produced by rotation of the ammonium heads and/or the pyridinium rings and tilting of BiI₆ octahedra, and the changes of the dynamics of hexane-1,6-diammonium cations are clearly established from our Raman analysis. We also discuss the nature of these transitions in terms of their activation energy and change in molecular orientations.

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Keywords: Single perovskites, Thermoelectric materials, Band Gap Engineering, Lead-Free Semiconductors.

Phonons and Structural Phase Transition Study of Hybrid Organic-Inorganic Perovskite-based Molecular Ferroelectrics

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As the global demand for sustainable energy grows, nuclear power emerges as a key alternative to fossil fuels, offering low-carbon electricity generation. Currently contributing 10% of global energy, nuclear power is projected to rise to 12% by 2050. However, the widespread adoption of this technology is challenged by the management of radioactive waste, particularly the release of hazardous iodine isotopes from reactor cooling systems into aquatic environments. These emissions pose serious environmental and public health concerns, underscoring the need for efficient iodine remediation strategies. Here, we report the development of four nonporous metal-organic coordination cages (MC1–MC4), assembled from Pd(II) nodes and -conjugated ligands, designed for effective iodine capture from both vapor and aqueous media. These robust cages exhibit remarkable iodine uptake capacities, reaching up to 3.38 g g⁻¹ in the vapor phase (75°C) and 2.73 g g⁻¹ in aqueous solutions—outperforming many existing MOF and COF systems in both rate and efficiency. Dynamic flow-through studies revealed sustained

adsorption, with MC2 achieving an elution volume of 7.8 L g⁻¹ from 0.5 mM I₃ solution. Importantly, these cages efficiently remove iodine from complex matrices like seawater and drinking water, reducing concentrations from ppm to ppb levels. Their scalability, recyclability, and versatility mark them as strong candidates for real-world iodine remediation.

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Keywords: coordination cages, iodine, dynamic adsorption, water purification

Integrating Hydrothermal Synthesis and Cold Sintering for Ultra-Low Energy Processing of High-Density BaTiO₃ Ceramics

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A sustainable processing route for barium titanate (BaTiO₃) ceramics is demonstrated by combining hydrothermal synthesis with cold sintering, significantly reducing both the processing temperature and associated energy consumption. Various sets of BaTiO₃ nano-powder were synthesized hydrothermally using Ba(OH)₂ · 8H₂O and TiO₂ (anatase) as precursors. In the absence of any additional alkaline agents, the resulting powder exhibited a predominantly cubic phase. To stabilize the ferroelectric tetragonal phase, the reaction environment was modified by varying the KOH-to-NaOH molar ratio

from 1:0 to 0:1. Rietveld refinement was employed to quantify the phase fractions and determine the optimal alkali ratio for tetragonal phase stabilization (Table 1). The off-center displacement of Ti^{4+} ions and unit cell polarizability were estimated using the Clausius–Mossotti relation. The BaTiO_3 powder exhibiting the highest tetragonality was selected for consolidation via the cold sintering process (CSP) using a transient flux without affecting the congruency of the composition. Cold sintering parameters, including pressure, temperature, and dwell time, were optimized to achieve high-density ceramics. Structural and microstructural properties of the sintered ceramics were evaluated using X-ray diffraction (XRD) and scanning electron microscopy (SEM), and their dielectric properties and energy storage performance were also assessed. The results demonstrate enhanced energy storage performance, confirming the viability of this low-temperature processing route for advanced dielectric applications.

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Keywords: Energy storage ceramics, Barium titanate, Hydrothermal synthesis, Cold sintering process, Dielectric properties, Energy storage performance, Rietveld refinement

Scalable Osmotic Energy Harvesting using Two-dimensional MoS Membranes

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The growing global demand for sustainable energy underscores the urgent need for innovative technologies that can provide clean, continuous, and scalable power. Salinity gradient energy, commonly referred to as “blue energy” harnesses the osmotic pressure difference between seawater and freshwater and offers tremendous potential, particularly in estuarine environments [1]. Two-dimensional (2D) materials have recently attracted attention as nanofluidic membranes, with monolayer molybdenum disulfide (MoS) standing out due to its atomic thickness, tunable surface charge, and exceptional mechanical stability [2][3]. In this work, we demonstrate scalable osmotic energy harvesting using CVD-grown monolayer MoS membranes suspended over 1 μm pores drilled in silicon nitride substrates via focused ion beam (FIB) milling. The membranes were transferred using a hybrid transfer method, and nanopores (20 nm) were subsequently fabricated with high precision using transmission electron microscopy (TEM). Ion transport measurements were performed in a diffusion cell containing KCl solutions with varying concentration gradients to evaluate osmotic power generation. Our results show that the harvested power scales with nanopore density, increasing from 84 nW for a single pore to 160 nW for two pores and 230 nW for four pores. Furthermore, the osmotic power output rises significantly with increasing salinity gradient (10 to 1000), confirming strong ion selectivity and efficient energy conversion in the MoS membranes. All measurements were performed using an automated experimental setup, which overcomes limitations of manual filling such as poor controllability, reproducibility, and reliability, thereby enabling accurate ion transport characterization. Notably, the experiments were carried out in a 10 L-capacity diffusion cell, rendering the study more representative of real-life operating conditions than conventional benchtop systems [4]. Collectively, these results demonstrate that CVD-grown MoS nanopore membranes, when integrated with automation and large-scale testing platforms, provide a promising route toward practical, modular, and high-efficiency blue energy harvesting devices.

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Keywords: Salinity gradient energy, MoS₂ membrane, Nanopore density, Scalable Osmotic Power.

Synthesis of a Novel Zirconium-Kaolin-reduced Graphene Oxide Composite for Multi-pollutant Adsorption from Water Samples

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This study presents the synthesis and performance evaluation of a novel Zirconium-Kaolin-reduced Graphene Oxide (Zr-Kaolin-rGO) composite, developed as a highly efficient, multi-functional adsorbent for water purification. The composite was fabricated using a simple hydrothermal method, leveraging the synergistic properties of its components. Zirconium was incorporated to enhance affinity for pollutants through Lewis acid-base interactions and complexation, while Kaolin provided a cost-effective structural support to mitigate rGO aggregation. The reduced Graphene Oxide (rGO) component significantly increased the composite's surface area and active sites, crucial for high adsorption capacity. The synthesised Zr-Kaolin-rGO was thoroughly characterised to confirm its structural and morphological properties. Scanning Electron Microscopy (SEM) was employed to visualize the surface topography and microstructure, providing crucial insights into the uniform dispersion of Zr and Kaolin on the rGO sheets. This confirmed the successful formation of the composite and its well-defined morphology. Furthermore, Brunauer-Emmett-Teller (BET) analysis was conducted to precisely measure the composite's specific surface area and pore size distribution. The results from BET analysis were vital, as a high surface area directly correlates with an increased

number of available active sites for adsorption, thereby explaining the material's high removal efficiency. Batch adsorption experiments were conducted to assess the removal efficiency for heavy metal ions: chromium, manganese, mercury, copper, and cobalt. Pollutant concentrations were precisely quantified using Microwave Plasma Atomic Emission Spectroscopy (MP-AES), confirming the composite's high efficacy. Results demonstrate the composite's exceptional adsorption capacity and rapid kinetics for both fluoride and heavy metal ions, showcasing superior performance across a broad pH range. The material also exhibited excellent reusability over multiple cycles, suggesting its potential as a sustainable adsorbent. Mechanistic studies indicate that adsorption occurs via a combination of electrostatic attraction, surface complexation, and ion exchange. The composite's remarkable performance, confirmed by its favorable textural properties and stability, positions it as a promising, cost-effective, and scalable solution for providing safe drinking water.

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Keywords:

Tuning Structural and Electronic Properties of AgSnSbTe₃ via Doping for Enhanced Thermoelectric Performance

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AgSnSbTe₃ and its doped variants are promising thermoelectric materials owing to their low thermal conductivity and tunable electronic properties [1]. In this work, we investigate structural, electronic, and transport properties of pristine and doped AgSnSbTe₃ samples using a combination of temperature-dependent synchrotron X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and transport measurements. Synchrotron XRD reveals the crystal structure (Fm-3m) and the lattice expansion of the material with increasing temperature. Valence band XPS shows a pronounced increase in electron population near the Fermi level in certain doped samples, suggesting potential enhancement in electronic conductivity and/or Seebeck coefficient. We aim to correlate these structural and electronic modifications with thermoelectric properties through measurements of thermal conductivity (LFA) and electrical conductivity and Seebeck coefficient (SBA Nemesis) on spark plasma sintered dense pellets. The combined study is expected to guide doping strategies for optimizing the thermoelectric performance of AgSnSbTe₃ based materials.

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Keywords: Thermoelectric materials; XPS; XRD; LFA.

Binary-Ternary complex Oxide nanoflower: Pulse Reverse electrodeposited electrode for designing supercapacitor prototype

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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 (NiCo₂O₄) manganese oxide (MnO₂) complex (NCMO) based electrodes, prepared by following three distinct electrodeposition recipes, have been studied, and their electrochemical energy storage properties have been evaluated. Films prepared through constant electrodeposition (CED), pulse potential (PP), and pulse reverse potential (PRP) show distinctly different morphology 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, the PRP mode results in a fully interconnected flake-flower-like nanostructured network. It delivers a high specific capacitance of 595.55 mF cm⁻², outperforming the other two electrodes. An asymmetric supercapacitor device, prepared using this electrode, exhibits device performance suitable for practical applications by showing a retention of 83% of its capacitance over more than 1000 charge-discharge cycles. A prototype device could operate a multipurpose digital display for several minutes, underscoring its practical viability for usage in appliances. This study offers a recipe to design and fabricate a solid-state supercapacitor for real-world applications as a next-generation energy storage system.

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Keywords: metal oxide composite; pulse reverse potential; supercapacitor; specific capacitance.

Eco-Friendly Water Cleanup: Nanotitania Composites for Sustainable Dye Degradation.

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This study explores the eco-friendly and sustainable synthesis of nanotitania (TiO₂) and its application in the efficient photocatalytic degradation of organic dyes. The conventional methods for TiO₂ nanoparticle production are often energy-intensive and involve toxic chemicals. In contrast, this study focuses on a "green synthesis" approach, utilizing natural, non-toxic, and biodegradable agents, such as plant extracts or microorganisms, as reducing and capping agents. This method yields highly crystalline, phase-pure anatase TiO₂ nanoparticles with a narrow size distribution and high surface area, crucial for enhanced photocatalytic activity. The synthesized green nanotitania is then modified with different clay materials and evaluated for its photocatalytic efficiency in degrading a model organic dye, such as methylene blue, under simulated UV light irradiation. The high surface area and well-defined crystal structure of the green-synthesized nanoparticles provide an abundance of active sites for the generation of reactive oxygen species. This research demonstrates that green-synthesized nanotitania is a highly effective, cost-efficient, and environmentally benign alternative to conventional photocatalysts, offering a promising solution for the treatment of textile and industrial wastewater.

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biomedical applications. *Environmental Science and Pollution Research*, 28(30), 41207-41223.

Keywords: Ultrahigh Seebeck coefficient, High figure of merit, Thermoelectric materials, Density functional theory (DFT).

Synergistic Effect of NiSb₂O₆ and rGO Nanocomposites for High-Performance Charge Storage Applications

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Over the past decade, supercapacitors, also called electrochemical capacitors, have been one of the most promising emerging energy storage devices due to their moderate energy density, high power density, fast charge and discharge rates, and long cycle lives[1]. From the materials' perspective, various carbonaceous materials, conducting polymers, and transition-metal oxides are fundamental candidates for supercapacitor electrode materials. In this study, we report the synthesis of nickel antimony oxide (NiSb₂O₆) through solid-state and physical mixture methods, and its composite with reduced graphene oxide (rGO). The synthesized materials were thoroughly characterized through structural, morphological, and elemental analyses. Additionally, the materials were fabricated onto nickel foam to evaluate their electrochemical properties. Electrochemical analysis revealed that the NiSb₂O₆-rGO composite exhibited a remarkable specific capacitance of 952.38 F/g at a mass-normalized current of 1 A/g, significantly surpassing the performance of bare NiSb₂O₆ [2]. A symmetric two-electrode device was also assembled using the NiSb₂O₆-rGO composite, demonstrating excellent capacity retention over 10,000 cycles. These results highlight the superior performance of the

NiSb₂O₆-rGO composite, suggesting its potential as an efficient material for electrochemical capacitors.

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Keywords: Supercapacitor; nickel antimony oxide; symmetric device; cyclic stability.

Harnessing Dual Ambient Energies: Magneto-Pyroelectric Hybrid Harvesters for Modern Electronics.

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Rising interest in sustainable energy has prompted exploration of often-ignored waste energy sources, particularly the thermal variations and stray magnetic fields generated by industrial equipment and consumer electronic devices. Traditional energy harvesters often primarily focus on a single energy source, and thus, this results in their low efficiency. In contrast, hybrid energy harvesting systems can have the ability to capture multiple sources of energy forms at the same time through combined effects[1]. In this study, we present a flexible nanogenerator that combines electrospun polyvinylidene fluoride (PVDF) nanofibers with magnetostrictive ferrite nanoparticles to work together in harnessing energy via both pyroelectric and magnetoelectric effects. The PVDF matrix, which has a high electroactive-phase content, effectively turns temperature differences into electrical energy. The dispersed ferrite nanoparticles convert weak ambient magnetic fields into mechanical strain. This strain can then be transformed into electricity through

PVDF's piezoelectric response. This dual harvesting method shows a notable improvement in voltage output compared to single-mode devices, as shown by controlled thermal and magnetic field cycling experiments. The ability of nanocomposites to be processed in solution and their mechanical flexibility make them especially suitable for conformal integration in industrial IoT sensors and wearable electronics[2]. *Keywords:* Supercapacitor; nickel antimony oxide; symmetric device; cyclic stability.

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2. S. K. Ghosh et al., Rollable magnetoelectric Energy Harvester as a wireless IoT sensor, *ACS Sustain. Chem. Eng.*, 2020, 8, 864–873.

Keywords: PVDF nanofibers, Ferrite composites, Magnetoelectric, Pyroelectric, Hybrid nanogenerator

Double-modified (Ag & Al) manganese with sufficient energy and power density for thermistor and supercapacitor applications

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Al-doped La_{0.9}Ag_{0.1}Mn_{1-x}Al_xO₃ (x = 0, 0.025, and 0.05) perovskite materials are synthesized using the sol-gel process, and their optical, electrical, electrochemical, structural, and morphological characteristics are investigated for potential energy storage uses. Single-phase rhombohedral (R-3c) structure development is confirmed by XRD. Well-defined nanoscale grains are visible in TEM and FESEM images. BET validates the increased surface area of LMAO5 (14.13 m²/g). Oxygen vacancies and stable bonding conditions are confirmed by FTIR and XPS. Dielectric loss decreases with increasing Al concentration and reaches a minimum at ambient temperature and 1 kHz, while all samples exhibit NTC behaviour. The LMAO5 electrode shows a specific capacitance of 158 F g⁻¹ at 5 mV s⁻¹, as revealed by CV,

GCD, and EIS analyses. This enhancement is attributed to the higher concentration of oxygen vacancies. EIS results further show low charge-transfer resistance ($R_{ct} = 1.01 \, \Omega$) and series resistance ($R_s = 1.06 \, \Omega$). A symmetric LAMAO5//LAMAO5 supercapacitor operating over a wide 1.1 V window achieves an energy density of $3.6 \, \text{Wh kg}^{-1}$ and a power density of $150 \, \text{W kg}^{-1}$, retaining 89% of its capacitance after 10,000 cycles. These findings indicate that Al-doped La–Ag manganites are promising multifunctional materials for thermistor and supercapacitor applications.

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Keywords: Energy storage device; Perovskite oxide; Energy density; Thermistor.

Flexible and wearable piezoelectric nanogenerator based on three-phase composite film for energy harvesting and mechanosensing

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A sustainable, self-powered energy source that addresses energy crises is highly sought after, given the current state of the energy industry. In this study, we demonstrate the fabrication of a flexible piezoelectric energy harvester based on a PVDF/ZnTiO₃/rGO composite, capable of harvesting energy from various mechanical stimuli as a sustainable energy source. We investigated the impact of the two fillers on the piezoelectric and dielectric properties of PVDF. The optimized composite film, composed of PVDF-5 wt% ZnTiO₃/1 wt% rGO (5PZTR1), exhibited good adaptability for flexible dielectrics with a higher dielectric constant (~ 10) and lower dielectric loss value (0.05 at 1 kHz). Considering its enhanced polarization,

the composite film is ideal for mechanical energy harvesting applications. The piezoelectric energy harvester (PEH) using 5PZTR1 generated an open-circuit peak-to-peak AC voltage of $\sim 37 \, \text{V}$ under repetitive human finger tapping, compared to 7 V and 28 V for pristine PVDF and PVDF/ZnTiO₃ (5 wt% of ZnTiO₃), respectively. For practical applications, commercial LEDs could be illuminated with a rectified voltage of $\sim 20 \, \text{V}$. Since the PEH responds to various types of applied mechanical stress and human body movements, it acts as a self-powered system with a maximum power density of $\sim 121 \, \mu\text{W/cm}^2$. This piezoelectric energy harvester is thus a promising alternative for self-sufficient monitoring systems.

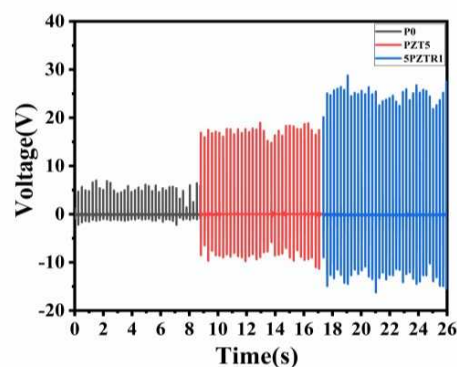


Figure 51:

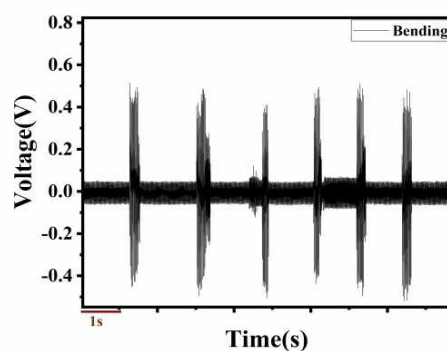


Figure 52:

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Keywords: Cu₂WS₄ nanocomposite, cellulose-based electrode, supercapacitor performance, hybrid energy storage material.

A Non-Enzymatic Glucose Sensor Based on AG Modified Electrode

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Diabetes mellitus remains one of the most prevalent metabolic disorders, requiring reliable and continuous monitoring of blood glucose levels. Conventional enzymatic glucose sensors often encounter drawbacks such as high production costs, poor stability, and susceptibility to environmental variations, which necessitate the development of robust nonenzymatic sensing platforms. Two-dimensional (2D) nanomaterials, particularly graphene-based derivatives, have emerged as promising candidates owing to their exceptional surface area, tunable defect density, electrochemical stability, and cost-effectiveness. In this study, we demonstrate the fabrication of a nonenzymatic glucose sensor based on activated graphene (AG) modified nickel foam prepared via an ultrasonication route. The conductive nanostructure provides abundant active sites and facilitates rapid electron transport, as confirmed through structural and spectroscopic analyses, including TEM, FTIR, Raman spectroscopy, and XRD. Optimization studies demonstrated that the electrolyte pH and the AG loading significantly influence electrochemical performance. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements highlighted the excellent redox activity, catalytic stability, and reproducibility of the electrode. The sensor exhibits a wide linear detection range spanning from 50 μ M to 500 mM, with a remarkably high

sensitivity of 4 mA mM⁻¹cm² obtained by DPV and a low detection limit of 0.20 mM (calculated as 3S/m). The glucose oxidation process at the defect-enriched graphene surface serves as the basis for the detection mechanism. Importantly, the electrode displays outstanding selectivity, effectively suppressing interference from common electroactive species such as dopamine, uric acid, ascorbic acid, folic acid, and sucrose. Practical applicability was further validated through measurements in simulated blood serum using the standard addition approach, achieving an excellent recovery rate of 98%, underscoring the reliability of the developed platform. Overall, this study establishes AG-modified nickel foam as a highly efficient nonenzymatic electrode for glucose detection. The outstanding sensitivity, broad dynamic range, selectivity, and real-sample applicability highlight its strong potential for integration into point-of-care diagnostic devices and pharmaceutical quality monitoring systems.

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Keywords: AG, Glucose, Non-enzymatic, Electrochemical sensor.

Two-dimensional Titanium Carbide MXenes for Efficient Water Electrolysis

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MXenes have emerged as one of the most versatile families of two-dimensional (2D) materials in recent years, with titanium carbide (Ti₃C₂) MXenes showing exceptional promise for applications in energy storage, sensors, and electrocatalysis. Their high electrical conductivity, hydrophilicity, and electrochemical stability make them particularly suitable as electrocatalysts for alkaline water splitting, including the hydrogen evolution reaction (HER) and oxygen

evolution reaction (OER), which are often limited by sluggish kinetics. However, conventional MXene synthesis methods rely on hydrofluoric acid (HF) or concentrated acids to etch the MAX phase (Ti_3AlC_2), raising significant safety and environmental concerns. In this work, we present an environmentally friendly, direct HF-free hydrothermal etching route using low concentrations of etchants, resulting in high-quality, delaminated $\text{Ti}_3\text{C}_2\text{T}_x$ MXene flakes (T_x = surface termination groups) with reduced reaction time and improved safety. To further enhance catalytic performance, we doped the MXenes with heteroatoms and studied their structural and morphological properties via X-ray diffraction, scanning electron microscopy, and atomic force microscopy to confirm successful etching and the pristine structure of MXenes. Electrochemical studies were conducted in an alkaline medium, which demonstrated that the doped MXenes exhibit significantly lower overpotentials for both HER and OER compared to pristine $\text{Ti}_3\text{C}_2\text{T}_x$. This enhancement is attributed to increased interlayer spacing, larger surface area, and the synergistic catalytic effects of the dopants. Overall, this scalable, green synthesis and doping strategy offers a promising platform for the development of high-performance 2D electrocatalysts, advancing clean hydrogen production and sustainable energy technologies.

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Keywords: Mxene, LaNiO_3 , Bifunctional electrocatalysis, Water splitting.

Impact of Temperature Variation on Functional and Electromechanical Properties of Lead-Based Ceramics

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In this work, the $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.75}\text{Ti}_{0.25}]\text{O}_3$ (PMN-25PT) ceramics are widely used in a multitude of applications as sensors, resonators, actuators, medical industrial ultrasonic devices, thermal detectors, tunable devices, energy harvesters, and solid-state cooling technologies etc, were synthesized using the solid-state reaction method and sintering process densification of the formed bulk material, which enhanced the electrical as well as mechanical properties. The cross-sectional microstructural characteristics of the PMN-PT ceramics were examined using scanning electron microscopy (SEM). For electrical characterization, both surfaces of the polished pellets were coated with silver paste and subsequently heat-treated at 200 °C for 30 minutes to ensure the formation of stable and well-adhered electrodes. The temperature-dependent dielectric constant (ϵ_r) and dielectric loss ($\tan \delta$) were measured over a frequency range of 100 Hz to 1 MHz in the temperature interval of 40 °C to 240 °C, which indicates a relaxor-type ferroelectric-paraelectric phase transition T_c at 130°C. To avoid electrical breakdown during the measurements, the ceramic samples were immersed in silicone oil. After DC poling for 30 minutes in silicone oil under an applied electric field of 10 kV/cm at room temperature, the temperature-dependent impedance spectra were measured across a range of frequencies from 230 kHz to 280 kHz, and the real part of the impedance (Z') was plotted as a function of frequency at various temperatures from 40°C to 110°C. We have studied the effect of temperature on ferroelectric and piezoelectric properties of the sample. The Strain – Electric field (S-E) plot represents a typical “butterfly” loop, a signature of a piezoelectric material. Interestingly, the explored composition can offer a high electro-caloric effect (ECE) output over a broad temperature range. It provides maximum entropy (S) and temperature (T) change i.e. 1.07 J/kg.K and 1.31 K for the applied electric field

of 17 kV/cm at 398 K temperature, respectively.

Keywords: Piezo-electric ceramic, Dielectric property, Pyroelectricity, Electro-mechanical properties.

Sulfonamide-derived Covalent Organic Frameworks (COFs) serving as efficient additives in polyethylene oxide (PEO) to enhance ionic conductivity

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Two novel amorphous Covalent Organic Framework (COFs) featuring sulfonamide functional groups have been successfully synthesised and integrated into a poly(ethylene oxide) (PEO) matrix, resulting in the development of advanced composite polymer electrolytes (CPEs) with exceptional properties. This newly synthesized COF demonstrates a remarkable ability to enhance key characteristics of the PEO matrix, significantly improving mechanical strength, ionic conductivity, which reaches an impressive level of 8.7×10^{-3} S/cm at ambient temperature, electrochemical stability with a notable oxidation resistance of up to 1.39 V against stainless steel electrodes, and thermal stability that withstands temperatures as high as 300 °C. The CPE exhibits a specific capacitance of 186 Fg⁻¹ and a coulombic efficiency of 99% at 1 V, with an ionic transport number of 0.998. The interaction between lithium ions (Li⁺) and the sulfonamide moiety (–SO₂NH–) plays a crucial role in optimising the performance of these electrolytes. This interaction facilitates the effective dissociation of lithium salts from their ion pairs, promoting ion mobility and overall conductivity. Differential Scanning Calorimetry (DSC) analyses reveal that there is no significant molten state during the conductivity measurements, indicating a stable amorphous structure. The observed enhancement in ionic conductivity can be attributed primarily to the synergistic effects between the COF additive and the PEO matrix. This research substantiates that sulfonamide-based COFs present a promising solution as high-performance additives in polymer-based solid electrolytes.

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Keywords: Covalent Organic Framework (COFs), Composite polymer electrolytes (CPEs), Electrochemical stability.

Cost-Effective and Durable AlN/Al/AlN Multilayer Coatings for Energy-Efficient Window Applications

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Energy-efficient glazing technologies are critical in reducing heat gain in buildings and vehicles while maintaining visible light transmittance. Low-emissivity (Low-E) coating are widely used for this purpose, typically consisting of silver (Ag) as an infrared-reflective layer encapsulated between multiple dielectric layers, usually oxides, to protect the metal from environmental degradation. However, Ag-based coating suffers from high material cost and long-term degradation due to environmental exposure. In this work, a novel cost-effective multilayer configuration consisting of aluminium nitride/aluminium /aluminium nitride (AlN/Al/AlN) is designed on the glass substrate using RF magnetron sputtering. Al is selected for its low cost, neutral appearance and self-passivating alumina layer, while AlN serves as an antireflective coating as well as protective layer for Al against environment degradation. Experimental results demonstrate an AlN/Al/AlN stack with 12nm Al realizing Tvis, infrared transmittance (TIR) and infrared reflectance (RIR) of 23.66%, 16.81% and 60%, respectively. Increasing the Al layer thickness to 16 nm resulted in an enhancement of RIR of 90% but reduces the visible and IR transmittance of 16.58% and 9.68%, respectively. Furthermore, varying AlN thickness is found to shift

the position of the visible transmittance maxima due to the interference effects, governed by the constructive and destructive interference of the electromagnetic radiation. These results show tunability in the optical performance through thickness control and demonstrate the potential of Al as a cost-effective, durable alternative to conventional Ag-based low-E coating for energy-saving window applications.

Keywords: Covalent Organic Framework (COFs), Composite polymer electrolytes (CPEs), Electrochemical stability.

Binary vs. Ternary MOF-on-MOF Architectures: Engineering Charge Dynamics for High-Efficiency Solar to Chemical Conversions

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The intrinsic limitations of single-component MOFs, such as limited visible-light absorption and inefficient charge separation, can be effectively addressed by constructing MOF-on-MOF heterojunctions. In this work, we strategically developed a binary MOF-on-MOF hybrid composed of NH₂–MIL–125(Ti) and ZIF-67 to form a solid-state Z-scheme photocatalyst, followed by rational integration of reduced graphene oxide (rGO) to yield a ternary hybrid with markedly superior photocatalytic performance. The binary heterojunction utilizes the redox asymmetry between NH₂–MIL–125(Ti) and ZIF-67 to establish an internal electric field that promotes spatial charge separation. However, due to the inherently insulating nature of MOFs, stemming from their organic linkers and localized electronic states, long-range charge transport remains limited, resulting in interfacial recombination losses. To overcome this, rGO, a π -conjugated, atomically thin conductor with a tunable work function, was introduced as an active electron mediator within the MOF-on-MOF matrix. Serving as a dynamic relay center rather than a passive additive, rGO bridges the conduction bands of NH₂–MIL–125(Ti) and ZIF-67, facilitating directional electron transfer and reinforcing a robust Z-scheme pathway that retains strong redox potentials. This ternary

architecture not only broadens light absorption and suppresses recombination but also redistributes reactive sites crucial for two-electron O reduction to H₂O₂ and proton reduction to H₂. The resulting ternary system delivers a H₂O₂ production rate of 2583 $\mu\text{mol g}^{-1} \text{h}^{-1}$, H₂ evolution of 471 $\mu\text{mol h}^{-1}$, and an AQE of 5.47% at 400 nm, nearly doubling the performance of the binary counterpart and affirming the essential role of rGO inclusion. This design evolution highlights a core principle: structural proximity alone is insufficient for efficient charge flow. Instead, performance enhancement arises from deliberate band alignment, conductive mediation, and interfacial energetic tuning, all embodied in the rGO-mediated ternary Z-scheme. The presented strategy offers a powerful blueprint for advancing MOF heterostructures in solar-driven chemical fuel production.

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Keywords: Metal-Organic-Frameworks, NH₂–MIL–125(Ti), Photocatalysis, energy generation.

Solvent-Controlled Self-Assembly and Chiral Induction in Pd(II) Coordination Cages

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Self-assembled coordination cages offer powerful platforms for molecular recognition, separation, and chirality control. In this work, we demonstrate the solvent-directed formation of two distinct Pd(II) coordination cages—Pd6L3 and Pd8L4—using a single ligand under varying conditions. The resulting polymorphic cages display size- and shape-selective guest encapsulation capabilities, enabling the efficient separation of benzene and cyclohexane, a classically challenging separation due to their similar boiling points and molecular volumes. In parallel,

we explore chiral induction in a Pd4L8 coordination cage assembled from achiral components. Upon binding optically active guest molecules, the cage exhibits emergent chirality, as revealed by circular dichroism (CD) spectroscopy. The extent and nature of this chiral induction depend on both the structure and stereochemistry of the guest, highlighting the cage's responsiveness and potential for enantioselective recognition. Together, these studies highlight the versatility of Pd(II)-based self-assembled cages, demonstrating how solvent effects and guest molecules can precisely modulate structural outcomes and chiral behavior. Such systems hold promise for applications in molecular separations, sensing, and asymmetric catalysis.



Figure 53: Solvent-induced reversible transformation between coordination cages and selective benzene-cyclohexane separation.

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Keywords: self-assembly, coordination cages, molecular separation, chiral induction.

Electronic structure and electrical properties of $\text{Bi}_{1-x}\text{Mn}_x\text{FeO}_3$ thin films.

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BiFeO_3 is a promising type-I multiferroic oxide perovskite (ABO_3) in the field of photovoltaic applications due to its anomalous photovoltaic effect[1]. However, the device aspect of pristine BiFeO_3 is limited by Bi volatility, weak ferromagnetism due to spin canting, and high leakage currents arising from oxygen vacancies generated by $\text{Fe}^{3+}/\text{Fe}^{2+}$ valence fluctuations[2]. To address these limitations, transition-metal doping at the Fe site has been widely explored. While several studies have reported improvements with lower percentages of Mn doping ($\leq 5\%$), the effects of higher Mn incorporation remain less explored, particularly in sol-gel spin-coated thin films where impurity phases often emerge. In this work, pristine and Mn-doped BiFeO_3 thin films ($\text{BiFe}_{1-x}\text{Mn}_x\text{O}_3$, $x = 0.1, 0.2, 0.3$) were fabricated on FTO/glass substrates via a facile spin-coating route, and their structural characterization was carried out by X-ray diffraction and Raman spectroscopy. The particle size was extracted from SEM analysis, and the band gap of the films was estimated from UV–VIS absorption studies. Electron paramagnetic resonance measurements and ferroelectric studies were performed to investigate the oxygen vacancy concentration and ferroelectric properties of the films, respectively. The 3+ oxidation states of the elements and local lattice distortions were determined from X-ray absorption studies. The J-V measurements were conducted in order to determine the electrical properties of the films. In conclusion, our results show that enhanced Mn doping in BiFeO_3 thin films decreases the particle size as well as the band gap, deteriorates the ferroelectric property (for Mn doping more than 10%), and improves the electrical conductivity, which will be discussed.

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Keywords: Mn doped BiFeO₃, Oxide perovskite, Oxygen vacancies.

Porous W₂N Fibrous-Nanograins and TiN Nanopyramids Framework for High Energy Density Flexible Asymmetric Supercapacitors

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Enhancing the energy density of flexible asymmetric supercapacitors (ASCs) necessitates developing and implementing high-performance anode materials for technological developments in wearable energy storage systems. Tungsten nitride (W₂N) offers enormous potential as an anode material for ASCs, ascribed to its substantial specific capacitance, massive electrical conductivity, and extended negative potential window. In this work, we fabricated a durable coin cell and flexible ASC utilizing W₂N/SSM fibrous-nanograins anode and TiN/SSM nanopyramids cathode deposited over a flexible stainless steel mesh (SSM) substrate by the DC magnetron sputtering technique. The W₂N/SSM // TiN/SSM ASC device demonstrates a high areal capacitance of 21.3 mF cm⁻², operating across a wide and stable electrochemical voltage window of 1.3 V with outstanding cycling robustness, demonstrating 89.09% retention over 8000 charge-discharge cycles. Notably, the ASC achieved a high energy density of 34.33 mWh cm⁻³ and a high power density of 17.32 W cm⁻³. The persistent electrochemical performance of the ASC is mainly attributed to the dominance of surface-controlled capacitive and pseudocapacitive charge storage kinetics of W₂N/SSM for Na⁺ ions, comprehensively examined employing 3D Bode and Dunn's

techniques. The flexible ASC shows remarkable mechanical stability of 92.36% up to 500 bending cycles. This study establishes W₂N nanograins' potential as a high-energy anode material, revealing the capability to increase the effectiveness of ASC for portable and miniaturized energy storage devices.

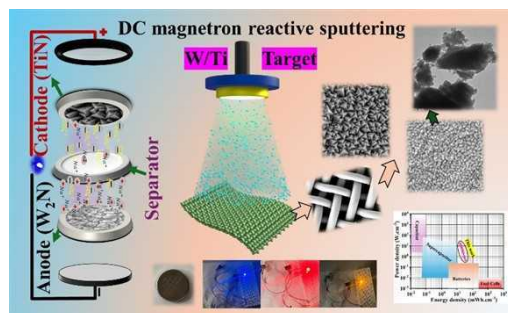


Figure 54: Solvent-induced reversible transformation between coordination cages and selective benzene–cyclohexane separation.

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Keywords: asymmetric supercapacitors, pseudocapacitive, miniaturized

Radiation Assisted Chemically Synthesized Tin Oxide Nanoparticles Towards Solid-State Supercapacitor

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This work introduced a new method to synthesize tin oxide (SnO_2) nanoparticles for supercapacitor applications using a special radiation-based technique, irradiated by cobalt-60 gamma radiation. The structural analysis, chemical composition, and morphological studies of radiation-synthesized SnO_2 were characterized by numerous analytical techniques including XRD, FTIR, FESEM, and HRTEM. The SnO_2 thin film was coated on a stainless-steel substrate using a simple and standard Dr. Blade technique for electrochemical measurement of both the electrode and solid-state device. At a 5 mV s^{-1} scan rate, the SnO_2 electrode delivered a specific capacitance of 84 F g^{-1} with 100% capacitive retention after 3000 cycles. Furthermore, the solid-state device displayed a potential window of 1.6 V and a specific capacitance of 51.9 F g^{-1} at 5 mV s^{-1} . Additionally, the device exhibited remarkable cyclic stability of 90% after 3000 cycles. The solid-state device, showcasing a device voltage of 1.6 V, successfully illuminated a VNIT LED panel and operated a miniature fan as a demonstration of practical application.

References:

Keywords: Magnetostriction; Strain mediated; Composite; Magnetodielectric.

Facile Hydrothermal Synthesis of ZnFe_2O_4 Nanoparticles with high specific Surface area for High Performance Supercapacitor Application.

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The growing demand for efficient energy storage technologies has established supercapacitors as one of the most promising solutions in sustainable nanotechnology. Binary transition metal oxides (BTMOs), particularly zinc ferrite (ZnFeO), are of great interest due to their high theoretical capacity arising from fast and reversible surface faradaic reactions. In this study, ZnFeO nanostructures were synthesized via a facile and scalable hydrothermal route with precise control

over reaction conditions to optimize the specific surface area, a critical factor for charge storage. The as-prepared material was extensively characterized by X-ray diffraction (XRD), Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), Brunauer–Emmett–Teller (BET) surface area analysis, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). These analyses confirmed the successful formation of the desired ZnFeO phase with high surface area, well-defined nanostructures, and appropriate oxidation states. Electrochemical performance was systematically evaluated in 3 M KOH electrolyte using cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. The ZnFeO electrodes demonstrated an excellent gravimetric capacitance of 612 F g^{-1} at 1 A g^{-1} and exhibited robust cycling stability with 92.5% capacitance retention after 2000 cycles.

References:

Keywords: Transition metal Oxides, Facile hydrothermal Synthesis, Supercapacitor.

From Charge to Waves: Fabrication and Fractional Dynamics Analysis of CuMnO_2 Symmetric Coin-cell Supercapacitor for Low-Frequency Oscillator application

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As supercapacitors become increasingly vital in modern electrical systems, understanding their complex nonlinear dynamics—governed by long-term memory effects—is crucial. Fractional calculus provides an effective tool for modelling such behaviour. In this work, a symmetric coin cell supercapacitor is first developed with lab-synthesized CuMnO_2 nanoplates using a facile hydrothermal method. Various characterization techniques such as PXRD, UV, FESEM, PL, Raman, and FTIR were used to investigate structural properties, whereas CV, GCD, and EIS were used to examine electrochemical performance. CuMnO_2 nanoplates, synthesized with 4.4 g of NaOH, exhibit the highest specific capacity of approximately 260 F g^{-1} at 7 A g^{-1} current density from GCD measurements in the presence of 3 M KOH electrolyte. The symmetric coin cell, prepared with CuMnO_2

nanoplates, possesses a specific capacity of approximately 75.2 F g^{-1} at 1 A g^{-1} , energy density of $\sim 19 \text{ Wh kg}^{-1}$, and power density of $\sim 501 \text{ W kg}^{-1}$. Through frequency-domain analysis of the lab-made symmetric supercapacitor with fractional dynamics, we established a framework to predict and tune oscillation frequencies. This study offers a systematic approach for designing oscillators with precise low-frequency performance, opening new possibilities for energy-efficient signal generation.

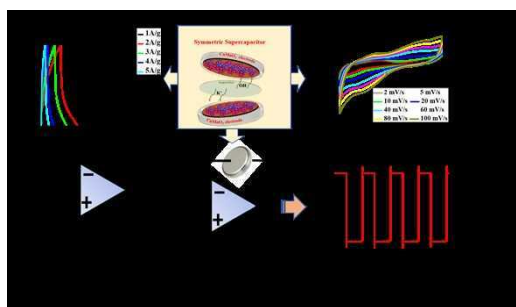


Figure 55:

References:

Keywords: Transition metal Oxides, Facile hydrothermal Synthesis, Supercapacitor.

Developing $\text{Rh}_{2-y}\text{Cr}_y\text{O}_3$ Cocatalysts to Outperform Platinum in Semiconductor-Based Photocatalytic H_2 Evolution

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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 semiconductors[1]. Traditionally, noble metal cocatalysts like Pt, Ru, Rh, and Ir—especially Pt 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 this context, $\text{Rh}_{2-y}\text{Cr}_y\text{O}_3$ 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 $\text{Rh}_{2-y}\text{Cr}_y\text{O}_3$ cocatalysts onto oxide-based photocatalysts via a facile impregnation method, producing a sophisticated core-shell motif. In this architecture, a catalytically potent Rh core facilitates proton reduction, while the Cr oxide shell acts as a protective layer, 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 the hydrogen evolution rate. Surpassing Pt-based systems in both activity and durability, the $\text{Rh}_{2-y}\text{Cr}_y\text{O}_3$ 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 toward next-generation photocatalysts that marry exceptional efficiency with longevity for scalable solar fuel production.

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Keywords: Cocatalyst; $\text{Rh}_{2-y}\text{Cr}_y\text{O}_3$, Photocatalyst, Hydrogen evolution.

Engineering Cation Vacancy Defects on LaNiO_3 for Efficient Oxygen Evolution Reaction

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Perovskite oxides (ABO_3) have been extensively studied as electrocatalysts for the oxygen evolution reaction (OER) due to their highly tunable and flexible electronic structures[1]. However, their practical use as electrocatalysts has been hindered by limitations such as low surface area and poor electrical conductivity[2]. In this work, LaNiO_3 (LNO) perovskite oxides were synthesized and modified by selectively removing A-site cations via etching with dilute acetic acid. This acid etching process induced cation and oxygen vacancies, resulting in increased surface area and enhanced surface wettability, which facilitated improved interaction with water molecules and promoted a higher density of catalytically active sites. These structural and surface modifications led to superior OER performance in alkaline media. The optimized catalyst, LNO-3M, demonstrated a reduced overpotential, smaller Tafel slope, higher turnover frequency, and greater mass activity compared to pristine LNO. Electrochemical measurements confirmed faster charge transfer and a higher density of active sites due to the increased electrochemical surface area. Furthermore, LNO-3M maintained excellent operational stability over extended periods. This study underscores the efficacy of a simple acid etching strategy to enhance the catalytic activity of LaNiO_3 for efficient water splitting applications.

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Keywords: Oxygen evolution reaction, Defect engineering, Perovskite oxide, Acid-etching

Superpower from Nature and Nanostructure: A Dual-Engineered Deformable Supercapacitor for Portable Electronics

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The ever-growing need for flexible, wearable, and portable electronics — ranging from rollable displays and smart wearables to health-monitoring devices — has driven demand for deformable energy storage devices with high energy and power densities. Designing systems that combine sustainability, flexibility, and long-term stability remains a major challenge. Here, we present a dual-engineering approach in an all-solid-state hybrid supercapacitor that harnesses both bio-derived materials and nanostructured engineering. We merged a bio-derived porous carbon cathode with an interfacially engineered MXene/metal-oxide anode to bridge the energy–power performance gap for wearable electronics. The cathode is derived from *Averrhoa carambola* (star-fruit) leaves via hydrothermal carbonization and thermochemical activation, yielding a porous, self-phosphorus-doped bio-carbon with an ultra-high surface area of $1576 \text{ m}^2 \text{ g}^{-1}$, enhanced wettability, and efficient ion transfer. On the anode side, we developed an in-situ carbon-doped ZnCo_2O_4 anchored on MXene, engineered via a twin-step annealing and electrostatic self-assembly process to ensure uniform doping, oxygen vacancies, and robust redox activity. The novelty of this work lies in the integrated use of a sustainable, self-doped bio-carbon cathode and a structurally engineered MXene-based hybrid anode within an all-solid-state flexible device framework. Owing to the synergy between natural architecture and synthetic precision, the device delivers a specific capacitance of 124.41 F g^{-1} , an energy density of $119.16 \text{ Wh kg}^{-1}$, and a power density of $3139.53 \text{ W kg}^{-1}$, with 90.55% retention over 20,000 cycles. Additionally, the device demonstrates mechanical stability by maintaining electrochemical performance under 100 twisting deformation cycles. By integrating sustainable biomass with advanced nanostructured materials, this work establishes a scalable, eco-conscious route toward next-generation deformable supercapacitors. The resulting device not only pushes the boundaries of hybrid supercapacitor technology

gies but also demonstrates structural robustness under dynamic deformation — underscoring its strong potential for integration into wearable, on-body, and flexible electronics applications.

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Keywords: Electrochemistry, flexible; biomass, asymmetric supercapacitor.

Layered Nb₂C and NiCo₂O₄ Nanocomposites for Enhanced Charge Storage in Supercapacitors

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The development of high-performance electrode materials is crucial for advancing next-generation supercapacitors with enhanced energy and power density. In this work, Nb₂C MXene was successfully synthesized by selectively etching the Al layer from the Nb₂AlC MAX phase using 50% concentrated hydrofluoric acid, followed by repeated washing. The resulting Nb₂C, possessing a large surface area, metallic conductivity, and a high density of active sites, served as the base material for composite formation. To enhance its charge-storage capability, Nb₂C was composited with NiCo₂O₄ nanoparticles, a redox-active bimetallic oxide known for its high theoretical capacitance and rich faradaic behaviour. Five different Nb₂C/NiCo₂O₄ composites were prepared by varying the NiCo₂O₄ content from 10 wt% to 50 wt%. Structural and morphological characterization confirmed the successful formation of the hybrid materials, with NiCo₂O₄ nanoparticles uniformly distributed across the Nb₂C layers while preserving the MXene's inherent lamellar architecture. The incorporation of NiCo₂O₄ significantly improved the electrochemical reactivity and ion accessibility of the composite electrodes. Electrochemical evaluations conducted in a three-electrode configuration using 3 M KOH electrolyte revealed a

substantial enhancement in charge storage with increasing NiCo₂O₄ content. Among all compositions, the Nb₂C@50%NiCo₂O₄ electrode delivered the highest performance, achieving a specific capacitance of 1312.08 F g⁻¹, an energy density of 45.55 Wh kg⁻¹, and a power density of 750 W kg⁻¹ at a current density of 3 A g⁻¹. The improved performance arises from the synergistic integration of electric double-layer capacitance from Nb₂C and redox-active pseudocapacitance from NiCo₂O₄ nanoparticles. This study clearly demonstrates that the electrochemical properties of Nb₂C can be effectively tuned through compositional engineering. The Nb₂C/NiCo₂O₄ hybrid system represents a promising pathway for the development of high-performance supercapacitor electrodes, combining the superior conductivity and structural integrity of MXenes with the rich faradaic activity of transition metal oxides.

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Keywords: Mxene, Nanoparticles, Specific Capacitance, Energy Density.

Synergistic Integration of NiNbO₆ and NbC MXene for Advanced Lithium-Ion Capacitor

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The rapid growth of portable electronics and electric vehicles has intensified the need for energy storage systems that can simultaneously deliver high energy and power densities. Lithium-ion capacitors (LICs), combining features of lithium-ion batteries (LIBs) and supercapacitors, offer a promising solution due to their hybrid charge storage mechanism. However, the development of high-performance anode materials with fast kinetics and stable cycling remains a key challenge. In this study, we report a novel dual-function composite anode, NiNb₂O₆@C/Nb₂C, engineered to enhance both energy and power performance in LICs. The material integrates nanostructured NiNb₂O₆ particles encapsulated in a conductive carbon matrix with Nb₂C MXene nanosheets. NiNb₂O₆ contributes high theoretical capacity through multivalent redox reactions, while the carbon coating improves electrical conductivity and structural stability. Nb₂C, a 2D transition metal carbide, provides high surface area, metallic conductivity, and rapid Li⁺ intercalation, enabling faster charge transport. The NiNb₂O₆@C composite achieves a high reversible capacity of 550 mAh g⁻¹ at 0.1 A g⁻¹, primarily due to its pseudocapacitive behaviour. When combined with Nb₂C, the resulting hybrid architecture facilitates efficient electron and ion transport, significantly improving electrochemical performance. Structural and morphological analyses (XRD, SEM/TEM, XPS) confirm the uniform distribution and successful integration of the composite. Electrochemical tests, including cyclic voltammetry and galvanostatic charge-discharge, demonstrate excellent rate capability and long-term cycling stability. When assembled into a full LIC with a porous carbon cathode, the device is expected to deliver a balanced energy-power profile suitable for fast-charging applications. This work highlights the synergistic roles of NiNb₂O₆ and Nb₂C in overcoming limitations of traditional anodes and offers valuable insights for designing next-generation high-

performance LICs. The detailed material synthesis and electrochemical performance will be discussed during the poster presentation.

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Keywords: 2D Materials, MXenes, Hybrid composite, NiNb₂O₆@C/Nb₂C, Synergistic effect.

Impact of Growth Conditions on the Structural and Magnetic Properties of -Fe_{3x}N Thin Films

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Iron nitrides exhibit valuable properties such as tunable magnetism, thermal stability, and corrosion resistance, making them attractive for both magnetic and protective applications. Among these, the ε -Fe_{3-x}N ($1 \geq x \geq 0$) phase features a trigonal (*P*3₁2) structure with a fixed nitrogen content, enabling compositional control over its magnetic properties. However, its thermal instability and the pronounced reduction in magnetic moment (ferromagnetic-to-paramagnetic transition) with increasing nitrogen content make it an important system for understanding the relationship between structure and magnetism in iron nitrides[1]. While the structure and magnetic behaviour of ζ -Fe₂N thin films[2,3] and bulk ε -Fe₂N have been explored[4], comprehensive studies on ε -Fe₂N thin films remain limited. In this work, thin films were synthesised using reactive DC magnetron sputtering by systematically varying the N₂/(

$\text{N}_2 + \text{Ar}$) gas ratio (R_{N_2}) and substrate temperature (T_s) to investigate their effect on phase formation. X-ray diffraction (XRD) measurements were performed on the prepared samples, as shown in (Fig.56). The XRD results confirm the formation of $\varepsilon\text{-Fe}_3\text{N}$ at $R_{\text{N}_2} = 40\%$, and the formation of the $\varepsilon\text{-Fe}_2\text{N}$ phase in the range of $R_{\text{N}_2} = 60\%$ to 100% , at a constant $T_s = 673\text{ K}$. At a fixed $R_{\text{N}_2} = 100\%$, the $\varepsilon\text{-Fe}_2\text{N}$ phase forms at $T_s = 673\text{ K}$ and 773 K , while a mixed $\varepsilon\text{-Fe}_2\text{N} + \text{FeN}$ phase appears at $T_s = 573\text{ K}$. Further, magnetic measurements (M-T and M-H) were carried out to distinguish the $\varepsilon\text{-Fe}_2\text{N}$ phase from the $\zeta\text{-Fe}_2\text{N}$ phase, as the latter exhibits a low Curie temperature ($\sim 35\text{ K}$). The $\varepsilon\text{-Fe}_2\text{N}$ films exhibit a paramagnetic-to-ferromagnetic transition below 160 K , consistent with the characteristic behaviour of the $\varepsilon\text{-Fe}_2\text{N}$ phase. These results demonstrate that deposition conditions—particularly N_2 content and substrate temperature—play a crucial role in controlling phase formation and the magnetic response in $\varepsilon\text{-Fe}_2\text{N}$ thin films.

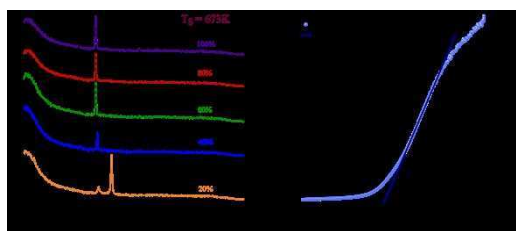


Figure 56: (a) XRD of the thin films deposited at $T_s = 673\text{ K}$ at different R_{N_2} ; (b) Curie-Weiss fit showing transition from Para magnetism to ferromagnetism.

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Keywords: thermal instability, magnetic behaviour, Curie temperature

Designing Defect-Rich Cobalt Oxide Nanostructures by Selective Cation Dissolution: A Template-Free Approach for Water Oxidation

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Water splitting is a promising route for sustainable hydrogen production, where the oxygen evolution reaction (OER) is a significant obstacle because of its slow kinetics [1]. Because of their stability, abundance, and tunable electronic structures, transition metal oxides (TMOs) have become effective and affordable OER catalysts [3]. Defect engineering, doping, and nanostructuring developments have greatly enhanced their catalytic performance. The integration of TMOs in scalable water-splitting systems holds great promise for enabling green hydrogen economies and addressing global energy and environmental challenges [2]. In this work, we developed a simple, template-free method to synthesize high surface area, defect-rich Co_3O_4 (AE- MgCo_2O_4) nanomaterials by selectively removing A-site cations from the MgCo_2O_4 spinel precursor. The acid-treated (AE- MgCo_2O_4) nanomaterials exhibit exceptional efficiency in the water oxidation reaction. They possess a surface area of $X\text{ m}^2/\text{g}$, which is nearly three times higher than that of Co_3O_4 nanoparticles synthesized via the citrate-gel method. Notably, the acid-treated sample (AE- MgCo_2O_4) demonstrates superior electrochemical performance, with a lower overpotential of 394 mV and a Tafel slope of $120\text{ mV}/\text{dec}$, outperforming the Co_3O_4 nanomaterials synthesized by the citrate-gel method (435 mV and $200\text{ mV}/\text{dec}$, respectively). This template-free approach, involving the selective removal of magnesium cations from the MgCo_2O_4 precursor, increases the catalyst's surface area, porosity, and anion vacancies, all of which collectively enhance water oxidation activity. Our template-free synthesis of high surface area, defect-rich nanomaterials provides a novel strategy for designing highly active catalysts for water oxidation and other catalytic applications.

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Keywords: Acid Etching (AE), Transition metal oxides (TMOs), Oxygen evolution reaction (OER).

Dual Functionality of Prussian Blue and Manganese-Doped Prussian Blue Materials for High-Performance Supercapacitors and Flexible, Low-Cost Screen-Printed Glutathione Sensors

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Prussian Blue (PB) and manganese-doped Prussian Blue (MnPB) nanocubes demonstrate dual functionality as advanced materials for both electrochemical energy storage and biosensing applications. This search has driven interest toward transition metal-based compounds, metal-organic frameworks, and Prussian Blue analogues as potential replacements. Unlike conventional metal compounds, MOFs facilitate more efficient surface redox reactions. MnPB nanocubes were synthesized with varying Mn concentrations via a facile reflux process, yielding crystals with tunable structural, optical, and electrochemical properties. XRD, FE-SEM, FTIR, and XPS confirmed phase purity and successful Mn incorporation, which reduced microstrain and defects, enhancing both capacitance and photoluminescence intensity. Electrochemical studies revealed that higher Mn doping led to increased specific capacitance, with MnPB(50%) achieving a peak value of 540.6

F/g and an energy density of 105 Wh/kg at a power density of 6882.5 W/kg, positioning it as a promising supercapacitor electrode material. Ragone and EIS analyses confirmed fast ion diffusion and robust charge-storage mechanisms, with distinct contributions from pseudocapacitive and electric double-layer processes. For biosensing, screen-printed flexible electrodes on OHP sheets employed MnPB(30%) as the active layer for glutathione (GSH) detection. UV-Vis and PL spectroscopy demonstrated high sensitivity and selectivity toward GSH, explained by changes in Fe redox states and lattice coordination, with MnPB(30%) showing the strongest spectroscopic and electrochemical response. This platform offers a low-cost, robust sensor for health applications, with mechanical flexibility validated under bending conditions. These findings underscore that composition tuning within the PB open framework enables multifunctional performance in both energy storage and biosensing, advancing sustainable and flexible device design.

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Keywords: Prussian blue, Metal organic framework, Electrochemical energy storage, Flexible sensor for Glutathione detection.

Magneto-Responsive Carbon:SPION Integrated Conducting Gel for Self-Powered Wearable Triboelectric Sensors

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Conducting gels have garnered considerable interest due to their outstanding conductivity, flexibility, and biocompatibility, making them suitable for various wearable health monitoring sensors. Despite progress in conducting gel, they exhibit limited electrical performance and sensitivity when integrated into a wearable system. To address these challenges, this study introduces a novel magneto-responsive, highly conducting gel by incorporating carbon: superparamagnetic iron oxide nanoparticles composite (C:SPION) in polyvinyl alcohol/silver nitrate (PVA/AgNO₃/C:SPION). The C:SPION is uniformly distributed into conducting gel, contributing to improved electrical conductivity due to the delocalized π electrons in carbon. The molecular interaction and magnetic domains of PVA/AgNO₃/C:SPION conducting gel were examined using Raman spectroscopy, vibrating sample magnetometer (VSM), and magnetic force microscopy (MFM). The resulting conducting gel exhibited high zeta potential, d_{33} coefficient, electronic conductivity, storage modulus, tensile strength, and magnetic moment of -0.13 mV, 26 pC/N, 38 kS/m, 6.6 kPa, 0.5 MPa, and 2.34 emu/g, respectively. This high-performance conducting gel was subsequently utilised to develop a wearable triboelectric nanogenerator (C-TENG), delivering a peak output voltage, current, and power density of 276 V, 8.6 μ A, and 1.67 mW/cm². C-TENG is efficiently capable to charge a 1 μ F to 10 μ F capacitor within 68 seconds. Beyond energy harvesting, the developed conducting gel showed potential application in wearable strain sensing, powering 39 LEDs, a capacitive screen sensitive, and real-time pulse detection.

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Keywords: Conducting Gels; Carbon; Superparamagnetic Iron Oxide Nanoparticles Composites (SPION); Triboelectric Nanogenerator (TENG); Self-Powered Sensor;

Tuning Lattice Thermal Conductivity through Selenium Substitution in Bi₂Te₃ Alloys

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Thermoelectric (TE) materials convert waste heat into usable electrical energy, offering a promising solution to increasing energy demand. Among thermoelectric material families, chalcogenides often exhibit strong energy-conversion performance in the mid- to high-temperature range. Bi₂Te_{3-x}Se_x alloys play a pivotal role in thermoelectric applications, where the intentional introduction of selenium (Se) into bismuth telluride (Bi₂Te₃) enables precise tuning of electronic and thermal transport properties. In this work, we synthesized Bi₂Te_{3-x}Se alloys via direct melt (sealed quartz tubes) and investigated heat transport and phonon behaviour using experiment-informed analyses in combination with first-principles calculations.

The phase identification and lattice parameter determination were carried out using the Rietveld refinement method with the FULLPROF software. Raman spectroscopy was employed to study the temperature-dependent Raman shifts. Furthermore, the shifts and broadenings in Raman modes were analyzed using the bond-order-length-strength (BOLS) correlation to extract composition-resolved Grüneisen parameters (γ), which provide insights into the material's anharmonicity, Debye temperature (θ_D), and effective phonon energy scale across the investigated temperature range. Consequently, the parameters, i.e., γ and θ_D obtained from the BOLS correlation, were utilized to estimate the lattice thermal conductivity (κ_l) via the Slack equation, which offers a material-specific, experimentally informed prediction of lattice thermal conductivity.

The phonon dispersion and thermal properties of the system were computed using PHONOPY interfaced with Quantum ESPRESSO (QE). Atomic vibrations were treated within the harmonic approximation by considering the second-order terms in the crystal potential energy, while higher-order interactions were evaluated using perturbation theory combined with the supercell finite-displacement approach. The force sets were generated from changes in the potential energy and subsequently used to calculate the phonon dispersion. The lattice thermal conductivity was then determined using the PHONO3PY software package interfaced with QE.

Keywords: Thermoelectric; Raman spectroscopy; BOLS theory; lattice thermal conductivity.

Investigation of Lattice Thermal Conductivity in SrSnO_3 : Combining Experiments, Theory, and Machine Learning Methodology

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Perovskite oxides represent a significant class of functional materials with broad applications in energy and electronic devices, where thermal transport is a key factor. This study investigates the lattice thermal conductivity (κ_L) of bulk strontium stannate (SrSnO_3) through a comprehensive approach combining experimental Raman spectroscopy, first-principles simulations, and machine learning (ML) techniques. Temperature-dependent Raman spectroscopy was conducted, and phonon frequency shifts were examined through the Bond-Order-Length-Strength (BOLS) model to quantify anharmonic phonon interactions and estimate the κ_L . Density functional theory-based Phono3py calculations were utilized to analyze phonon dispersion, lifetimes, and κ_L , offering detailed insight into phonon scattering processes in SrSnO_3 . Concurrently, machine learning models

trained on extensive perovskite oxide datasets predicted κ_L trends and identified key structural and chemical factors influencing heat transport. The combined analysis of experimental Raman-based BOLS modelling, Phono3py simulations, and machine learning predictions demonstrates that SrSnO_3 possesses relatively low κ_L compared to similar perovskites, attributed mainly to its pronounced anharmonicity and heavy atomic constituents. This integrative framework underscores the prospective utility of SrSnO_3 in thermal management applications and exemplifies the efficacy of combining spectroscopic characterization, first-principles computational methods, and data-driven modeling to elucidate thermal transport phenomena in complex oxide systems.

Keywords: Raman spectroscopy, Lattice Thermal Conductivity, Density Functional Theory, Machine Learning.

Employing Coumarin Framework for the Development of Insensitive Energetic Materials

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Once seen only as symbols of war and violence, energetic materials are gaining significant attention due to their wide range of potential applications in the civil sector (such as controlled demolition, mining, and aerospace propulsion) and the military domain. Well-known benchmark explosives like RDX, HMX, and CL-20 were developed in the 20th century and are still used due to their excellent energetic performances. However, their high sensitivity poses significant risks of accidental detonation during transportation, storage, and handling. This highlights the need for developing safer and more stable energetic materials, but the inverse relationship between energy and stability makes it challenging to synthesize compounds with optimal balance. In this regard, fused cyclic energetic materials have emerged as promising alternatives to conventional energetic compounds, owing to their coplanar molecular frameworks, resulting in enhanced π - π stacking and denser crystal packing, leading to superior energetic performance, improved thermal stability, and reduced sensitivity

to external stimuli. Among fused cyclic compounds, the coumarin framework is known to be a unique class of large, conjugated, oxygen-rich scaffolds that can be used to synthesize novel energetic materials, which not only offer good detonation performance but are also stable enough to meet modern safety and sustainability standards. In this study, coumarin-based compounds 4,7-dihydroxy-3,6,8-trinitro-2H-chromen-2-one (2) and 7-hydroxy-4-methyl-3,6,8-trinitro-2H-chromen-2-one (10) were synthesized using a cost-effective route and readily available starting materials. The presence of a hydroxyl group adjacent to the nitro substituents on the coumarin ring enables hydrogen bonding, enhances overall stability, and also provides modification sites to further improve the properties of the parent compounds through salt formation. Notably, except for neutral compound 2, all synthesized compounds were found to be insensitive to external stimuli. However, the potassium salt of compound 2 showed the highest decomposition temperature ($T_d = 297\text{ }^\circ\text{C}$), highlighting its potential as a promising heat-resistant explosive. This novel class of oxygen-rich, fused polycyclic Coumarin-based compounds is being explored for the first time in the field of energetic materials. All the compounds were thoroughly characterized through IR, multinuclear NMR spectroscopy [^1H , $^{13}\text{C}\{^1\text{H}\}$], HRMS, and elemental analysis. The structure-property relationships were investigated through Hirshfeld surface, noncovalent interaction (NCI) analysis, and electrostatic potential (ESP) mapping.

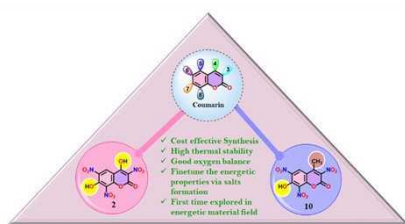


Figure 57: Representative examples of coumarin-derived energetic molecules.

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Keywords: Fused cyclic energetic materials; Coumarin;oxygen rich; reduced sensitivity.

Harnessing the mechanical and magnetic energy with PMN-PT/Ni-Mn-In based flexible piezoelectric nanogenerator

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Multifunctional piezoelectric nanogenerators (PENG) hold significant potential in developing smart sensing technologies for the military, healthcare, and industrial sectors. Here, we present the efficient energy harvesting from mechanical and magnetic stimuli in 0.67Pb(Mg_{1/3}Nb_{2/3})O₃-0.33PbTiO₃ (PMN-PT) / Ni₅₀Mn₃₅In₁₅ (Ni-Mn-In)-based PENG fabricated on a flexible nickel substrate using the DC/RF magnetron sputtering technique. The performance of the device has been assessed by imparting forces in the range of 0.12 to 0.61 N using various weights, finger tapping, bending, and magnetic fields. The device generates the maximum open circuit voltage (V_{oc}) of 9.3 V and 6 V with 0.61 N of force and finger tapping, respectively. The corresponding short circuit current (I_{sc}) has been obtained as 1.33 μA (0.61 N) and 0.9 μA (finger tapping). The device shows a maximum V_{oc} of 10.6 V and I_{sc} of 1.51 μA at the bending angle of 120°. Furthermore, the V_{oc} and I_{sc} have increased from 0 mV and 0 nA to 240 mV and 35 nA under the presence of 0 Oe to 500 Oe of DC magnetic field, respectively. The fabricated device exhibited a power density of 2.7 $\mu\text{W}/\text{cm}^2$ with a high mechanical stability of 2500 cycles. Additionally, LEDs of green, red, yellow, and white colour have been illuminated. The receptiveness of the fabricated PENG towards mechanical and magnetic stimuli highlights its potential in areas such as tactile sensing, wearable electronics, human-machine interfaces, and biomedical devices.

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Keywords: PMN-PT, Ni-Mn-In, Nanogenerator, Tactile sensor, Flexible

Improved Ionic Conductivity and Phase Stability in Sm and W Co-Doped $\text{La}_2\text{Mo}_2\text{O}_9$ Electrolytes

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Lanthanum molybdenum oxide ($\text{La}_2\text{Mo}_2\text{O}_9$ or LAMOX) has emerged as a promising oxide-ion conductor for use as an electrolyte in intermediate-temperature solid oxide fuel cells (IT-SOFCs). The ionic conductivity of LAMOX is closely linked to its crystal structure, which transforms from a low-conducting monoclinic α -phase (P2_1) to a highly conductive cubic β -phase (P2_13) around 580°C. This β -phase offers enhanced oxide-ion mobility due to structural disorder. However, its instability below the transition temperature leads to reduced conductivity, limiting practical SOFC applications. To overcome this drawback, the present study explores a co-doping strategy aimed at stabilizing the β phase at lower temperatures and boosting ionic conductivity. In this work, a new series of Sm and W co-doped LAMOX compounds was synthesized, where samarium (Sm^{3+}) was partially substituted at the lanthanum (La^{3+}) site, and tungsten (W^{6+}) was introduced at the molybdenum (Mo^{6+}) site. The structural phase evolution and dopant incorporation were confirmed using X-ray diffraction (XRD) followed by Rietveld refinement. The analysis revealed that the co-doped compositions retained the cubic structure even at room temperature, indicating successful suppression of the $\alpha \rightarrow \beta$ transition. Raman spectroscopy was employed to probe the local lattice dynamics and coordination environment around the MoO_6 units. The synthesized pellets were found to be highly dense and mechanically stable, making them suitable for conductivity measurements. Electrochemical impedance spectroscopy (EIS) was

performed to evaluate the ionic transport behavior of the co-doped systems in the temperature range of 350°C to 650°C. The results revealed a remarkable improvement in ionic conductivity in the co-doped samples compared to the undoped LAMOX. Specifically, the conductivity of the undoped $\text{La}_2\text{Mo}_2\text{O}_9$ was measured to be $8.99 \times 10^{-3} \text{ S}\cdot\text{cm}^{-1}$ at 650°C. In contrast, the co-doped composition (LMXS15) exhibited an enhanced conductivity of $1.36 \times 10^{-2} \text{ S}\cdot\text{cm}^{-1}$ at the same temperature, an improvement of over two orders of magnitude in certain cases. To further understand the relaxation behavior and conduction mechanism, the Distribution Function of Relaxation Times (DFRT) analysis was performed. The enhanced conductivity is attributed to the combined effect of Sm^{3+} and W^{6+} dopants, which help stabilize the cubic structure, create favorable defect chemistry, and reduce the energy barriers for ion migration. Overall, this study demonstrates that co-doping is an effective strategy to improve the structural and electrical performance of LAMOX-based electrolytes for IT-SOFCs.

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Keywords: Co-doped LAMOX; Ionic Conductivity; Impedance Spectroscopy; Distribution of Relaxation Time

Volume Percentage Doping Effects of Fe_3O_4 Nanoparticles in P(VDF-TrFE) Matrix: Enhanced Magnetoelectric Coupling in Nanocomposite Films prepared by solution casting method

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Magnetoelectric (ME) nanocomposites comprising magnetostrictive and piezoelectric phases are promising for multifunctional device applications due to their ability to couple magnetic and electric properties in a single material platform [1]. In this work, we systematically investigated the effect of varying Fe₃O₄ nanoparticles volume fraction on the room-temperature ME response of P(VDF-TrFE) matrix [2]. Nanocomposite films were fabricated by incorporating Fe₃O₄ nanoparticles at multiple volume percentages (0.5%, 1%, 1.5%, 2% and 2.5%) into the ferroelectric P(VDF-TrFE) matrix using the solution-casting technique. Scanning Electron Microscopy (SEM) confirmed homogeneous nanoparticle dispersion at low loadings, whereas higher concentrations led to aggregation of nanoparticles within the matrix. XRD and FTIR analyses showed preservation of the electroactive β -phase, with subtle changes in crystallinity at elevated filler contents. Dielectric measurements show an enhancement in the relative permittivity from 5.5 for pure P(VDF-TrFE) to 11 for 2.5% Fe₃O₄ doped P(VDF-TrFE) with increasing Fe₃O₄ content. Magnetic characterization demonstrated that saturation magnetization (M_s) scaled proportionally with increasing Fe₃O₄ content, confirming retention of nanoparticle magnetic functionality within the polymer scaffolds. Importantly, dynamic ME measurements displayed a non-linear dependence on nanoparticle loading, with a maximum ME voltage coefficient of ~ 180 mV/Oe.cm at 1.5 vol.% under a bias DC field of 2000 Oe superimposed with an AC field of 1.05 Oe at frequency 10 kHz, applied perpendicular to the plane of sample. Beyond 1.5%, aggregation reduced effective stress transfer, leading to a slight decline. These results highlight Fe₃O₄/P(VDF-TrFE) nanocomposites as promising candidates for smart materials, spintronic devices and energy harvesting applications.

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Keywords: Magnetoelectric, magnetostrictive, ferroelectric, piezoelectric etc.

Electrospun Highly Porous N-doped Carbon Nanofibers for High Performance Supercapacitor Application

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The distinctive features of one-dimensional porous heteroatom-doped carbon nanofibers, such as their high surface area, fibrous morphology, numerous active sites (heteroatom centers) facilitating surface redox reactions, and impressive mechanical strength, render them appealing candidates for capacitive energy storage. This study presents an electrospinning-mediated two-step synthesis approach for highly porous carbon nanofibers. In the first step, electrospinning of polyacrylonitrile (PAN), polyvinylpyrrolidone (PVP), and nitrogen-doped carbon (CN) followed by carbonization was employed to prepare CN-carbon nanofibers (CN-CNF-x_c, where x = amount of CN). The second step, involving high temperature KOH activation, leads to the formation of highly porous carbon nanofibers (CN-CNF-x) with an exceptionally high specific surface area (SSA) of 2000.8 m² g⁻¹ coupled with a micropore volume of 0.67 cc g⁻¹. The as-synthesized porous carbon fibers were then utilized in energy storage applications. The CN-CNF-x demonstrated a maximum specific capacitance (C_s) of 483 F g⁻¹ and 456 F g⁻¹ at 1 A g⁻¹ in basic and acidic media, respectively. This capacitance performance was nearly three times higher than the non-activated carbon nanofibers without CN i.e., CN-CNF-0_c (C_s = 178 F g⁻¹ at 1 A g⁻¹ in 6M KOH) and other reported electrospun carbon nanofibers. The symmetric device fabricated using the CN-CNF-x exhibited an 85% capacitance retention

in an alkaline medium over 5000 cycles, along with a peak energy density (ED) of 12.22 Wh kg^{-1} and a maximum power density (PD) of 2500 W kg^{-1} . Therefore, incorporating CN into the PAN/PVP nanofibers, combined with KOH activation, presents a promising avenue for enhancing their performance in energy storage applications. The collaborative effects of high SSA, an abundance of micropores, porous nanofiber morphology, and N, O doping work synergistically to improve electrochemical performance, ultimately leading to the fabrication of superior supercapacitor devices.

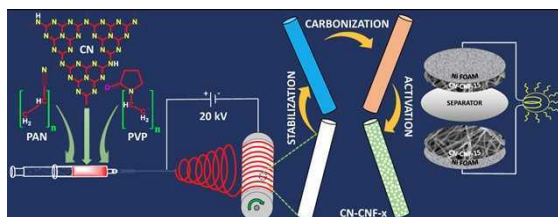


Figure 58:

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Keywords: Electrospinning; Porous nanofibers; N-doped carbon; Supercapacitor.

Nanostructure Engineering of Pt-Shell-Decorated PdPt Alloy for Highly Efficient Oxygen Reduction Catalysis

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Rational design of Pt nano-shell onto Pd-based nanostructure delivers an effective way for significantly boosting catalytic performance. Herein we report a facile solvothermal approach for synthesizing anisotropic Pt-skin PtPd core-shell nanocatalysts (NCs) with low Pt amount. Meanwhile, maximizing Pt utilization efficiency in PdPt@Pt NCs can be further gained through strategic morphology modifying, precise control over atomic arrangements like numerous

twinned structures, surface defects and modulation of electron transfer properties. This strategy not only changes the charge-transfer mechanism to modulate the formation of active catalytic centers but also efficiently regulates the physicochemical properties of the designed electrocatalysts which plays crucial role for enhancing their overall catalytic performance. Due to the distinct surface site reactivities, the growth of the Pt shell can be precisely regulated by adjusting the loading of Pt amount. Interestingly, Pt tends to favorably form a shell structure (PdPt@Pt) at low Pt amount instead of PdPt alloy. Consequently, the anisotropic Pt-skin on PtPd core-shell nanostructure offers noteworthy catalytic advantages by inducing compressive surface strain in the Pt-skin layer, which effectively weakens the chemisorption of oxygenated intermediates and increases greatly the catalytic performances for ORR.

Keywords: Oxygen reduction reaction; Core-shell nanocatalyst; Catalytic activity and stability enrichment; Morphological engineering; Electrocatalyst optimization

Piezopolarization Induced High Rate Solar N_2 -to- NH_3 Conversion in Vacancy Engineered AgCu-Modified BiFeO_3

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The sustainable production of ammonia via the nitrogen reduction reaction (NRR) under ambient conditions remains a formidable challenge due to the inertness of N_2 molecules and sluggish reaction kinetics. In this work, we present a multifunctional photocatalyst vacancy-engineered AgCu-modified BiFeO_3 (AgCu@BiFeO_3) that harnesses the synergistic effects of piezopolarization, photocatalysis, and the localized surface plasmon resonance (LSPR) effect to achieve enhanced solar N_2 -to- NH_3 conversion. The incorporation of Ag and Cu nanoparticles introduces strong LSPR absorption, extending visible light harvesting and promoting hot electron generation, while simultaneously activating surface plasmon-driven charge transfer. Vacancy engineering induces oxygen deficiencies within the BiFeO_3 lattice, creating

active sites for efficient N_2 adsorption and activation. Furthermore, the intrinsic piezopolarization of $BiFeO_3$ under mechanical stress induces an internal electric field, which dramatically enhances charge separation and directs photogenerated electrons toward the NRR pathway. The resulting composite exhibits a significantly improved NH_3 yield rate of $278 \mu\text{mol g}^{-1} \text{h}^{-1}$ under simulated solar irradiation and mild ultrasonic agitation. This study underscores a rational design strategy integrating plasmonic modulation, defect engineering, and piezoelectric polarization to unlock the full potential of advanced hybrid photocatalysts for green ammonia synthesis.

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Keywords: piezopolarization, Photocatalysis, NRR, Vacancy Engineering, LSPR Effect

Color tunable $CsPbX_3@MOF$ nanocomposites as a temperature sensor and stable electrospun microfibers for fabrication of down-converting WLEDs

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All inorganic $CsPbX_3$ ($X = \text{I, Br, Cl}$) nanocrystals (NCs) have achieved remarkable progress in numerous optoelectronic applications owing to their suitable photophysical properties. However, they are prone to degrade due to the ionic nature and halide ion migration among the NCs that hinders the sensing and lighting applications. To tackle such issues, we encapsulated perovskite NCs with different amounts of metal-organic frameworks (MOFs).

The optimized $CsPbBr_3@MOF$ nanocomposites (NCPs) resulted in superior stability with a maximum photoluminescence quantum yield (PLQY) of $\sim 94\%$ in the green spectral region. Red-emitting $CsPbBr_xI_{3-x}@MOF$ NCPs were synthesized by halide exchange process of $CsPbBr_3@MOF$ NCPs. Such NCPs are comparatively stable even at higher temperatures and tested as a temperature sensor which demonstrated superior temperature sensitivities. The NCPs were further embedded inside flexible poly(methyl methacrylate) microfibers that was grown via an electrospinning process, to enhance the stability against water. Finally, we fabricated down-converted WLEDs by incorporating green and red-emitting flexible $CsPbX_3@MOF@Fibers$ that were deposited on a glass substrate and excited by a blue LED chip. The optimized WLED device exhibited a CIE chromaticity coordinate of (0.30, 0.33) at 80 mA driving current with a correlated color temperature (CCT) value of ~ 6808 K. Our research work provides very insightful ideas for synthesizing stable color-tunable perovskite MOF NCPs that can be utilized as a temperature sensor, and also feasible for fiber-based futuristic lighting and display technologies.

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Keywords: $CsPbX_3$ nanocrystals; metal-organic frameworks; polymeric fibers; WLEDs.

Exploring the Reactivity of Oxygen and Ozone in C_2N Monolayer and its Photocatalytic activity for Water Splitting: A First Principles Study

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Understanding the interaction of various environmental oxidizing agents is important in determining the physical and chemical properties of two-dimensional (2D) materials. Its impact holds great significance for the practical application of these materials in nanoscale devices functioning under ambient conditions. This study delves into the influence of O₂ and O₃ exposure on the structural and electronic characteristics of the C₂N monolayer, focusing on the kinetics of adsorption and dissociation reactions. Employing first-principles density functional theory calculations alongside climbing image nudged elastic band calculations, we observe that the C₂N monolayer exhibits resistance to ozonation, evidenced by energy barriers of 0.56 eV, respectively. These processes are accompanied by the formation of C–O–C groups. Furthermore, the dissociation mechanism involves charge transfers from the monolayer to the molecules. Notably, the dissociated configurations demonstrate higher band gaps compared to the pristine C₂N monolayer, attributed to robust C–O hybridization. Interestingly, the oxidized and ozonized C₂N monolayer exhibited enhanced band edge positions spanning the oxidation/reduction potential of water along with its optical absorption lying in the visible region, thus ensuring its potential application in photocatalytic water splitting. These findings suggest the robustness of C₂N monolayers against oxygen/ozone exposures, ensuring stability for devices incorporating these materials along with its promising application for photocatalytic water splitting.

Keywords: Photocatalytic activity, Water Splitting, DFT.

Vacancy-Tailored low-dimensional 2D perovskite inspired Halide CsAgBr₂ for Next-Generation High-Performance Supercapacitor

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The search for cutting-edge supercapacitor materials has become increasingly urgent due to the rising global demand for fast, reliable, and sustainable energy storage solutions. Although carbon nanostructures, transition-metal oxides, conducting polymers, and 2D MXenes have significantly advanced supercapacitor technology because of their high surface area, rapid ion diffusion, and strong redox activity, low-dimensional halide materials remain largely unexplored. Their limited use is mainly attributed to structural instability, poor charge transport, and weak electrode–electrolyte compatibility. In this study, we report the synthesis of the two-dimensional halide CsAgBr₂ using a simple solution-based method and demonstrate its capability as an efficient supercapacitor electrode material. Structural phase purity and morphology were validated through XRD, XPS, and FE-SEM analyses. Electrochemical characterization in a three-electrode setup (1 M KOH, 0.1–0.6 V vs Ag/AgCl) indicates that charge storage occurs predominantly via vacancy-assisted pseudocapacitance, where halide vacancies act as energetically favorable sites for OH[−] intercalation, while reversible Ag⁺/Ag⁰ redox transitions support rapid faradaic charge transfer, effectively bridging surface ion adsorption and bulk redox processes. Owing to this synergistic mechanism, CsAgBr₂ delivers a high specific capacitance of ~567 F g^{−1} at 2 mV s^{−1}. Additionally, an asymmetric device (CsAgBr₂//activated carbon with PVA–KOH gel electrolyte) exhibits excellent energy and power performance with strong cycle stability, retaining ~70% capacitance after prolonged charge–discharge cycling. These results highlight the potential of CsAgBr₂ to overcome key limitations of halide-based electrodes and position two-dimensional halides as promising candidates for next-generation supercapacitor technologies.

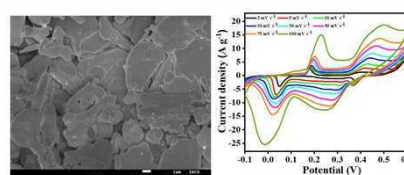


Figure 59: FESEM image and CV profile of CsAgBr₂

Keywords: 2D halide; Vacancy-assisted pseudo-capacitance; asymmetric supercapacitor; charge-transport

Simple and Template-free Approach for Synthesis of High Surface Area and Defect NiO from Olivine Precursor for Efficient Water Oxidation

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Water splitting is an efficient and promising technique for producing sustainable hydrogen fuel, but its major bottleneck is the sluggish and energy-intensive oxygen evolution reaction (OER)[1]. Although catalysts based on RuO_2 and IrO_2 are highly effective, their high cost and scarcity hinder large-scale application, while cheaper alternatives lack comparable efficiency. To address this challenge, porous materials have gained attention due to their high surface area and rapid mass diffusion characteristics, making them ideal candidates for developing affordable and efficient OER catalysts. Herein, we report a simple, template-free strategy to synthesize high-surface area porous NiO nanomaterial from an olivine-type precursor (NaNiPO_4). The acid-treated AT-NNP nanomaterials exhibit exceptional water oxidation efficiency, displaying a nine-fold increase in surface area compared to NiO nanoparticles produced by the citrate-gel method. The acid-treated sample (AT-NNP) further shows superior electrochemical performance, featuring a lower overpotential (340 mV) and Tafel slope (118.7 mV/dec) relative to conventional NiO nanomaterial (520 mV and 190.4 mV/dec). The selective removal of sodium ions during acid treatment enhances surface area, porosity, and anion vacancies, which synergistically improve OER activity. Overall, this template-free method provides a new pathway for designing high-surface area, defect-rich materials for highly active water oxidation and other catalytic applications.



Figure 60: Graphical Abstract

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Keywords: Oxygen Evolution Reaction (OER), electrocatalyst, acid-etching, overpotential.

Multicomponent entropy stabilized ceria based rare earth oxides for photocatalytic hydrogen production and dye degradation applications

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Ceria is a well-known and widely used catalyst for optical applications such as in, thermochemical hydrogen production and CO_2 splitting, respectively, due to its attractive redox properties. Significant efforts are being carried out to further enhance the catalytic performance through chemical doping. Multicomponent ceria-based high-entropy rare earth oxides (HEOs) represent a significant advancement in photocatalytic materials, demonstrating remarkable potential in hydrogen production and dye degradation applications. These

materials are characterized by the incorporation of multiple rare earth elements, which enhance their chemical and structural properties. The unique architecture of HEOs facilitates improved oxygen vacancy concentrations, crucial for effective photocatalytic activity. Recent studies indicate that ceria-based HEOs exhibit higher efficiency in photocatalytic hydrogen evolution under various conditions, surpassing conventional catalysts due to their superior light absorption capabilities and charge carrier dynamics. Moreover, their application in dye degradation processes reveals enhanced catalytic performance, enabling the breakdown of hazardous organic pollutants in aqueous solutions. The synergistic effects of different metal ions in the ceria framework contribute to optimized lattice structures and increased specific surface areas, which are pivotal for both photocatalytic reactions.

In this work, ceria-based entropy stabilized rare earth oxides were synthesized using solid-state method, using commercially available, less expensive carbonate precursors. The as-synthesized materials are found to be in single-phase, which is evident from the X-ray diffractograms of calcined samples. The powder morphology and the chemical composition were studied using a field emission scanning electron microscope (FESEM) and energy dispersive spectroscopy (EDS). The atomic arrangements, band-gap and elemental analysis were examined using high-resolution transmission electron microscopy (HRTEM) and electron energy loss spectroscopy (EELS), respectively. The catalytic performance of as-synthesized HEO materials was correlated with the oxygen vacancies, through Raman spectroscopic analysis and further substantiated with HRTEM images. The photo dye degradation activity of the HEOs is active in the visible range, which is in concomitant with UV-vis band-gap calculations. BET studies were carried out to evaluate the surface area of as-synthesized samples. Electron paramagnetic resonance (EPR) studies were conducted on as-synthesized samples which confirmed the presence of un-paired electrons as well as the presence of oxygen vacancies. Finally, the as-synthesized HEO was then examined for hydrogen generation through photo-catalytic water splitting reaction.

Keywords: Rare-earth oxides; dye degradation; hydrogen production.

Tailoring Gold Corroles via Regioselective Nitration: Near Infrared Emission, Singlet Oxygen Sensitization, and Photocatalytic Oxidation of Sulfides

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A regioselective β -nitration of gold(III) corrole using nitrosonium ion is reported, the first such example. The reaction proceeds via a one-electron oxidized intermediate, $[(\text{corrolato}^{2-})\text{Au}^{\text{III}}]^+$, characterized by UV-Vis, EPR, and DFT studies. Introduction of two nitro groups significantly increases the electron-withdrawing nature of the corrole, shifting its redox potentials. The resulting 3,17-dinitro-gold(III) corrole shows partial inverse hypercorrole character and corrole-to-nitro charge-transfer transitions. These complexes exhibit near-IR phosphorescence (~ 920 nm), high singlet oxygen sensitization ($\sim 50\%$), and efficiently catalyze selective sulfide oxidation to sulfoxides with air and light, showing $>99\%$ selectivity and TONs of 1300–1800, outperforming many known systems.

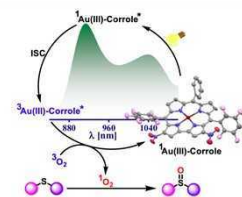


Figure 61: Regioselective β -nitration of gold(III) corrole yielding NIR-phosphorescent complexes for efficient photocatalytic sulfide oxidation.

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Keywords: Gold(III) corrole; NIR-phosphorescence; Singlet oxygen sensitization.

EVAPORATION-DRIVEN HYDROVOLTAIC DEVICES: HARNESSING ENGINEERED CARBON FOR SUSTAINABLE ENERGY

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The escalating global energy demand and the pressing need to mitigate environmental challenges associated with fossil fuels have intensified the search for sustainable and renewable energy alternatives. Hydrovoltaic technology has emerged as a promising avenue, harnessing the latent heat absorbed by natural water bodies and converting it into electrical power. By considering the abundance of water and its intrinsic capacity to absorb solar energy, hydrovoltaic systems offer an eco-friendly solution aligned with green energy principles. Among these, evaporation-driven hydrovoltaic devices are particularly noteworthy, as they mimic Earth's natural water cycle to transform ambient thermal energy into electricity. This approach has garnered significant attention for its potential to power self-sustaining systems, particularly in remote or off-grid locations, where low-energy devices can operate independently of external power sources. Recent advancements in hydrovoltaic energy harvesting emphasize the critical role of material innovation in enhancing conversion efficiency. In this study, commercially available carbon powder was chemically oxidized in an acidic medium to tailor its surface properties for improved energy generation. The functionalization process imparted advantageous attributes including increased surface area, enhanced hydrophilicity, superior porosity, and improved wettability, thereby facilitating more effective water absorption and charge generation. The surface modified materials were systematically characterized through various characterisation techniques like XRD, SEM, FT-IR and Raman spectroscopy to investigate its crystallinity,

morphology, and to analyze chemical functionalities. Contact angle measurement was also carried out to further assess its surface wettability. The multipronged design and evaluation strategy underscores the potential of chemically engineered carbon materials in enabling scalable and efficient hydrovoltaic systems. By optimizing water-surface interactions at the nanoscale, this work contributes to the advancement of next-generation energy harvesting platforms that are sustainable, environmentally benign, and adaptable for diverse real-world applications. The findings highlight not only the fundamental material-property relationships critical for hydrovoltaic energy conversion but also the broader role of nanostructured carbon-based systems in shaping the future of renewable energy technologies.

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Keywords: Hydrovoltaic effect; water evaporation; electrical double layer; hydrovoltaics

Influence of Nanoconfined Gold Nanoparticles on Phase Transformation and Enhanced Pyroelectric Response in PVDF Nanofibers

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Polyvinylidene fluoride (PVDF) nanofibers are widely recognized for their potential in sensing and energy-harvesting applications, primarily due to their electroactive β -phase.^{1,2} This study explores the nanoconfinement of gold nanoparticles (Au NPs) in PVDF nanofibers via electrospinning, aiming to maximize the β -phase content and improve device performance. The addition of Au salt during electrospinning not only increases the proportion of the electroactive

β -phase, as confirmed by FTIR and XRD analyses, but also results in finer, bead-free fibers with improved crystallinity. The Au NPs are prepared *in situ*, with DMF acting as a reducing agent and PVDF as a stabilizing agent. TEM and XPS studies further verify the successful integration and interaction of Au NPs within the PVDF matrix. Electrical and electroactive property assessments included dielectric spectroscopy and piezoresponse force microscopy (PFM) under applied bias. Au NP-doped PVDF nanofibers exhibited significantly higher dielectric permittivity and enhanced piezoelectric response compared to neat PVDF, demonstrating easier dipole switching and a marked increase in the piezoelectric coefficient from 4.9 pm/V for neat PVDF to 44 pm/V for the composite fiber. PEDOT:PSS was employed as a flexible, highly conductive electrode material, ensuring robust charge collection and mechanical stability in the assembled devices. Pyroelectric measurements reveal a significant improvement in the electroactive response of Au NP-doped PVDF fibers compared to neat PVDF. The enhanced β -phase content, crystallinity, and plasmonic properties of Au NPs facilitate superior pyroelectric output under thermal fluctuations. The pyroelectric coefficient of Au-doped PVDF is calculated to be $83 \mu\text{C}/\text{m}^2\text{K}$, which is among the highest reported so far in PVDF fiber-based pyroelectric devices.³ The devices also exhibit rapid response times of 120 ms and long-term operational stability. Overall, this work highlights the effectiveness of Au NP incorporation and optimized electrode integration in advancing PVDF-based devices for next-generation sensing and energy-harvesting technologies.

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Keywords:

Self-powered PVDF@MoSSe based TENG enabled Wireless Braille Typing System with Integrated Auditory Feedback for Assistive Communication Systems

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Advancements in touch-sensitive human-machine interfaces (HMIs) have transformed communication, education, and health-care, driven by the rise of the Internet of Things (IoT) and 5G technologies. A critical need exists for assistive technologies that enable independent communication for individuals with visual or speech impairments through auditory feedback. This study introduces a portable, self-powered smart Braille typing system powered by a triboelectric nanogenerator (TENG), eliminating reliance on external power sources. The development of an efficient tactile sensing system necessitates the integration of a high-sensitivity tactile sensor and a circuit optimized for weak current signal processing. For this purpose, we developed a PVDF@MoSSe nanofiber composite-based TENG, fabricated via a combination of the hydrothermal method and electrospinning, paired with silk cloth. To determine the most effective filler concentration, MoSSe nanocomposites with varying filler loadings (1, 2.5, and 5 wt%) were characterized for their structural, morphological, dielectric, and surface potential properties. The 2.5 wt% MoSSe-based TENG achieved a peak-to-peak open-circuit voltage (V_{OC}) of 754.35 V and a short-circuit current (I_{SC}) of $14.45 \mu\text{A}$, with a maximum power density of $7.36 \text{ W}/\text{m}^2$. The sensitivity was found to be $32.3 \text{ V}/\text{kPa}$ up to an external pressure of 0.18 kPa. The resulting PVDF@MoSSe-based tactile sensor exhibits high sensitivity, low-pressure responsiveness, and robust durability. A prototype integrating six contact-separation triboelectric sensors for Braille input and a seventh confirmation triboelectric sensor was developed, enabling tactile-to-auditory translation for accessible communication. The system currently allows input using English letters and numbers. This work highlights the successful integration of a tactile Braille typing system with a modern in-built Bluetooth-based microcontroller (ESP32) and demonstrates the potential of 2D materials in advancing auditory feedback-based HMIs for assistive technologies.

Keywords: Triboelectric nanogenerator (TENG); PVDF@MoSSe2D nanofiber; Braille; Auditory feedback;

Keywords: Photoelectrochemical; Water splitting; Cu SPR; Plasmonic heterostructure.

Electronic Charge Transportation in Plasmonic NrGO/NiFeTb LDH@Cu Heterostructure for Enhanced Photoelectrochemical Water Oxidation

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This work reported the cost-effective plasmonic NrGO/NiFeTb-LDH@Cu photoelectrode prepared via the light-mediated photodeposition method as a potential photoelectrocatalyst for PEC water-splitting. The significant finding of the work is an enhancement in light-harvesting capability, improved interfacial charge-transfer dynamics, and stabilization of the defect regions over NrGO and NiFeTb-LDH by incorporating metallic Cu nanoparticles into the NrGO/NiFeTb-LDH hybrid. This NrGO/NiFeTb-LDH@Cu photoelectrode exhibits an exceptional photocurrent density of 19.92 mA/cm² at 2 V vs. RHE and a solar-to-hydrogen (STH) conversion efficiency of 2% at 0.80 V (vs. RHE), outperforming NrGO/NiFeTb-LDH (11.49 mA/cm² at 2 V vs. RHE; 1% at 0.80 V vs. RHE) and NiFeTb-LDH (5.55 mA/cm² at 1.78 V vs. RHE; 0.5% at 0.80 V vs. RHE). Additionally, the transient photocurrent behaviour and stability of NrGO/NiFeTb-LDH@Cu maintain a constant current flow, remaining stable for up to 6 h of continuous light exposure. Notably, the NrGO/NiFeTb-LDH@Cu hybrid displays an incident photon-to-current efficiency (IPCE) of ~13%, attributed to the superior photocurrent density arising from the rapid electron transfer facilitated by the plasmonic Cu nanoparticles incorporated into the coupled system. Hence, this approach can be considered an effective strategy for enhancing PEC performance in NrGO/NiFeTb-LDH-based photoelectrocatalysts.

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Pseudocapacitive nanoparticles of cadmium hydroxide – cobalt hydroxide composite electrodes for supercapacitor application

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Present work explores the growth of unique cadmium hydroxide–cobalt hydroxide nanoparticles using a two-step method through chemical bath deposition followed by ion exchange at room temperature. The detailed explanation of crystal structure with functional group analysis has been confirmed through XRD and FTIR analysis. The nanoparticle-type morphology with elemental composition was carried out through FESEM and EDX analysis. The three-electrode configured electrochemical analysis revealed the areal capacitance of 512.97 mF/cm² at 5 mVs⁻¹ through cyclic voltammogram study. The galvanostatic charge–discharge (GCD) analysis was used to obtain an areal capacitance of 176.4 mF/cm² at a current density of 8 mA/cm². The electrochemical impedance analysis was plotted to give solution resistance (R_s) and charge transfer resistance (R_t) of 1.87 and 7.85 Ω /cm², respectively. The electrode's long-term stability with good cyclic retention was carried over 5000 CV cycles, showing an 80.36% retention rate.

Keywords: FESEM,EDX,

Oxy – hydroxyl manganese tungsten anchored on multi-walled carbon nanotubes with hybrid surface architecture towards flexible solid-state device grade supercapacitor

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Hydroxylated mixed phase tungsten oxide comprising manganese tungsten oxide (MnWO) and hydroxyl manganese tungsten oxide (MnWO·(OH)) were grown on MWCNTs for the first time using simple, low cost, and low temperature chemical bath deposition (CBD) method. The resulting film exhibited distinctive hybrid morphology, characterized by cuboidal and micro-flower nanoarchitectures. Monoclinic and cubic crystal phases with floral and cuboidal morphology were observed in field emission scanning electron microscopy (FE-SEM). In aqueous 1 M KOH electrolyte, the electrode exhibited a wide operational voltage window of 0.98 V and delivered a high specific capacitance of $2215.34 \text{ F}\cdot\text{g}^{-1}$ (with an areal capacitance of $1063.36 \text{ mF}\cdot\text{cm}^{-2}$) at a scan rate of $2 \text{ mV}\cdot\text{s}^{-1}$. Both surface capacitive and diffusion-controlled charge storage mechanisms were quantitatively analysed. A symmetric flexible solid-state pouch cell was further fabricated using polyvinyl alcohol–LiClO₄ gel electrolyte, extending the voltage window to 1.9 V. The device achieved an impressive specific capacitance of $337.92 \text{ F}\cdot\text{g}^{-1}$ (areal capacitance of $162.20 \text{ mF}\cdot\text{cm}^{-2}$) at $2 \text{ mV}\cdot\text{s}^{-1}$. Moreover, the device exhibited excellent electrochemical and mechanical stability of 90.54% at 5000 CV cycles and 101.40% at 170° bending angle. It achieved maximum energy and power densities of $15 \text{ Wh}\cdot\text{kg}^{-1}$ and $303.88 \text{ W}\cdot\text{kg}^{-1}$, respectively. Its practical viability was demonstrated by powering an LED panel and a miniature DC fan, underscoring its potential for next-generation flexible energy storage applications.

Keywords: CBD,floral,electrolyte

Micro-sampling of dilute analytes using metal-organic framework

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Metal–organic frameworks (MOFs) are crystalline porous material with high surface areas, tunable pore architectures, and chemically functionalizable pore surfaces, making them ideal candidates for selective adsorption and molecular separation. It is feasible predictively design MOF void space, for targeted applications related to capture [1], diffusion [2] and release of specific chemical (isomers) [3]. Recent advances have demonstrated the utility of MOFs in capturing biomolecules and small molecule biomarkers [4], yet integration into microscale devices for low-volume sampling remains challenging. Herein, we present a glass capillary system coated with MOFs via a stepwise growth strategy [5], designed for micro-sampling (<10 μL) and selective enrichment of trace analytes. By leveraging the high adsorption enthalpy and tunable pore chemistry of MOFs, our device facilitates preconcentration of dilute biomarkers, enhancing detection sensitivity for applications in early-stage diagnostics and minimally invasive testing. Demonstrations with ZIF-type MOFs highlight the potential of this approach for efficient biomarker capture, separation, and downstream analysis, bridging a critical gap between MOF materials research and practical biological sensing.

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Keywords: ZIFs, Micro-sampling, Biomarker, Sensing

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Keywords: Bi-functional catalyst, photocatalysis, coin cell supercapacitors, p-n junction

Self-sacrificial template-induced fabrication of sustainable micro-junction towards energy conversion and storage

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Energy storage and conversion remain central challenges in the pursuit of sustainable and green chemistry solutions, attracting increasing interest in recent years. Among emerging materials, heterostructures have gained prominence due to their engineered interfaces, robust architectures, and synergistic charge dynamics; however, the complex interplay between their structure and performance requires deeper investigation. In this study, a novel diode-type interfacial micro-junction based on FeCo-layered double hydroxide (LDH) is synthesized using a self-sacrificial template-induced method. The resulting micro-junction significantly enhances electronic conductivity, enabling efficient charge separation and rapid ion diffusion. Owing to these features, the material exhibits dual functionality in both energy storage and conversion. As a supercapacitor electrode in coin-cell configuration, it delivers an exceptionally high specific capacitance of 1814.14 F g⁻¹ at 1 A g⁻¹, an energy density of 61.6 Wh kg⁻¹, and retains 90.7% of its capacitance after 15 000 cycles, demonstrating outstanding durability. Concurrently, its improved light absorption and facilitated charge transport enable efficient photocatalytic hydrogen evolution with a rate of 577.8 μmol h⁻¹. This work not only advances the development of multifunctional materials for clean energy technologies but also provides new insights for designing high-performance systems for energy storage and conversion.

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From Nano to Wearable: Multimodal Energy Harvesting Using Axially Confined Chalcogenide in Ferroelectric Polymer

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Low-power electronic devices play a pivotal role in the advancement of next-generation flexible electronics with impactful applications spanning artificial intelligence, biosensing, and energy harvesting. Among emerging energy conversion technologies, piezoelectric and pyroelectric nanogenerators have shown great promise for efficiently converting mechanical and thermal energy into usable electrical signals [1]. In this regard, one-dimensional (1D) and two-dimensional (2D) nanomaterials are distinguished by their exceptional characteristics, including high charge carrier mobility and outstanding thermoelectric properties. In particular, 1D semiconducting monochalcogenides such as tellurium (Te) have attracted significant attention as promising materials for piezoelectric, ferroelectric, and optoelectronic applications [2]. In this work, a facile synthesis method is presented for 1D tellurium nanorods (Te-NRs) exhibiting a non-centrosymmetric crystal structure, conferring strong piezoelectric and pyroelectric properties. Axial nanoconfinement within poly(vinylidene fluoride) (PVDF) nanofibers facilitates improved alignment of nanorods for optimized piezoelectric and pyroelectric responses, enabling the fabrication of a high-performance hybrid nanogenerator (HyNG). The resulting HyNG demonstrates a peak-to-peak voltage, V_{OC} , of approximately 8.5 V and a short-circuit current, I_{SC} , of 1.2 . Furthermore, by employing organic PEDOT:PSS/Xyl electrodes, superior photothermal heat localization is achieved compared to traditional metal electrodes, which amplifies the

pyroelectric response and enables the detection of small thermal variations. As a proof of concept, the HyNG was successfully utilized for physiological signal monitoring, highlighting its potential as a self-powered biomedical sensor. The integration of monoelemental Te-NRs with ferroelectric PVDF nanofibers not only enhances device stability but also broadens the operational scope, making the system suitable for mechanical and thermal energy harvesting, infrared sensing, and respiratory monitoring.

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Keywords: 1D-Tellurium, Nanofiber, Hybrid nanogenerator, Healthcare monitoring.

Stability and Thermal Transport Features of Cubic HfO₂ and MgO₂ Monolayers: A DFT Approach

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This study presents a first-principles investigation of the structural, electronic, and thermodynamic properties of single-layer HfO₂ and MgO₂ chalcogenide oxides, using Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) as implemented in the WIEN2k code. The materials are modeled in their respective cubic crystal structures, with HfO₂ crystallizing in the Fm-3m (No. 225) space group and MgO₂ in Pa-3 (No. 205). Structural optimization and energy-volume fitting using the Birch-Murnaghan equation of state confirm the mechanical stability of both single-layer configurations. Electronic structure analysis reveals that both compounds exhibit indirect electronic transitions. The valence bands are primarily derived from oxygen

2p orbitals, while the conduction bands are influenced by Hf 5d and Mg 3s states, respectively. The clear separation between these bands suggests the possibility of tuning electrical conductivity through external doping or strain, which is significant for improving thermoelectric performance. This study highlights the promising nature of 2D HfO₂ and MgO₂ as thermally stable, tunable oxide materials. Thermodynamic properties such as heat capacity, entropy, bulk modulus, Debye temperature, and thermal expansion coefficient were examined over a wide temperature range. The results indicate that HfO₂ exhibits higher lattice stiffness and thermal stability, whereas MgO₂ shows greater entropy and thermal expansion, suggesting enhanced anharmonic phonon interactions. These characteristics are favorable for materials intended for heat dissipation or thermoelectric conversion at elevated temperatures. Their favorable mechanical and electronic features, combined with the ability to tailor thermal behavior, make them strong candidates for future applications in thermoelectric devices and energy-harvesting technologies. The suitability of their thermoelectric behaviour for energy conversion technologies is also analyzed.

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Keywords: Density functional theory (DFT), Thermoelectric materials, Chalcogenide, thermodynamic properties

Neuromorphic Performance of Organic FEFETs Using Novel Ferroelectric Compounds: Towards In-Memory Computing

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Neuromorphic computing architectures that mimic brain-like information processing offer significant advantages for energy-efficient artificial intelligence and in-memory computing. This work investigates the neuromorphic performance of organic FEFETs fabricated using novel solution-processable ferroelectric materials based on metals. Electrical characterization demonstrates stable ferroelectric switching with well-defined memory windows. Neuromorphic measurements reveal long-term potentiation/depression (LTP-LTD), spike-timing dependent plasticity (STDP), and paired-pulse facilitation/depression (PPF-PPD), confirming synaptic emulation capabilities. Memory retention and endurance testing show device longevity, while performing suitable handwritten pattern recognition. These insights will directly contribute to advancing neuromorphic device technology and accelerating the development of energy-efficient in-memory computing systems that can overcome the limitations of conventional von Neumann architectures.

Keywords: Ferroelectric materials, organic field-effect transistors, neuromorphic devices, solution processing, synaptic plasticity

Piezopolarization Induced High Rate Solar N₂-to-NH₃ Conversion in Vacancy Engineered AgCu-Modified BiFeO₃

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The sustainable production of ammonia via the nitrogen reduction reaction (NRR) under ambient conditions remains a formidable challenge due to the inertness of N₂ molecules and sluggish reaction kinetics. In this work, we present a multifunctional photocatalyst

vacancy-engineered AgCu-modified BiFeO₃ (AgCu@BiFeO₃) that harnesses the synergistic effects of piezopolarization, photocatalysis, and the localized surface plasmon resonance (LSPR) effect to achieve enhanced solar N₂-to-NH₃ conversion. The incorporation of Ag and Cu nanoparticles introduces strong LSPR absorption, extending visible light harvesting and promoting hot electron generation, while simultaneously activating surface plasmon-driven charge transfer. Vacancy engineering induces oxygen deficiencies within the BiFeO₃ lattice, creating active sites for efficient N₂ adsorption and activation. Furthermore, the intrinsic piezopolarization of BiFeO₃ under mechanical stress induces an internal electric field, which dramatically enhances charge separation and directs photogenerated electrons toward the NRR pathway. The resulting composite exhibits a significantly improved NH₃ yield rate of 278 $\mu\text{mol g}^{-1} \text{h}^{-1}$ under simulated solar irradiation and mild ultrasonic agitation. This study underscores a rational design strategy integrating plasmonic modulation, defect engineering, and piezoelectric polarization to unlock the full potential of advanced hybrid photocatalysts for green ammonia synthesis.

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Keywords: piezopolarization, Photocatalysis, NRR, Vacancy Engineering, LSPR Effect.

Deciphering the S-scheme Carrier Transfer Dynamics at CdS-ZnCdS Heterojunction for Enhanced Hydrogen Evolution: An Ultrafast Approach

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The S-scheme heterojunction proves its proficiency by segregating photogenerated carriers at high redox potentials, paving the way for environmental remediation by effectively enhancing photocatalytic performance. Here, we have combined two broadly absorbing photocatalysts, CdS and ZnCdS (ZCS), to fabricate an S-scheme contact interface via an *in situ* hydrothermal method. The introduction of ZCS resulted in improved hydrogen evolution rates for the CdS/ZCS heterostructure.

Photoluminescence studies highlighted suppressed recombination, suggesting a staggered-type band alignment. XPS spectroscopy revealed the underlying mechanism for directional carrier migration pathways at the heterojunction. Femtosecond transient absorption spectroscopy was employed to gain insights into the photophysical properties of the photoexcited carriers, and the normalised kinetic profiles indicate interfacial electron transfer from CdS to ZCS upon illumination.

The cascade of spectroscopic characterisations confirms the S-scheme charge separation mechanism at the CdS/ZCS heterojunction for enhanced photoactivity. This work emphasises rational interface engineering to correlate ultrafast carrier dynamics with the catalytic capacities of photocatalysts, thereby enabling the design of a progressive S-scheme-based photocatalyst.

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Keywords: S-scheme, Heterojunction, Hydrogen Evolution, XPS spectroscopy.

Symposium: D

2D h-BN Reinforced Protein Scaffold/Films for Biomedical and Thermoelectric Applications

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2D nanomaterials such as hexagonal boron nitride (h-BN) combined with protein-based scaffolds and biopolymer thin films offer notable

advantages in biomedical engineering[1]. When embedded with hydroxyapatite, proteins like collagen render them osteoconductive, bioactive scaffolds suitable for bone tissue regeneration[2]. Similarly, chitosan-based nanocomposite thin films integrated with 2D nanomaterials enhance mechanical strength, functional properties, and biocompatibility, including enzyme immobilization and UV-blocking abilities [3]. These composite systems are suitable for applications in biosensing, wound healing, bone repair, and controlled drug delivery, making them highly valuable for next-generation biomedical and flexible electronic devices [3,4].

In this study, we propose two distinct types

of biomaterials: a 3D scaffold and a biopolymer thin film, each designed for multifunctional biomedical and energy applications. The scaffold was fabricated using hydroxyapatite, collagen, and pristine hexagonal boron nitride (h-BN), targeting a porous structure appropriate for drug delivery. FTIR analysis revealed characteristic functional groups, suggesting successful component integration, while SEM morphology confirmed a highly porous architecture suitable for operative drug loading and sustained release, as verified using ciprofloxacin.

In parallel, an eco-friendly nanocomposite thin film was fabricated by combining pristine BN and hydroxyl-functionalized BN (h-BNf) into a chitosan-collagen matrix via the solution casting method. The addition of h-BNf prominently improved the mechanical strength, reaching 20.1 MPa. Surface wettability experiments confirmed a shift from hydrophobic behavior (contact angle: 93.4°) in h-BN-loaded films to more hydrophilic behavior (73.1° – 85.3°) in h-BNf-based films, which is advantageous for biomedical interfacing. FTIR analysis revealed the presence of functional groups and active bonding between the nanofillers and biopolymers, while SEM morphology indicated uniform filler dispersion and improved film morphology in h-BNf-based films. Conformational studies further evidenced molecular-level interactions between collagen and h-BNf, corresponding to enhanced film stability.

The nanocomposite films also demonstrated extensive thermal stability and UV-blocking characteristics. To assess thermoelectric functionality, the films were integrated into a thermoelectric generator (TEG) setup, and current–voltage curves were recorded under a temperature gradient, confirming their energy conversion potential. Biocompatibility assays further confirmed that both the scaffold and thin films are safe for biomedical use, highlighting their potential as sustainable, multifunctional materials for next-generation thermoelectric and bioelectronic devices.

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Keywords: Collagen, Hexagonal Boron Nitride, Biomedical, Thermoelectric material

Sericin–polyethylene glycol hydrogel as an innovative excipient for progesterone delivery: formulation development, characterization, molecular docking and toxicity evaluation

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The development of biocompatible and sustainable drug delivery systems is a growing area of interest in biomedical research [1]. Sericin (SS), a silk-derived protein, possesses numerous advantages such as biocompatibility and non-toxicity, making it a promising material for hydrogel fabrication in biomedical and pharmaceutical fields [2]. Progesterone (PRO), a natural hormone essential for regulating key physiological functions such as preparing the female body for conception and pregnancy, faces challenges due to its low water solubility [3]. Therefore, effective formulations are required to enhance its solubility and bioavailability. In this study, a hydrogel was synthesized through a simple blending method at room temperature using SS and polyethylene glycol (PEG), a widely used synthetic polymer in biomedical fields. The primary objective of this formulation was to

achieve controlled release of PRO, thereby improving its therapeutic efficacy and patient compliance. Various characterization techniques, including Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), nuclear magnetic resonance spectroscopy (NMR), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA), were employed to evaluate the hydrogel's structural, morphological, and thermal properties. The swelling behaviour and drug release kinetics of the hydrogel were analysed, confirming its suitability for controlled delivery of PRO. Furthermore, toxicity studies demonstrated the hydrogel's significant non-toxic behaviour. Most importantly, the synthesized hydrogel offers potential applications in the biomedical field due to its simple fabrication process, biocompatibility, and effective controlled release of hydrophobic drug PRO, making it a promising candidate for controlled drug delivery systems.

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Keywords: Sericin; Polyethylene glycol; Progesterone; Drug delivery system

Development of a Simple and Efficient Method for the Micropatterning of Silk Fibroin

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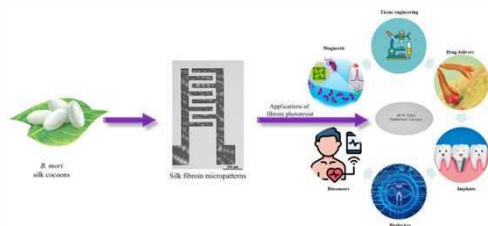
Microfabrication has been a widely used technique for the development of microelectronics due to its applications in health monitoring, diagnosis, treatment, and drug delivery [?]. Conventional materials for fabricating such devices often have biocompatibility issues, leading to tissue rejection. Thus, there is a shift towards using naturally available materials that are biodegradable, exhibit less tissue rejection, and require non-toxic chemicals for microfabrication.

Silk fibroin (SF) has been employed in tissue engineering, drug delivery, wound healing, and tissue repair [?]. Its high biocompatibility, low immunogenicity, and excellent mechanical stretchability make it an attractive candidate for microfabricating electrodes [?]. Current microfabrication technologies, such as 3D bioprinting, X-ray lithography, and E-beam lithography, provide lower resolution and are not scalable for industrial production. This study aims to develop a photolithography-based microfabrication method for SF that is scalable, nanoscale-capable, and sustainable.

Methacrylated SF (SFGMA) patterns were microfabricated on silicon wafers and characterized for their chemical, morphological, mechanical, cytotoxic, and biological properties. FTIR and NMR analyses confirmed methacrylation of SFGMA by detecting methacrylate groups in SFMA. The microfabrication process involved using 0.7% SFMA solution with 0.2% Irgacure and exposure to UV light for 40 s. Pattern development was performed using LiCl for 1.5 hrs.

Mechanical testing of SFGMA films revealed a Young's modulus of 2689.29 MPa in the dry form and 0.01 MPa in the wet form. Cytotoxicity studies showed cell viability of 136.9% for SF and 148.9% for SFGMA. Morphological analysis of cell adhesion assays demonstrated that SFMA promotes cell proliferation. Biodegradability studies using proteinase K enzyme indicated that SF underwent 100% mass loss by the 9th day, whereas SFMA underwent 50% mass loss by the 15th day.

These observations indicate that modified SF exhibits enhanced mechanical properties, good stretchability, and improved surface characteristics. Overall, this study demonstrates an optimized method for microfabricating SFMA using photolithography, resulting in improved mechanical, morphological, biological, and degradation properties.



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Keywords: silk fibroin, methacrylation, photolithography, microfabrication, biocompatible

Ligand-Dependent Regulation of Copper Nanocluster–DNA Binding and Its Relevance in Targeted Biology

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This study explores how surface ligands influence the binding interactions between copper nanoclusters (CuNCs) and deoxyribonucleic

acid (DNA), with an emphasis on their potential in biotherapeutic applications. CuNCs were synthesized using three chemically distinct ligands, tannic acid (TA), chitosan (Cht), and cysteine (Cys), and characterized through a range of analytical techniques. Binding interactions were examined at both ensemble and single-molecule levels using various spectroscopic and microscopic approaches. Results revealed that cysteine-stabilized CuNCs (Cys-CuNCs) interact with DNA via a one-step binding process, while tannic acid- (TA-CuNCs) and chitosan-coated CuNCs (Cht-CuNCs) follow a two-step mechanism. Circular dichroism studies further demonstrated the effect of CuNCs on the structural integrity of DNA. Fluorescence correlation spectroscopy provided single-molecule insights, showing distinct interaction pathways for each type of CuNC. Notably, Cht-CuNCs promoted DNA base accumulation and exhibited weak intermolecular interactions, suggesting their strong potential in gene therapy. In contrast, TA-CuNCs and Cys-CuNCs preserved DNA structure and demonstrated good biocompatibility, making them more suitable for bioimaging and biosensing applications. Overall, these findings highlight the pivotal role of surface ligands in modulating DNA–nanocluster interactions and underscore their relevance in advancing targeted biomedical applications.

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Keywords: silk fibroin, methacrylation, photolithography, microfabrication, biocompatible

Wound Healing Activity of Nanocellulose-Graphene Oxide Hydrogel by Excision Model in Rats

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Chronic wound management, with its significant burden on the healthcare sector, has become a challenge that demands the development of advanced treatments. This study presents a systematic in vivo assessment of the wound healing efficacy of bacterial nanocellulose (BNC) hydrogels formulated with graphene oxides (GOs) derived from graphite (G-GO) and coal (C-GO). In vitro findings have indicated that C-GO hydrogels with edge functionalization facilitate enhanced cell migration capacity[1].

To validate these findings in vivo, the excision wound healing model on Wistar Albino rats was used. Animals were divided into five groups, each consisting of six rats: Group I (untreated), Group II (BNC hydrogel), Group III (BNC-G-GO hydrogel), Group IV (BNC-C-GO hydrogel), and Group V (standard treatment with commercially available povidone iodine ointment). Daily treatment was administered for

28 days, and wound contraction rates were monitored.

Upon completion of the study, skin tissues and internal organs (brain, heart, liver, and kidneys) were collected for histological analysis and molecular studies. Data were expressed as mean $\pm$ SD of six animals per group and statistically analyzed using Student's paired t-test and one-way analysis of variance (ANOVA), with $P < 0.05$ considered significant. Histological analysis of healed skin tissues revealed increased collagen deposition, promoted epithelial regeneration, and reduced inflammation[2].

In vivo biocompatibility assessment of the liver, kidney, heart, and brain revealed no abnormalities. Additionally, molecular analysis confirmed that C-GO hydrogels resulted in a significant reduction in interleukin (IL)-6 and matrix metalloproteinase (MMP)-9 markers, indicating their effectiveness in reducing inflammation. In conclusion, BNC-C-GO hydrogel accelerated wound healing and exhibited superior performance compared to BNC and BNC-G-GO hydrogels, aligning with the standard treatment, while maintaining a moist wound environment. These findings highlight the critical importance of optimized GO synthesis and demonstrate the effectiveness of BNC-C-GO hydrogels in wound healing, suggesting their valuable potential for advancing regenerative medicine.

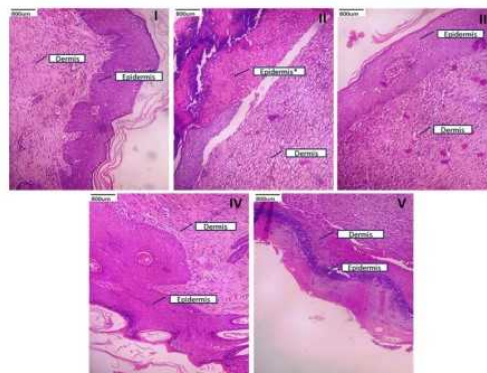


Figure 62: Histology of skin tissue after 28th day from the healed area of the wound showing dermis and epidermis of (I) control animal; (II) animal treated with BNC-Hydrogel; (III) animal treated with G-GO Hydrogel; (IV) animal treated with C-GO Hydrogel; (V) animal treated with commercial povidone iodine

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Keywords: Wound Healing; Bacterial Nanocellulose (BNC); Coal-derived graphene oxide(C-GO); Hydrogel; In vivo studies.

MXene as a new candidate for Photoacoustic Transducers for High-Resolution Diagnostic Imaging

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Photoacoustic imaging (PAI) combines optical excitation with ultrasonic detection, enabling high-resolution and deep-tissue visualization that overcomes the penetration limits of conventional optical techniques. This makes PAI a valuable tool for early detection of solid cancer, rheumatoid arthritis, inflammation due to an unknown disease, etc. Although the physicochemical properties of MXene have been widely investigated, their exploration in the fields of sensing and device applications is in its infancy, with many potential opportunities yet to be realized. Hence, in this work, it is demonstrated that MXene, an emerging 2D material, is a potential candidate for the development of a high-frequency and broad-bandwidth pure MXene-based photoacoustic transducer, capable of high resolution diagnostic imaging. These findings establish MXene as a promising material platform for next-generation photoacoustic transducers and biomedical imaging devices.

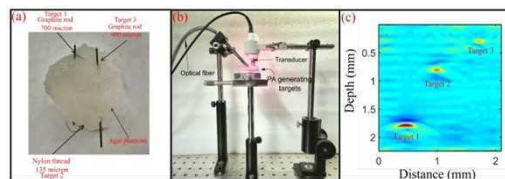


Figure 63: Figure (a) shows the photoacoustic imaging of an agar phantom containing three different targets: (1) a graphite rod (700 μm), (2) a nylon thread (135 μm), and (3) a graphite rod (400 μm). Figure (b) depicts the photoacoustic setup used for signal detection, consisting of a laser, a transducer, and the phantom used for imaging. Figure (c) presents the reconstructed image of the phantom, where all three targets are clearly visible, highlighting the importance of the pure MXene-based transducer for high-resolution photoacoustic imaging.

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Keywords: MXene; Photoacoustic Imaging; High-frequency; Broad-Bandwidth; Transducers.

A Covalent Organic Framework-Based Triad Sensor for Early Turner Syndrome Diagnosis

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Turner Syndrome (TS) affects ~ 1 in 2000 female births, resulting from partial (mosaicism) or complete (monosomy) loss of an X chromosome. It contributes to $\sim 10\%$ of miscarriages, with only 1% of affected fetuses surviving to term. TS leads to diverse complications, including short stature, ovarian insufficiency, sensory loss, type-2 diabetes, cardiac and renal abnormalities, and tumors such as gonadoblastoma, making clinical differentiation from other conditions challenging. While cell-free DNA analysis and ultrasound can aid detection before birth, confirmatory tests such as karyotyping, exome sequencing, chorionic villus sampling, and amniocentesis remain necessary, and no point-of-care test currently exists for rapid TS diagnosis.

Here, we present a non-invasive, multiplexed sensor targeting TS-specific genes—*SHOX*, *ARSE*, *XIST*, and *VAMP7*—using oligonucleotides conjugated to a thiol-modified imine-based covalent organic framework (COF) probe. Binding of target genes induces aggregation-induced emission (AIE), which is measured via fluorescence spectroscopy. Functionalization with gold nanostars (AuNS) enables near-infrared absorption and a photoacoustic (PA) response, while UV-Vis and PA spectroscopy characterize agglomeration. These spectral changes allow quantification of gene expression, facilitating TS diagnosis through detection of genetic dysregulation.

This platform demonstrates promise for early screening and intervention in TS by enabling rapid, accurate molecular sensing.

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Keywords:

Stimuli-Responsive Defective $\text{NaNbO}_{3-x}/\text{CuIn}_2\text{S}_{4-y}$ Binary Hybrid for Photo-Chemodynamic Antimicrobial–Antibiofilm Therapy

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The alarming rise of microbial and biofilm-associated infections necessitates the development of multifunctional materials capable of dual-action therapy. In this study, we report a novel stimuli-responsive dual-defective binary hybrid, comprising oxygen-vacancy (O_v)-rich NaNbO_3 (NNO_3) and sulfur-vacancy (S_v)-enriched CuIn_2S_4 quantum dots (CIS_{4-y} QDs), engineered for multifunctional applications in photo-chemo-dynamic antimicrobial and antibiofilm therapy. Upon light irradiation, the binary hybrid exhibits pronounced antimicrobial and antibiofilm activity against standard *Escherichia coli* (*E. coli*) and *Staphylococcus aureus* (*S. aureus*) through reactive oxygen species (ROS)-mediated cell damage.

The material demonstrates a self-supplied H_2O_2 generation ability of $1938 \mu\text{mol h}^{-1} \text{g}^{-1}$ within 1 hour. The deliberate introduction of oxygen and sulfur vacancies enhances charge-carrier separation, light absorption, and ROS generation. Under IR irradiation, the $\text{NNO}_{3-x}/\text{CIS}_{4-y}$ heterojunction facilitates efficient electron transfer and photoinduced Fenton-like reactions, amplifying ROS-mediated oxidative stress.

This dual-mode approach not only disrupts bacterial membranes but also effectively penetrates and eradicates biofilms through enhanced peroxidase-mimicking activity. The hybrid exhibits potent antibacterial activity against both Gram-positive and Gram-negative bacteria, along with significant inhibition of biofilm formation and dispersion. Our findings demonstrate that defect engineering and heterostructure formation synergistically elevate antimicrobial efficacy, providing a promising avenue for treating persistent infections and addressing antibiotic resistance.

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Keywords: S-scheme pathway, PDT, CDT, antimicrobial-biofilm therapy

Activated Carbon/PNIPAM Nanocomposite Hydrogel Derived from Rice Straw for Effective Dye Adsorption

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Synthetic dyes are persistent and hazardous pollutants widely discharged into water bodies from industrial sources, and their removal is crucial for environmental sustainability. In this study, we present a green and efficient strategy for dye adsorption using a novel nanocomposite hydrogel composed of poly(*N*-isopropylacrylamide) (PNIPAM) and activated carbon (AC) derived from rice straw. Rice straw, an abundant agricultural byproduct, was pyrolyzed and chemically activated with KOH to obtain porous, graphitized AC with an average particle size of 26 nm. The AC was then incorporated into the PNIPAM matrix via free-radical polymerization to form a stable, elastic hydrogel. Comprehensive material characterization was performed using PXRD, ATR-IR, Raman spectroscopy, FESEM, HRTEM, and BET analyses.

The nanocomposite hydrogel was evaluated for its adsorptive performance toward two common synthetic dyes, rhodamine B (cationic) and congo red (anionic). The hydrogel exhibited high adsorption efficiencies of 71% and 94% for rhodamine B and congo red, respectively, within 24 hours. Maximum dye loading capacities were 208 mg g⁻¹ for rhodamine B and 282 mg g⁻¹ for congo red. The adsorption mechanism is attributed to synergistic effects involving π - π interactions, electrostatic forces, and enhanced dye diffusion through the hydrogel's porous network.

This research demonstrates a sustainable valorization of agricultural waste into a multifunctional adsorbent for wastewater remediation. The PNIPAM/AC nanocomposite hydrogel offers a cost-effective, reusable, and scalable solution for removing diverse dyes from aqueous environments, contributing to the development of responsive materials for environmental applications.[1]

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Keywords: activated carbon; nanocomposite hydrogel; dye adsorption; rice straw.

Rapid detection of fatty acids using gemini lipidoid based sensor: Application in quality checking of edible oils and profiling bacterial drug resistivity

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Fatty acids are vital biomolecules that serve as a primary energy source, contribute to the stability and fluidity of cell membranes, and play a key role in regulating gene expression, thereby influencing processes such as metabolism, inflammation, and overall cellular function.[1] Cis-unsaturated fatty acids offer significant health benefits, whereas trans fats pose health risks by elevating low-density lipoprotein (LDL) levels and increasing the likelihood of chronic diseases. Hence, the rapid and efficient detection of different fatty acids based on their geometric orientation and hydrophobic strength is essential for monitoring health and metabolic processes. Traditional detection methods rely on fatty-acid derivatization followed by gas chromatography-mass spectrometry (GC-MS), procedures that are often complex, costly, and time-consuming.

In this work, we designed a gemini lipidoid (GL) platform consisting of a polyethylene glycol (PEG)-based hydrophilic backbone and two identical hydrophobic units on either side. The hydrophobic components were meticulously designed (after extensive screening) to prevent GL from self-assembling independently, ensuring that vesicle-like structures form only in the presence of an external hydrophobic source. The extent of vesicle formation varied depending on the nature of the hydrophobic source, *i.e.*, different fatty acids, and these differential interactions between the fatty acids and GL were monitored using various hydrophobic dyes. In a multichannel sensor array employing three different dyes,[2] six fluorescence signals were collected through excimer formation and Förster resonance energy transfer (FRET). These signals were subjected to linear discriminant analysis (LDA) to generate canonical patterns for six different analytes, enabling successful discrimination of *cis*, *trans*, and saturated fatty acids with 100% classification accuracy.

Furthermore, the method was applied for detecting fatty acids in serum media at biologically relevant concentrations. As the sensor platform could distinguish between *trans* and *cis* fatty acids, it was further utilized for the successful identification of *trans*-fat contamination in edible oils. Additionally, the method was extended to detect drug-resistant bacteria based on variations in their lipid content.

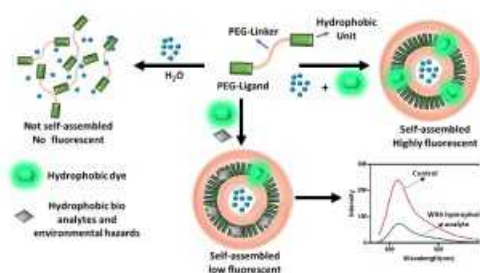


Figure 64: Schematic representation of vesicle formation from gemini lipidoid assisted by external hydrophobic source

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Keywords: LDL, PEG, chromatography.

Design and development of Chitosan-Based Conductive Hydrogels for Biocompatible and Self-Healing Human-Machine Interfaces

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Biopolymer-based conductive hydrogels have broad applications in various advanced bioelectronic devices, such as flexible wearable electronics, artificial biological soft tissues, and implantable biomedical devices. For such applications, these hydrogels must exhibit good mechanical strength, stability, electrical conductivity, and flexibility. However, most available hydrogels fail to integrate all these essential features, which limits their performance in engineering and biological systems.

In this study, a conductive hydrogel was synthesized from chitosan, acrylamide, and maleic anhydride through a sequential synthesis process carried out in a single reactor. The resulting hydrogel exhibits inherent conductivity, self-healing capability, biocompatibility, and antioxidant properties. FTIR analysis confirms successful hydrogel formation through chitosan modification, as indicated by characteristic peaks corresponding to crosslinking and the formation of amide and ester bonds. XRD analysis reveals a crystallinity index of 30.56%, confirming the semi-crystalline nature of the hydrogel. SEM photomicrographs show an interconnected porous network with an average pore size of 550 nm and a porosity of 77.45%. TGA results indicate sequential thermal stability.

The hydrogels demonstrate good biocompatibility toward the 3T3-L1 cell line, exhibiting 84.46% cell viability after 24 h. Moreover, they display minimal haemolytic activity of 3.57% at higher concentrations, and DPPH assay results confirm significant antioxidant behavior. The prepared hydrogel also functions effectively as a stylus or touchscreen pen for mobile-device

interaction, serving as a human-machine interface (HMI). These findings suggest that the developed hydrogel is a promising candidate for advanced bioelectronic applications, including biosensors, biomedical devices, and flexible bioelectronic systems.

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Keywords: Biopolymer, Conductive Hydrogel, Self-healing, Biomedical device

How Dental Biomaterials Wear under Saliva and Temperature Changes

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This study examines the influence of artificial saliva (Nanochemazone) and elevated temperatures (up to 70 °C) on the wear and frictional behavior of orthodontic biomaterials, using human cadaver canine teeth as a biological benchmark. Six materials were evaluated: alumina fiber-based composite, zirconia molar crown, sintered alumina bar (sintered at 1550 °C), sodium tripolyphosphate (STTP)-coated alumina, cadaver canine teeth, and artificial saliva (Nanochemazone). The phase composition was characterized using X-ray diffraction (XRD), while tribological behavior was assessed with a PON tribometer under simulated oral conditions. Surface morphology and microstructural changes after wear were analyzed through scanning electron microscopy (SEM), and the surface roughness of the wear tracks was measured using a profilometer.

The objective was to investigate how saliva exposure and temperature variations—mimicking oral conditions during food intake—affect the tribological performance of these materials in orthodontic applications. Findings revealed that elevated temperature significantly influences the coefficient of friction, with STTP-coated alumina exhibiting superior wear resistance at higher temperatures. The zirconia crown showed low frictional values but displayed temperature-dependent wear behavior in the presence of saliva. Comparison with natural canine teeth indicated distinct wear mechanisms, underscoring the importance of biomimetic design in the development of advanced dental materials. Overall, this study provides critical insights into enhancing the durability and biocompatibility of orthodontic biomaterials under realistic oral conditions.

References:

Keywords: Alumina composites; Artificial saliva; Coefficient of friction; Tribology.

Cost-Effective porous metal oxides and mixed metal oxides coatings for Ti- 6Al-4V biomedical implants

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Titanium metal and its alloys, such as Ti-6Al-4V, are widely used for fabricating biomedical implants due to their excellent mechanical and antibacterial properties. However, these implant materials require surface modifications to address limitations in corrosion resistance and biocompatibility. In this regard, porous coatings are essential, as they significantly promote the survival of bone-forming cells (osteoblasts) and support tissue ingrowth into the implant. This leads to improved implant stability and a reduced risk of implant loosening.

This study focuses on modifying Ti-6Al-4V surfaces using a cost-effective bottom-up sol-gel method to prepare TiO₂, Ta₂O₅, and TiO₂-Ta₂O₅ nanocomposites in 1:2, 1:1, and 2:1 ratios. A spin-coating technique with optimized

rotational speed and deposition time was employed to deposit uniform films onto the Ti–6Al–4V substrate. Microstructural characterization of the prepared films revealed porous architectures with varying pore sizes, uniform film thickness, and stoichiometric formation of the desired metal oxides and their composites.

A detailed corrosion study was conducted in Hank's solution and simulated body fluid (SBF). Tafel plots and electrochemical impedance spectroscopy (EIS) demonstrated high corrosion resistance, with I_{corr} values on the order of 10^{-8} A cm⁻² for the coated samples. Pull-off adhesion testing confirmed excellent film-to-substrate adhesion, effectively overcoming one of the most common limitations of sol-gel-derived coatings.

The prepared porous films also exhibited enhanced cell viability and attachment compared to bare Ti–6Al–4V when tested with MG-63 (cancerous osteoblast) and NIH3T3 (fibroblast) cell lines over 1, 3, and 7 days. Overall, this study highlights the efficacy of the cost-effective coating technique and demonstrates the superior surface properties of TiO₂, Ta₂O₅, and TiO₂–Ta₂O₅ composite films relative to bare Ti–6Al–4V implants.

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Keywords: Tantalum pentoxide (Ta₂O₅); Titanium dioxide (TiO₂); sol-gel; cost-effective.

Laser-scribed graphene microelectrode for non-enzymatic glucose detection

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Electrode geometry plays a pivotal role in electrochemical measurements, as the electrochemical reaction occurs over the surface area of the electrodes. Transforming the sensing area geometry from macro- to micro-/nano-scale dimensions can elevate the Faradaic current over

the capacitive current[1]. Herein, we fabricated graphene-based microelectrodes using direct laser writing, a unique technique for scalable fabrication of graphitic carbon materials known as laser-scribed graphene (LSG), and implemented these electrodes for glucose detection. LSG possesses specific properties such as high specific surface area, excellent electrical conductivity, and tunable surface chemistry, making it highly suitable for electrochemical sensing applications[2].

Furthermore, the catalytic activity of LSG was enhanced by the conformal attachment of highly catalytic copper oxide (CuO) nanoparticles via a simple dip-coating process followed by sunlight-assisted oxidation. The resulting non-enzymatic glucose sensor (CuO/LSG) demonstrated excellent reproducibility and long-term stability, exhibiting a linear glucose detection range from 1 μ M to 70 mM with high sensitivity and a low detection limit.

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Keywords: Microelectrode, laser-scribed graphene, glucose, sensitivity, catalytic activity

Development of Physically Crosslinked PVA–Gelatin Hydrogels Loaded with Piperine for Enhanced Wound Healing Applications

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This work presents the synthesis of physically crosslinked polyvinyl alcohol (PVA)–gelatin hydrogels incorporated with piperine at different concentrations (2%, 4%, and 6%) using the freeze–thaw method for wound healing applications. PVA and gelatin were selected due to their excellent film-forming ability, hydrophilicity, biodegradability, and biocompatibility. Piperine is a bioactive alkaloid derived from black pepper, known for its

well-documented anti-inflammatory, antimicrobial, and antioxidant properties, making it a promising phytochemical for wound care formulations. The freeze–thaw process provided a safe and effective means of hydrogel formation by inducing physical crosslinking without the use of cytotoxic chemical crosslinkers.

The resulting hydrogels were clear, elastic, and exhibited high mechanical strength and structural stability. Swelling studies confirmed the hydrophilicity of the hydrogels, which is essential for maintaining a moist wound environment conducive to healing. Scanning electron microscopy revealed a porous morphology that supports nutrient diffusion and fluid exchange. Biological assessments demonstrated that the presence of piperine significantly enhanced the antimicrobial and antioxidant activities of the hydrogels in a concentration-dependent manner. Specifically, the 5% and 3% piperine-loaded formulations showed superior performance compared to the 1% formulation, as evidenced by larger zones of inhibition against wound-associated pathogens and higher free-radical scavenging activity.

Overall, the developed PVA–gelatin–piperine hydrogel system represents an effective and affordable wound dressing strategy, offering a biocompatible platform with enhanced therapeutic potential resulting from the synergistic interaction between the polymer matrix and the incorporated phytochemical.

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Keywords: Freeze-Thaw ; Gelatin ; Hydrogel ; Piperine

Synthesis of ZnO-TiO₂ Heterojunction Nanocomposite for Dye Removal and CO₂ Adsorption

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The current scenario of environmental risk driven by persistent pollutants demands sustainable materials with multifaceted applications. ZnO and TiO₂ are well-known photocatalytic materials, but their performance is often limited by electron–hole pair recombination[1] and low CO₂ adsorption capacity. In this work, we incorporated zinc acetate and TiO₂ nano-precursors to form a heterojunction nanocomposite [2] under a consistently low temperature (65 °C) without the use of any external capping agent.

The resulting material was characterized using several advanced analytical techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer–Emmett–Teller (BET) surface area analysis, X-ray photoelectron spectroscopy (XPS), Fourier-transform infrared (FTIR) spectroscopy, and UV–Vis spectroscopy. XRD analysis confirmed the presence of both ZnO and TiO₂ nanoparticle phases. SEM revealed surface morphology, while TEM enabled visualization of the formed heterojunction. XRD and XPS further validated the crystallographic structure and elemental states of the material, respectively.

The synthesized heterojunction nanocomposite was subsequently utilized for adsorption and combined adsorption–degradation of the cationic dye methylene blue and the anionic dye Congo red. Using photoluminescence spectroscopy (PL) and time-resolved photoluminescence spectroscopy (TRPL), the reaction mechanism was proposed. The degradation pathway was further elucidated using LC–MS analysis, where degradation intermediates were identified from aliquots of the reaction mixture. Additionally, the heterojunction nanocomposite was evaluated for CO₂ adsorption, and its adsorption behavior was systematically studied.

In conclusion, the prepared nanocomposite demonstrated dual functionality, exhibiting ef-

ficient dye removal as well as CO₂ adsorption capability.

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Keywords: Nanocomposite; Heterojunction; Dye Removal; CO₂ adsorption

Silk Fibroin-PEDOT: PSS Composite Coatings for Enhanced Stimulation Performance of Silver Microelectrodes with Neural Interfaces

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The long-term success of neural stimulation devices critically depends on the development of microelectrodes that exhibit high electrochemical performance, mechanical durability, and biocompatibility with neural tissue. Conventional metal electrodes, such as platinum and iridium, while stable, suffer from low charge injection limits (CIL) and elevated impedance, particularly at microscale dimensions, leading to inefficient stimulation and potential tissue damage. Conductive polymers such as poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) offer enhanced electrical performance, but their long-term mechanical and structural stability remains a challenge due to swelling, cracking, and delamination in aqueous environments. To address these limitations, we developed a hybrid conductive composite by integrating PEDOT:PSS with silk fibroin functionalized with glycidyl methacrylate (SF-MA), a biomaterial known for its superior biocompatibility, flexibility, and mechanical adaptability.

In this study, we report that silver microelectrodes (70 μm diameter) coated with the SF-MA/PEDOT:PSS composite form covalent bonds with the silver surface, enabling superior electrochemical performance and biological stability. Our investigations reveal that impedance was substantially reduced (from 120 Ω for bare silver to 100 Ω after coating) at the clinically relevant frequency of 1 kHz, and the charge storage capacity (CSC) increased approximately six-fold—from 47 $\mu\text{C}/\text{cm}^2$ to 294.2 $\mu\text{C}/\text{cm}^2$ —compared to uncoated electrodes. Additionally, the CIL was significantly enhanced, allowing safer and more efficient neural stimulation. These improvements are attributed to the synergistic effects of the composite: PEDOT:PSS facilitates rapid charge transfer and high conductivity, while SF-MA enhances film adhesion, structural integrity, and resistance to mechanical and electrochemical degradation.

Surface morphology analysis confirmed that the composite formed a uniform, hydrogel-like layer that increased the effective surface area and promoted ion exchange. The SF-MA component contributed to improved anchoring of the PEDOT:PSS network, mitigating the delamination and structural collapse commonly observed in pure PEDOT-based coatings. Furthermore, the composite exhibited stable electrochemical performance under repeated stimulation cycles, indicating its suitability for chronic applications.

In summary, this work presents a novel, biocompatible, and electrochemically robust electrode coating based on SF-MA and PEDOT:PSS. The composite significantly enhances key performance parameters—impedance, CSC, and CIL—while offering improved mechanical stability and biocompatibility. These findings support the potential of SF-MA/PEDOT:PSS composites for developing next-generation neural microelectrodes capable of chronic, safe, and efficient electrical stimulation, marking a significant advancement in neural interface technology.

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Keywords: Neural Stimulating Probe, Biomaterial, Conducting Polymer, PEDOT: PSS, Silk Fibroin

Active Particles Knead Three-Dimensional Gels into Porous Structures

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Colloidal gels are prime examples of functional materials exhibiting disordered, amorphous, yet metastable forms. They maintain stability through short-range attractive forces and their material properties are tunable by external forces. Combining persistent homology analyses and simulations of three-dimensional colloidal gels doped with active particles, we reveal novel dynamically evolving structures of colloidal gels. Specifically, we show that the local injection of energy by active dopants can lead to highly porous, yet compact gel structures that can significantly affect the transport of active particles within the modified colloidal gel. We further show how passive interfaces play a topologically significant role in interacting with active particles in 3D. The results open the door to an unexplored prospect of forming a wide variety of compact but highly heterogeneous and percolated porous media through active doping of 3D passive matter, with diverse implications in designing new functional materials for active ground remediation.

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Keywords: Colloidal gels, Active Matter, Persistent Homology

Biomaterialization, Antifungal, Antibacterial and Cytotoxicity Investigation of Larnite/Nano Titania Composite via Sol-gel Combustion Method

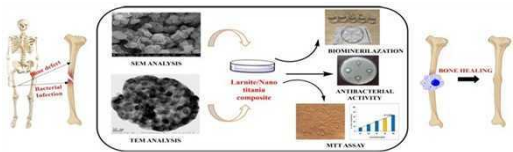
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Biomaterials research represents an imminent vocation in modern healthcare. The multidisciplinary nature of biomaterials necessitates collaboration among scientists, engineers, and physicians. Scientists design and synthesize the material, engineers fabricate prostheses, and physicians study the response of natural tissues to artificial biomaterials implanted in the body. Globally, it has been reported that approximately 60% of artificial bone substitutes are composed of bioceramics. Consequently, there has been significant interest in exploring various bioceramics for bioactive fixation of artificial implants. The most critical criteria in biomedical materials for hard tissue engineering are biocompatibility and mechanical stability.

The present work focuses on the synthesis and characterization of a Larnite/nano titania (TiO₂) composite (Ca₃SiO₄/TiO₂) via a facile sol-gel assisted combustion route using L-alanine as fuel, reported here for the first time. Analytical techniques such as powder X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), and scanning electron microscopy (SEM) were employed to study the characteristic behaviour of the synthesized composite. High-resolution transmission electron microscopy (HR-TEM) and selected area electron diffraction (SAED) using an FEI-Tecna G2 20S-TWIN at 200 kV were used to examine particle morphology and crystallinity. In-vitro biomaterialization was evaluated on the scaffold surface after 9 days of immersion in simulated body fluid (SBF). Additionally, the antibacterial properties of four Larnite/nano titania samples were tested against *Staphylococcus aureus*, *E. coli*, *Klebsiella pneumoniae*, and *Bacillus subtilis* using the well diffusion method. Cytotoxicity was assessed via the MTT assay [3-(4,5-dimethylthiazolyl)-2,5-diphenyltetrazolium bromide] to evaluate in-vitro biocompatibility.



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Keywords: Bioceramic composite, antimicrobial, cytotoxicity, biomineralization, sol-gel combustion

Active Ornstein-Uhlenbeck particle under stochastic resetting

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We investigate the dynamics of an inertial active Ornstein-Uhlenbeck (AOU) particle in the presence of stochastic resetting. Using a renewal approach, we compute the mean displacement, mean square displacement (MSD), and position probability distribution in both overdamped and underdamped regimes in both viscous and viscoelastic mediums. In contrast to a normal AOU particle in a viscous medium, the MSD of an AOU particle with resetting displays an initial diffusive and long-time or steady state nondiffusive behavior. The steady-state MSD has a dependence both on the resetting rate and the persistent duration of activity. It decreases with an increase in the resetting rate and approaches zero for an infinitely large resetting rate. Moreover, steady-state MSD has a nonmonotonic impact on the duration of activity. These results are further supported by the position probability distribution function, which initially grows wide with increasing activity time, shows a maximum spread, and narrows with further increase

in the duration of activity. Moreover, when the particle is suspended in a viscoelastic medium, the MSD interestingly develops an intermediate-time plateau due to the memory effect, and the plateau depends on the strength of the viscoelasticity and the viscoelastic relaxation time. With an increase in strength of the viscoelasticity, the width of the plateau increases and the MSD suppresses. Further, for slow viscoelastic relaxation, the memory effects become weaker and the intermediate plateau disappears. Similarly, for slow resetting, the intermediate plateau is more distinct, whereas fast resetting results in the system approaching steady state faster, overcoming the intermediate plateau in MSD. This emerging behavior might be due to the complex interplay between the resetting mechanism, activity, and memory effects. Finally, our analytical results are in good agreement with numerical simulation.

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Keywords: Active Ornstein-Uhlenbeck particle; Stochastic Resetting; Viscoelastic medium

Bioconversion of Paper Mill Wastewater into Bioplastic using a Novel strain isolated from soil

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This study aims to valorise paper mill wastewater as a bacterial substrate for the production of the bioplastic polyhydroxybutyrate (PHB). A novel *Bacillus* strain was isolated from soil and demonstrated a strong potential to metabolise wastewater for PHB accumulation. The strain was taxonomically confirmed by 16S rRNA gene sequencing, and the data were submitted to GenBank. Fermentation parameters were optimised to maximise the PHB yield by the *Bacillus* strain using wastewater as the sole carbon source.

Extraction of PHB was performed using a probe sonicator instead of the conventionally used sodium hypochlorite. A comparative analysis of the produced PHB with a standard sample using FTIR, XRD, and NMR confirms the polymer's chemical identity and crystallinity. These analyses further reveal that the produced polymer possesses physicochemical properties comparable to industrial PHB.

Keywords: Waste valorisation; wastewater; Polyhydroxybutyrate (PHB); *Bacillus* strain.

Rhodamine-Appended Fluorescent Probe for Selective Iron Sensing and Theranostic Applications of the corresponding Iron Complex

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The development of functional organic molecules for advanced biological and environmental applications is of growing interest, particularly in the context of metal ion sensing and therapeutic delivery. In this context, the rational design of suitable organic probes offers

a promising strategy. Rhodamine-based fluorescent compounds have been widely studied due to their well-defined absorption and emission properties.

In this study, a rhodamine-based fluorescent probe (RhB-A) was designed and synthesised, exhibiting strong fluorescence upon excitation at 400 nm. The probe displays exceptional selectivity toward Fe³⁺ ions, with significant fluorescence quenching observed even in the presence of 16 competing metal ions, yielding a limit of detection (LOD) of 0.195 ppm in a semi-aqueous medium, which is well below the WHO guideline value of 0.3 ppm for iron in drinking water.

Furthermore, the Fe³⁺-coordinated complex was isolated in single-crystalline form, and structural analysis confirmed a 1:2 metal-to-ligand binding ratio. UV-Vis absorption studies further validated a reversible binding mechanism, supporting the probe's potential as a reusable sensor. Importantly, the synthesised Fe³⁺ complex was successfully applied in treating lead-induced anaemia in *Drosophila melanogaster*. Biological evaluation demonstrated that the complex effectively delivers iron to deficient cells in a controlled and targeted manner.

Thus, both the rhodamine-based probe (RhB-A) and its iron complex exhibit strong potential for dual applications: as a selective Fe³⁺ sensor and as a therapeutic agent for anaemia management.

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Keywords: Schiff base, LOD, fluorescent probe, *Drosophila*

Symposium: E

Fused Hollow Cathode Plasma Source for Plasma-Enhanced Chemical Vapor Deposition of Carbon Nanostructures

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One special form of carbon that interests many scientists worldwide is the sp^2 -hybridized carbon. Among the various sp^2 -hybridized carbon nanostructures, graphene oxide (GO) and carbon nanotubes (CNT) are particularly important materials for multiple applications, including quantum physics, nanoelectronics, energy research, catalysis, and the engineering of nanocomposites and biomaterials. While conventional synthesis techniques such as Brodie, Staudenmaier, and Hummers (for the synthesis of GO) and arc discharge, laser ablation, and chemical vapor deposition (CVD) (for the synthesis of CNTs) are well established, they are unrelated to each other and material-specific. This work focuses on developing an adaptable and unified plasma-enhanced chemical vapor deposition (PECVD) process for the synthesis of both GO and multi-walled CNTs by controllably varying plasma parameters. The primary aim of this work is to study the fundamental role of plasma in the controlled deposition of the nanomaterials. Optical Emission Spectroscopy (OES) is employed to diagnose the plasma and determine key parameters such as electron temperature (T_e) and electron density (N_e). By correlating these parameters with the resulting material characteristics, we gain critical insights into the underlying synthesis mechanisms. This process would be advantageous in low-temperature material processing, high growth rates, and controlled nanostructure formation for these functional materials with tailored properties for targeted applications.

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Keywords:

Ex-situ XRD Analysis of Phase Transitions in P2-Type $\text{Na}_{0.67}\text{Ni}_{0.33}\text{Mn}_{0.67}\text{O}_2$ for Symmetric Na-ion Batteries

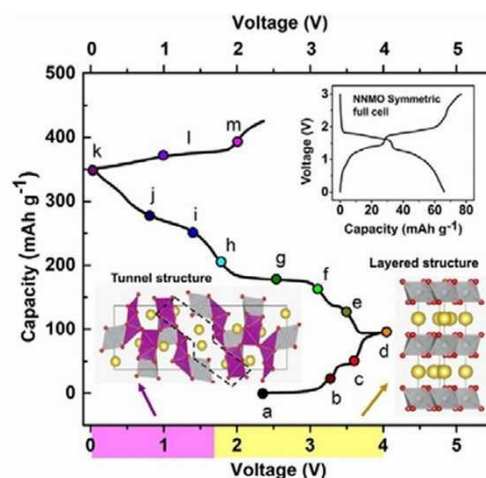
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P2 type $\text{Na}_{0.67}\text{Ni}_{0.33}\text{Mn}_{0.67}\text{O}_2$ (NNMO) is a well-established layered oxide cathode material for sodium-ion batteries, valued for its broad electrochemical stability window, favourable specific capacity, and robust structural integrity during cycling. Interestingly, NNMO exhibits bipolar electrochemical behavior, attributed to the redox activity of both Ni and Mn ions, enabling its application as positive and negative electrodes in symmetric sodium-ion cells. In this study, we systematically investigated the structural evolution of NNMO during electrochemical cycling between 0.01 V and 4.0 V using ex-situ X-ray diffraction (XRD) and Rietveld analysis to assess its viability as a bipolar electrode. Our results reveal a reversible phase transition from a hexagonal layered structure to an orthorhombic tunnel-type framework during the $\text{Mn}^{4+}/\text{Mn}^{3+}$ redox process (1.8 V–1.4 V), which facilitates enhanced Na^+ intercalation. The reversibility of this structural transformation demonstrates the potential of NNMO for use in symmetric full-cell configurations.



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Keywords: Na-ion batteries, ex-situ XRD, phase transition, bipolar materials

Raman at the Frontier of 2D Materials Research

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Two-dimensional (2D) materials have attracted significant attention owing to their tunable structures, diverse electronic properties, and potential in next-generation energy and electronic devices. Among the various characterization tools, Raman spectroscopy stands out as a highly sensitive and non-destructive technique capable of probing vibrational, structural, and electronic features of layered materials. Its ability to distinguish crystal phases, defect densities, and interlayer coupling makes it indispensable in the exploration of 2D systems. In this contribution, I will present Raman spectroscopic investigations of two representative families of 2D materials: transition metal dichalcogenides (TMDCs) and MXenes. For TMDCs, the focus will be on molybdenum disulfide (MoS₂), which exists in multiple polymorphic forms including semiconducting 2H, metallic 1T, and mixed-phase 1T/2H structures. Raman spectroscopy provides distinct fingerprints for each phase, enabling precise identification of structural transitions, electronic modifications, and their correlation with material performance. The analysis of frequency shifts, peak broadening, and intensity variations sheds light on how these phases influence lattice dynamics and defect-induced modifications. In parallel, I will discuss Raman studies on niobium carbide (Nb₂C), a MXene synthesized through selective etching of the parent Nb₂AlC MAX phase. Raman spectra play a crucial role in confirming the successful removal of Al layers, revealing changes in local bonding environments, and identifying surface terminations that strongly impact electrochemical behavior. By correlating Raman features with structural and electronic properties, this

work demonstrates how the technique provides a comprehensive understanding of phase, composition, and functionality, thereby advancing the rational design of 2D materials for energy and electronic applications.

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Keywords: Raman, 2D Materials, TMDCs, Mxene

Thermal phonon induced resonant Fano interaction in V₂O₅ under off-resonant excitation

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Understanding electron-phonon interactions, particularly Fano resonance, is critical for optimizing materials for optoelectronic applications. Raman spectroscopy serves as a powerful tool to probe these interactions in materials like orthorhombic V₂O₅ microcrystals. This study investigates the B_{1g}/B_{3g} Raman mode at approximately 702 cm, revealing an asymmetric Raman line-shape indicative of Fano resonance under 532 nm resonant excitation. Through carefully designed wavelength- and temperature-dependent Raman measurements, we demonstrate that off-resonant excitation can also induce an asymmetric Fano line-shape at elevated temperatures, driven by sufficient thermal phonon populations in V₂O₅. These thermal phonons act as a mediator, facilitating quantum interference between discrete phonon states and the electronic continuum. A non-linear temperature dependence of the Fano coupling parameter is observed, highlighting the dynamic role of thermal phonons. We propose a quantum mechanical framework to explain the temperature-dependent Fano resonance under off-resonant conditions, offering insights into tailoring electron-phonon interactions for enhanced optoelectronic performance.¹

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Keywords: Resonant Fano, Thermal phonon, V_2O_5 , Electron Phonon interaction

Estimating dielectric function of quantum dots

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Kramers-Kronig relations are frequently used for estimating the refractive index from the absorption coefficient and vice-versa. Absorption spectrum of a material is a conveniently measurable experimental quantity, so it is used for estimating refractive index in this poster. Quantum dot absorption spectrum is measured and converted to refractive index by a home developed Matlab program, based on the subtractive Kramers-Kronig relations. The measured refractive index is compared with the experimental refractive index data of quantum dots, measured via spectroscopic ellipsometry. The validated Matlab program generates the refractive index spectrum with absorption co-efficient as the input. Using this program, our team plans to build a database of optical materials for future research.

Keywords: absorption, refractive index

Advanced Corrosion Protection Using In-Situ Synthesized Fe/Mg-Doped Polyaniline-Polyimide Composite Coating

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Metal-doped polyaniline (PANI) is a promising material for anticorrosion coatings due to its ability to passivate the metal surface and potentially release corrosion inhibitors. In this study, an in-situ synthesized metal-doped polyaniline-polyimide (PANI-PI) composite coating is developed to enhance corrosion resistance [1][2]. Herein, two different types of metals are doped with PANI, such as iron (F1-PANI, F3 PANI, F5-PANI) and magnesium (M1-PANI, M3-PANI, M5-PANI) with different weight percentages. The incorporation of metal dopants into the polyaniline enhances the passive film formation on metal substrates, reducing localized corrosion and increasing the charge carrier mobility within the polymer matrix, improving electron transfer kinetics in electrochemical applications. To prepare polyimide composites, in-situ polymerization of polyamic acid (PA) and metal-doped PANI (PA, PANI/PA, F5 PANI/PA, M5-PANI/PA) have been performed. Further, it is coated on cold rolled cold annealed (CRCA) grade steel substrate and cured to prepare polyimide composite coatings. The polyimide matrix synergistically improves the coating's conductivity, adhesion, and barrier properties. Polyimide ensures thermal and mechanical stability, while polyaniline provides active corrosion inhibition through redox behavior[3][4]. Electrochemical impedance spectroscopy (EIS), potentiodynamic polarization studies, and salt spray tests confirm the superior anti-corrosion performance of the synthesized coating. Electrochemical studies revealed that the F5-PANI/PI composite exhibited a higher I_{corr} at 82.90 nA and a corrosion rate of $37.87 \text{ e}^{-3} \text{ mpy}$. In contrast, the M5-PANI/PI composite showed the lowest corrosion current at 32.70 nA and a corrosion rate of $14.94 \text{ e}^{-3} \text{ mpy}$ among all the coated samples, indicating superior corrosion protection performance. The metal-doped polyaniline-polyimide composite exhibits higher charge transfer resistance, reduced corrosion current density, and prolonged durability in aggressive environments as compared to normal PANI/PI.

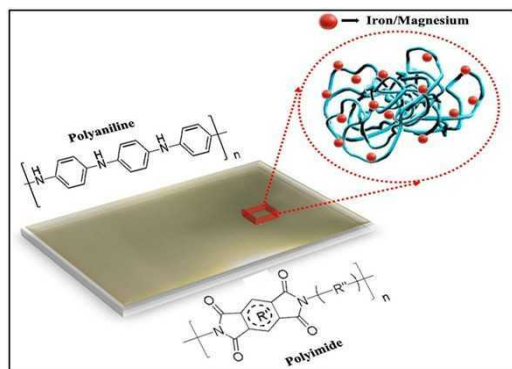


Figure 65: Schematic representation of metal-doped PANI/PI composite on steel substrate.

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Keywords: Polyaniline; composites; In-situ polymerization; Anticorrosion.

Symposium: F

Self – Sterilizing Nanofiber Air filter for PM_{2.5} Filtration

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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.

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Keywords: Electrospinning; PM particles; Air filtration; Anti-bacterial activity

The Age hardenability and Colour differences of 22k gold micro alloyed with Sc, Zr and some rare earth elements

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India has one of the largest gold jewellery markets in the world, reflecting the deep affinity Indians have for gold. 22k gold is occupying the major portion of it and the recent surge in gold price globally, has increased the demand for light weight and hard gold. The regular 22k gold has Cu and Ag as alloying elements with 5.8 wt% and 2.5 wt% respectively and is having a hardness of 85-90 HV (Vickers Scale). Increasing the hardness to 150 HV allows 20 to 30% weight saving in cast, hand-made and studded jewellery with high strength. In the present work we have attempted to improve the hardness of 22 karat gold by micro-alloying with some transition elements along with some rare earth elements via age hardening treatment (precipitation strengthening). The peak aging time and temperature was optimized through the aging kinetics studies. The colour of the hard- 22 karat gold was measured using CIE lab spectrophotometer, reflectivity using UV-Visible reflectance spectrometer and Hyper Spectral Imaging, and compared with that of the existing regular 22 karat alloy. It is observed that at micro-addition levels, the transition elements efficiently age hardens Au at shorter time. The a^* and b^* values of most alloys were very close to the regular 22k alloy and the brightness (l^*) of the alloys were correlating with the UV-VIS reflectance spectrometer analysis.

Keywords: age hardenability, hard gold, rare earth elements, CIE lab spectrophotometry

Tarnish Resistance Mechanism in Ag-4Cu-2.5Zn-1Ge novel Alloy: A Comprehensive Experimental and Computational Study

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Silver and its alloys undergo tarnishing with time, which is a black stain on its surface which diminishes the luster. The reaction of atmospheric Sulphur with Silver causes the formation of Ag_2S compound that gives the black colour. Developing a tarnish resistant silver alloy was attempted by many researchers by alloying silver with oxidizing elements that form a passive oxide layer on the surface and prevent the Ag_2S formation. The element germanium is proven to provide better tarnish resistance to sterling silver alloy (92.5wt.% pure) which is commercially exploited and available under the trade name of Argentium© However the mechanism behind its tarnish resistance behaviour is still unknown. In the present work, the tarnish resistance behavior of silver alloy containing copper, zinc, germanium, and boron was investigated. The alloys were prepared by melting and casting route, followed by passivation heat treatment (PHT) to create the oxide layer. Accelerated tarnish test was carried out to the alloy as a function of time to investigate its tarnishing behavior. The temperature for PHT was optimized using Thermogravimetry Analysis (TGA) for various isothermal durations. And to more accurate the time and temperature of PHT were optimized by investigating the passive oxide layer formed systematically using micro-Raman spectroscopy. In our present study high tarnish resistance was obtained for the Ag-4Cu-2.5Zn-1Ge which was confirmed by the light reflectivity measurement used for the samples exposed to accelerated tarnished testing environment. The mechanism behind the tarnish resistance of the present composition was derived using Density Functional Theory (DFT) by comparing sulphide and oxide binding energies (BE) on these alloys. The composition Ag -4.2Cu-2.8Zn 1.4Ge has S_2 (B.E)/ O_2 (B.E) of about 132% which is much less than the ratio of 222% for pure silver.

Keywords: alloys, PHT

Multiple recycled triboelectric nanogenerators for smart waste management

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A multiple recycled triboelectric nanogenerator (MRTENG) derived from mixed plastic waste has been fabricated to achieve an environmentally sustainable energy harvesting device with an increase in lifetime in an order of magnitude. The triboelectric layer is prepared from plastic waste using a novel material design in the presence of a compatibilizing agent derived from e-waste for high stability and mechanical performance. This increases the lifetime of the energy harvester for ten rounds of recycling. The current collector is extracted by high-temperature pyrolysis of segregated mixed plastic waste, depolymerized polyester, and multiple recycled triboelectric layer that acts as a conducting layer in the single-electrode triboelectric nanogenerator. The fabricated device shows high performance and is used as a waste disposal sensor in smart dustbins for digitalizing waste management using machine learning.

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Keywords: Recycling, energy harvesting, triboelectric nanogenerator, plastic waste management

Microstructural Evolution and Magnetic Properties of As Cast and Melt-Spun Co–Zr Alloys

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In this study, the as-cast microstructures and magnetic properties of Co-rich Zr alloys, specifically Co-x at.% Zr (x = 13, 15, 17), were investigated along with their rapidly solidified ribbons of the same compositions. The phase evolution was analyzed using X-ray diffraction, scanning electron microscopy, and transmission electron microscopy. The results showed that the microstructures of the alloys in the as-cast state vary significantly with increasing Zr content, accompanied by a reduction in the volume fraction of the α -Co phase. As a result, the room-temperature magnetization decreases with increasing Zr concentration. A similar trend was observed in the melt-spun ribbons, where the high cooling rate during rapid solidification not only modified the phase evolution but also refined the microstructure. The magnetic properties of the ribbons were found to strongly depend on the relative volume fractions of the constituent phases. Compared to the as-cast alloys, the ribbons exhibited lower magnetization and higher coercivity, the latter being attributed to the finer scale of the microstructure produced under rapid solidification conditions.

Keywords: X-ray diffraction, phase evolution

Structural, Magnetic and Thermoelectric properties of Al-Cu-Fe quasicrystal reinforced at various concentration of Sn and CNT

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We investigate structural, magnetic, and thermoelectric properties of Al-Cu-Fe icosahedral quasicrystals (IQC) reinforced with tin (Sn) and carbon nanotubes (CNT) at varying concentrations. Mechanical milling followed

by controlled annealing was employed to synthesize the composites and to achieve homogeneous dispersion of the reinforcements within the IQC matrix. X-ray diffraction and electron microscopy confirmed phase stability, grain refinement, and uniform distribution of Sn and CNT. The addition of Sn enhanced electrical conductivity by reducing grain boundary scattering, while CNT provided conductive pathways thereby enhancing charge carrier transport. Thermal conductivity was effectively suppressed due to phonon scattering at the interfaces of the reinforcements and the IQC matrix. This interplay between electrical and thermal transport yielded a remarkable improvement in the electrical-to-thermal conductivity ratio (σ/κ) [1]. For Sn-reinforced samples, σ/κ values were observed as 0.0059 S-K/W, 56.06 S-K/W, and 1644.23 S-K/W at 10, 20, and 30 vol% of Sn, respectively, indicating progressive enhancement with increasing concentration. For CNT-reinforced systems, σ/κ values of 20.28 S-K/W and 0.27 S-K/W were obtained at 1 and 2 vol% of CNT, respectively, suggesting that an optimal CNT concentration is critical for maximizing transport performance. Magnetic measurements revealed soft ferromagnetic behavior with low coercivity and retentivity at 300K and 2K. Law of Approach to Saturation (LAS) was applied to evaluate the magnetic anisotropy constant (K) in our system [2]. For IQC, K is $1.2 \times 10^3 \text{ erg/cm}^3$ at 300 K and $1.5 \times 10^3 \text{ erg/cm}^3$ at 2 K. For IQC-Sn composites, K values decreased with increasing Sn concentration: 23.5×10^3 , 14.7×10^3 , and $8.8 \times 10^3 \text{ erg/cm}^3$ at 2 K, and 9.1×10^3 , 6.2×10^3 , and $2.6 \times 10^3 \text{ erg/cm}^3$ at 300 K, for 10, 20, and 30 vol% Sn, respectively. Conversely, for the IQC-CNT system, K values increased with CNT concentration, measured as 11.2×10^3 and $15.510^3 \text{ erg/cm}^3$ at 2 K, and 3.9×10^3 and $6.9 \times 10^3 \text{ erg/cm}^3$ at 300 K, for 1 and 2 vol% CNT, respectively. These results clearly demonstrate that Sn reduces magnetic anisotropy due to dilution of magnetic exchange interactions and enhanced lattice disorder, while CNT enhance it as the CNT-matrix interfaces act as pinning centers and induce structural anisotropy, thereby enhancing magnetic alignment [3]. This reveals a contrasting influence of different reinforcements on the spin dynamics of the system. This observation suggests the presence of competing exchange interactions within the reinforced IQC matrix. These findings demonstrate that the interplay between structural anisotropy, reinforcement type, and concentration critically governs

the coupled thermoelectric and magnetic behavior of IQCs. The results confirm that magnetic anisotropy plays an important role in determining thermoelectric efficiency, particularly in quasicrystalline systems where electron-phonon and spin interactions are strongly interlinked. These findings provide valuable insights for the engineering of multifunctional IQC-based materials with tunable thermoelectric and magnetic properties, making them promising candidates for applications in energy conversion, spintronics, and advanced magnetic devices.

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Keywords: Quasicrystals, ferromagnetism, anisotropy, thermoelectricity.

Study of bubble growth response in VCrFeNiCu High Entropy Alloy

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High Entropy Alloys (HEAs), a novel class of metallic materials leverage the complex interactions among multiple principal elements to achieve remarkable properties [1,2]. HEAs exhibit enhanced mechanical properties due to solid solution strengthening, lattice distortion, and sluggish diffusion effects. The concept of the "cocktail effect" underscores the synergistic benefits derived from this multi-elemental mixture. Generally, Fe based alloys along with other principal elements like Ni and Cr leads to exceptional mechanical strength, thermal stability, and corrosion resistance, resulting in structural applications [3,4]. In this present work,

a five component equiatomic HEA, VCrFeNiCu was chosen considering the properties required for applicability as a nuclear structural material. Vanadium, known for its low induced radioactivity [5] and Cu, which enhances precipitation strengthening in the alloy [6], were chosen. VCrFeNiCu synthesized using arc melting technique was subjected to 5% cold working. Defect recovery studies in the alloy were performed using both positron lifetime and depth resolved positron beam based Doppler broadening measurements. It is well known that Positron Annihilation Spectroscopy is a powerful tool to study defects in atomic level and provides unique insight into the nature, type and distribution of vacancy-type defects [7]. These studies show formation of Cu nano precipitates above 673 K and dissolution of these precipitates at higher temperatures in the cold-rolled sample [8]. In this work, the 5% cold-rolled sample was subjected to He ion implantation and studied using depth resolved Doppler broadening measurements [9] after each isochronal annealing from 300- 1373 K. Here, the bubble growth response in He ion implanted VCrFeNiCu, in presence of the thermally evolved Cu nano precipitates, using positron beam, will be presented.

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Keywords: High entropy alloys; Cu nano precipitates; He bubbles; positron annihilation spectroscopy.

A Novel Melt-Route Approach for the fabrication of uninterrupted and interrupted silver foams for jewellery applications

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A novel approach for the development of silver foams through the melt route has been successfully demonstrated. Silver foam offers reduction in weight and material usage jewellery, while maintaining design flexibility. The foam fabrication was achieved through both uninterrupted and interrupted foaming methods, utilizing carefully selected gas-releasing agents to generate porosity. To control the foaming temperature and improve compatibility with the gas-releasing agents, new silver alloy compositions were designed. An experimental setup with multiple furnaces was developed to address the challenges associated with the high density of silver and to ensure stable processing conditions. Foam stability was further enhanced through the incorporation of ceramic particles as stabilizing agents, whose effectiveness was optimized by tailoring their wettability with the silver. The proposed method enables the reliable fabrication of silver foams in diverse shapes such as idols, articles and jewellery ornaments, highlighting its potential in jewellery and decorative applications. Beyond aesthetics, the approach offers scalability and economic advantages over conventional foam production methods, positioning silver foams as a material of dual importance combining functional performance with commercial potential.

Keywords: Closed cell silver foam, foam stabilization, uninterrupted foaming, uninterrupted foaming, blowing agent, melt route.

Integrated PANI and Carbon Quantum Dots in UiO-66-NH₂ for Superior Conductive and Photoluminescent Sensing Performance

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Semiconductor composites are emerging as multifunctional materials for optoelectronic device applications due to their tunable charge transport and photophysical properties. The integration of redox-active emeraldine Polyaniline (PANI) into an insulating Zr-based metal-organic framework (UiO-66-NH₂), along with carbon quantum dots (CQDs), resulted in a conductivity enhancement of 10,000 times. This significant improvement arises from synergistic interactions between the host MOF and the guest molecules (PANI and CQDs). XPS and FT-IR spectroscopy confirmed that PANI

and CQDs strongly interact with the anchoring groups of UiO-66-NH₂, while *in situ* polymerisation of PANI within the CQD@MOF composite blocked the pores, establishing an effective charge-transfer pathway. Optimisation of the PANI@(CQD@UiO-66-NH₂) composite reduced the resistance drastically, from $7.05 \times 10^8 \Omega$ in the pristine MOF to $7.46 \times 10^4 \Omega$ in composite 2. Beyond electrical enhancement, the composite also demonstrated solvent-dependent photoluminescence behaviour. In the presence of ammonia, the material exhibited pronounced PL enhancement due to strong acid-base interactions with PANI, whereas it showed selective fluorescence quenching toward Pd²⁺ ions among various tested metal ions. This dual response highlights the high selectivity and sensitivity of the composite for both ammonia and palladium detection, establishing its strong potential for multifunctional environmental and chemical sensing applications.

Keywords: Polyaniline, MOF, Carbon Quantum Dots, Conductivity, Ammonia sensing, Palladium quenching.

Symposium: G

Phonon Dispersion in Superconducting NiBi₃ system

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We report a systematic study of NiBi₃ thin films with nanorod morphology grown by co-deposition of Ni and Bi and subsequently modified by 100 MeV Ag ion implantation at varying fluences, with structural, morphological and vibrational characterization. X-ray diffraction establishes the NiBi₃ phase and baseline crystallinity, while SEM clearly shows fluence-dependent nanorod morphological evolution. The observed Raman peaks match DFT-calculated phonon frequencies for NiBi₃, and temperature-dependent Raman measurements reveal systematic, fluence-dependent shifts and broadenings of phonon modes consistent with phonon renormalization and increased lattice disorder. Implantation also induces XRD peak

broadening and strain signatures that corroborate defect accumulation and the morphological changes seen in SEM. By linking DFT-validated phonon assignments and temperature-dependent Raman shifts, we disentangle contributions from modified electron-phonon coupling and enhanced defect scattering. These results demonstrate that high-energy Ag implantation is an effective route to controllably tune lattice dynamics and electronic structure in NiBi₃ nanostructures. We also plan systematic transport (R-T) and magneto-transport (magnetoresistance, critical field) measurements across fluences and temperature to directly correlate the phonon and structural modifications with changes in superconducting properties and magneto-transport behavior, informing strategies for engineering NiBi₃-based nanoscale superconducting devices.

Keywords: ion implanatation, DFT, magnetoresistance

Enhanced EMI Shielding in Flexible Carbon Black/LSMO Reinforced PVDF Composites for Protection Against Electromagnetic Pollution

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Electromagnetic interference (EMI) from external radiation sources can significantly affect the proper functioning of electrical and electronic devices. In military systems, EMI can affect the dependability of weapons, leading to problems including erroneous intelligence, missed targets, and uncontrollable aircraft movements. Long-term exposure to this unwanted electromagnetic radiation has also been associated with negative health impacts; epidemiological studies show that vulnerable groups, especially pregnant women, newborns, and those with pre-existing medical issues, are more at risk. In this context, electromagnetic wave-absorbing materials play a crucial role in mitigating electromagnetic interference (EMI). A novel smart tertiary PVDF–LSMO–Carbon Black composite film was created using a straightforward solvent casting method. In accordance with the observed dielectric behaviour, FTIR studies showed that raising the carbon black content encourages the production of electroactive phases, whereas XRD examination validated the single-phase synthesis of LSMO. Mostly due to Shielding effective absorption (SEA), the CB70 composition (PVDF–10 wt% LSMO–70 wt% CB) demonstrated an impressive total EMI shielding efficiency (SET) of 30.50 dB. The fabrication of layered-structure films also showed a significant improvement in shielding performance, with the three-layered structure achieving SET of 55.56 dB. The results indicate that the layered PVDF–LSMO–CB composites constitute a viable next-generation smart material platform for high-efficiency electromagnetic absorption, effectively mitigating pollution arising from intense electromagnetic radiation.

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Keywords: Flexible; Carbon Black; EMI Shielding; Tensile Strength

Ex-Situ Phase Evolution Study of Indigenous Lanthanum Carbonate Hydrate and Synthesis of Lanthanum Oxide and Lanthanum Hydroxide

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Lanthanum oxycarbonate, lanthanum oxide, and lanthanum hydroxide are known for their environmental and engineering applications, such as their use as a sensing material, catalyst, special optical glass making, and water treatment. These materials are being synthesised by different routes, typically involving lanthanum nitrate for lanthanum oxide and lanthanum hydroxide for lanthanum oxycarbonate. In India, lanthanum carbonate is produced as a byproduct from a mineral called monazite, which can be used as an alternative precursor for synthesising lanthanum oxide. In this work, the single-step processing of lanthanum carbonate is explored and intensively investigated by calcination in the 300–1000 °C range for deriving lanthanum oxycarbonate and lanthanum oxide. In addition, atmospheric exposure studies were conducted to determine the minimum time required to produce lanthanum hydroxide effortlessly. As-synthesised materials were ex-situ investigated by X-ray diffraction, revealing lanthanum oxycarbonate and lanthanum oxide phase stabilisation above 500 °C and 800 °C, respectively. The lanthanum hydroxide phase was first observed upon atmospheric exposure for 6 hours; however, complete conversion occurs within 24 hours. X-ray photoelectron spectroscopy was carried out to observe changes in the doublet peak in lanthanum 3d orbital, which varies from 3.5 eV to 4.4 eV, then to 4.6 eV,

and subsequently to 3.9 eV, further helping in distinguishing the evolved phases during calcination and hydrolysis. In addition, scanning electron microscopy, transmission electron microscopy and UV-visible spectroscopy were used to investigate the as-synthesised materials.

Keywords: Lanthanum carbonate, Calcination, XPS, XRD

MOF-Derived Porous Carbons and Hybrids for Microwave Absorption: A Comprehensive Review

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The prompt development in technology has brought a great convenience to humans. In civil as well as military aspects, the introduction of electronic gadgets, from hand held devices to RADARs, has proven useful. In a war scenario, it becomes crucial to put ships, submarines, and aircrafts out of the sight of RADARs. Hence, Microwave Absorbing Materials (MAM) have generated a world-wide interest to eliminate the potential threats to National Assets. The basic properties that any MAM should have are the microwave attenuation capability, environmental stability, lightweight and wider absorption bandwidth [1–3]. From the conventional carbon materials and ferrites to recently explored Metal Organic Frameworks (MOFs) and MXenes, many materials have shown promising results. MAM should have magnetic as well as dielectric loss to counter the electric and magnetic components of Electromagnetic (EM) waves. MOFs are highly crystalline structures with metal centres coordinated to organic linkers. MOFs have high porosity and surface area that can be tuned to achieve application-specific properties. Fe-, Co-, and Ni-based MOFs are extensively studied for Microwave (MW) absorption because of the intrinsic magnetic properties exhibited by the metal centres. Xiang *et al.* synthesized $\text{Fe}_3\text{O}_4@\text{NPC}$ showcasing a RL of -65.5 dB and a 4.5 GHz electromagnetic absorption bandwidth (EAB) [4]. Huang *et al.* tuned synthesis parameters precisely to obtain different morphologies of the Co-based MOF ZIF-67 and established that different morphologies exhibited different MW absorption [8]. Carbon-based materials have relatively higher complex permittivity

and hence need to be combined with magnetic lossy materials to achieve impedance matching and microwave attenuation [5]. From a synthetic point of view, MOF-derived porous carbon (PC) materials have advantages over conventional carbon/magnetic structures [3]. When pyrolyzed at high temperatures under inert conditions, a metal/carbon composite is generated that retains the unique microstructure of the MOF, with magnetic metal atoms uniformly dispersed, thus improving the absorption performance. By changing the pyrolysis temperature, the crystallinity, degree of graphitization, magnetism, and porous microstructure can be varied to achieve targeted properties [3,5]. Wu *et al.* synthesized Ni/C microspheres by pyrolysis of Ni-based MOF at temperatures 600C, 700C and 800C. PHNiC700 showed an EAB of 3.8 GHz and a Return Loss (RL) of -55.4 dB at a thickness of 1.56 mm, while for PHNiC800 the RL was above -10 dB [6]. Wang *et al.* also investigated the effect of temperature on MW absorption properties by pyrolyzing ZIF-67 at three different temperatures: 500C, 700C and 900C. It was found that the resultant honeycomb-like Co/C composite calcined at 700C exhibited the best performance, giving an EAB of 4.6 GHz and RL of -50.7 dB [7]. MOFs can further be combined with other materials such as MXenes for enhanced microwave absorption properties. Han *et al.* reported a MXene/Co composite that showed an RL of -60.09 dB and an EAB of 9.3 GHz [9]. Hence, MOF-derived porous carbons and MOF-based composites exhibit significant potential for stealth applications due to their tunable structure and excellent electromagnetic absorption properties. Precise control over synthesis parameters enhances their efficiency, making them ideal candidates for advanced defence technologies.

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Keywords: Microwave Absorbing Materials, Metal organic frameworks, Return Loss, Electromagnetic Absorption Bandwidth.

Defect-Driven Anharmonic Phonon Dynamics in Ag-Implanted Bi₂Se₃

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Bismuth selenide (Bi₂Se₃), a prototypical topological insulator, hosts protected surface states under time-reversal symmetry and, together with favorable charge transport, is a promising candidate for visible-infrared photodetection and thermoelectric devices [1]. Here, ~40 nm Bi₂Se₃ films were grown by RF magnetron sputtering; X-ray diffraction and scanning electron microscopy confirm single-crystalline character and smooth surfaces. Temperature-dependent Raman spectroscopy

(80–300 K) was employed to probe lattice dynamics: the 2A_{1g} and 1E_{2g} modes show progressive broadening of the FWHM and red-shifts upon cooling, consistent with enhanced phonon–phonon interactions and anharmonicity in this layered system. Prior theoretical work indicates that intercalation or ion implantation can introduce foreign species into layered lattices while largely preserving the host framework, enabling emergence or tuning of phenomena such as superconductivity and ferromagnetism [2,3]. Motivated by this, films were irradiated with 90 keV Ag ions. Implantation strongly modifies the low-frequency Raman-active modes— notably the breathing- and shear-like interlayer vibrations—which display pronounced anharmonic behavior that is well described by a two-phonon decay channel. Increasing Ag dose produces systematic red-shifts, revealing softening of weak van der Waals interlayer coupling. Room-temperature photoluminescence exhibits an emission corresponding to an indirect bandgap of ≈0.835 eV. These observations demonstrate that Ag implantation effectively tailors both vibrational and electronic properties of (orthorhombic) Bi₂Se₃, with implications for defect-engineered thermoelectric, magnetic, and optoelectronic applications.

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Keywords: Topological insulator; Anharmonic phonon decay

Rare Earth Elements in Coalmine Overburden: Future Possibilities for Recovery

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Rare earth elements and yttrium (REY) are essential for numerous sophisticated technologies, especially in the field of electronics, and are key to the economic development of any nation. Coalmine by-products can be potential precursors to these commodities and other natural resources. Although coal and coal fly ash have been evaluated for REY content, coalmine overburden (OB) or waste has not yet been investigated as a source of rare earth elements. In this study, we analysed coalmine OB samples randomly collected from Tikok colliery of the Makum coalfield. The presence, distribution, and chemical speciation of REY in coalmine OB were characterized employing various sophisticated analytical methods, including X-ray Photoelectron Spectroscopy (XPS), Field Emission Scanning Electron Microscopy (FE-SEM), and High-Resolution Transmission Electron Microscopy (HR-TEM), to shed light on the geochemical behaviour and commercial potential of REY. The XPS spectra display Sc(2p) peaks at 399 eV (Sc), 400 eV (ScN), 402 eV (Sc₂O₃), and Gd(4d) peaks at 140 eV (Gd) and 141.5 eV (Gd₂O₃), predominantly exhibiting a +3 oxidation state [1]. The HR-TEM image shows the presence of mixed-layer minerals at 200 nm with disordered crystal fringes, having d-spacing values of 3.57 Å (002 planes, possible kaolinite, Al₂Si₂O₅(OH)₄), 1.25 Å (304 planes, quartz, SiO₂), and 1.82 Å (220 planes, rutile, TiO₂), showing a strong association with REY [1]. The mean value of REY in the study area is 237.37 mg kg⁻¹ on an entire sample basis, with cerium having the highest concentration (198.23 mg kg⁻¹). Moreover, the concentration of critical REY and the prospect coefficient are both well above 30% and 0.7, respectively, indicating potential sources for REY recovery [2–3]. In this study, we also performed ultrasonic-assisted leaching of REY from OB under different time and frequency conditions, achieving 6–10% recovery of REY.

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Keywords: Overburden, rare earth elements, sustainable recovery, economic potential

Controlled micro and nanodome formation by proton irradiation on ZnTe thin film

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This work investigates the impact of low-energy hydrogen (proton) ion implantation on ZnTe thin films, focusing on the controlled formation of micro- and nanodome (bubble) structures mediated by hydrogen accumulation. By systematically varying the proton implantation doses, the study demonstrates the evolution of surface morphology, crystal strain, and optoelectronic properties of the films, by using characterization techniques including FESEM, AFM, XRD, Raman spectroscopy, and photoluminescence (PL). The controlled formation of domes is correlated with enhanced and tunable PL emission, attributed to the interplay between defect states and bubble-induced strain in the ZnTe matrix. The results reveal an optimal dose range where PL intensity is maximized, alongside observations of changes in crystallinity and the emergence of luminescent features precisely localized at the periphery of formed domes because of the hydrogenated ZnTe matrix. The methodology enables the scalable fabrication of light-emitting arrays and periodic strain fields, opening avenues for nanoscale optoelectronic devices, sensors, and nanoreactor applications. The domes are attributed to hydrogen bobbles, which can be a suitable hydrogen storage application of energy harvesting. Furthermore, the approach is generalized as a potential platform

for strain engineering and device innovation in other 2D materials.

Keywords: optoelectronic, crystallinity, AFM, XRD

Effect of Gamma Irradiation on Radiation Shielding, Thermal and Optical Properties of Bismuth Modified Barium Zinc Borosilicate Glasses

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Shielding materials are essential in areas such as hot cells, nuclear medicine facilities, and radiography laboratories to protect personnel and equipment from the harmful effects of ionizing radiation. Glasses containing heavy metal oxides like BaO, Bi₂O₃, and PbO are considered effective for shielding high-energy gamma radiation due to their high density and good transparency in the visible region [1, 2]. In this study, we report the effect of Bi₂O₃ addition on BaO-ZnO-B₂O₃-SiO₂ glasses for gamma ray shielding applications. Glasses with 0, 5, and 10 mol% Bi₂O₃, designated as BZ0, BZ5, and BZ10, were synthesized by the melt-quench technique. Pre- and post-irradiation in a Co-60 gamma source were characterized for optical and thermal properties. All the glasses were transparent and bubble-free. Density increased from 4.3 g/cm³ (BZ0) to 5.1 g/cm³ (BZ10) with the addition of Bi₂O₃. Shielding parameters were calculated using XCOM. Half value layer (HVL) thicknesses were 3.14, 2.74, and 2.54 cm for BZ0, BZ5, and BZ10 glasses at 1.33 MeV gamma energy. The glass transition temperature (T_g) was measured using the DTA technique and found to be approximately 485°C for BZ10 glass. T_g decreased with increasing Bi₂O₃ concentration in the glasses. UV-Visible data revealed a red shift in the absorption edge with increasing Bi₂O₃ content. Gamma-irradiated glasses showed a color change from transparent to grey for BZ0

and yellow-brown for BZ10, as shown in Figure 1. After gamma irradiation, the absorption spectra showed a redshift in the absorption edge of approximately 76 nm for BZ0, 152 nm for BZ5, and 175 nm for BZ10 glasses. This study demonstrated that glasses with 10 mol% Bi₂O₃ possess better shielding capability, comparable to commercial RS360 and RS520 glasses; however, radiation-induced browning also became more pronounced.

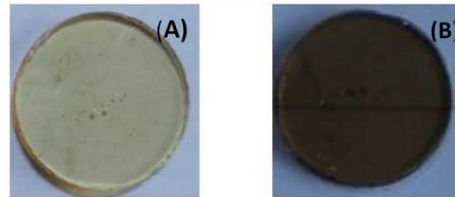


Figure 66: Digital photographs of glass with 10 mol% Bi₂O₃ before (A) and after (B) gamma irradiation.

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Keywords: High Density Glasses, Radiation Effects, Optical Properties

Magnetic Field Simulation for Ion Beam Transport and Implantation: Development using COMSOL

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Ion beam implantation is a widely employed technique for modifying the electrical, structural, and optical properties of materials, particularly in semiconductor device fabrication. However, precise beam control during transport remains a major challenge due to divergence effects and the coexistence of multiple charge states in the ion source plasma. In this work, we present the simulation and design of a beam-line system capable of handling a variety of ion species, including H, He, Ar, Si, and Ge. The plasma generated at the source produces ions of different charge states (e.g., Si, Si²⁺, Si³⁺), which cannot be distinguished by mass or charge alone. An analyzing bending magnet, operating

on the Lorentz force principle, is therefore employed to separate ions according to their mass-to-charge ratio.

Following acceleration, the beam tends to diverge within the transport tube, leading to reduced implantation efficiency and poor dose uniformity at the target. To counter this effect, we investigate the use of electromagnetic quadrupoles arranged in triplets as focusing elements. The simulation work, carried out using COMSOL Multiphysics, emphasizes the ability of quadrupole configurations to alternately focus and defocus the beam, thereby achieving overall confinement and controlled delivery at the target plane. The bending system, currently designed with permanent magnets, faces limitations due to remanence and performance degradation over time. We therefore propose the transition to an electromagnet-based design, which offers stability, tunability, and scalability for bending heavier ions, including rare gases (Ne, Kr, Xe) and higher-mass elements.

Keywords: Analyzing bending magnet; Electromagnetic Quadrupoles; COMSOL Multiphysics

Surface Plasmon Resonance study of Au plasmonic structures with Cr adhesion layers

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Surface Plasmon Resonance (SPR) is an extremely sensitive optical technique for detecting changes in the refractive index near a metal-dielectric interface, making it highly effective for biosensing, chemical detection, and thin-film characterization. In order to stabilize the plasmonic structures on the substrate and to ensure

their robust structural applications, an adhesion layer is often introduced underneath the plasmonic layer. However, the damping effect of such adhesion layers on plasmon modes are not yet fully understood. In this study, we investigate the influence of Chromium (Cr) adhesion layer on the SPR response of the gold (Au) plasmonic structures. Thin films of Cr and Au were sequentially deposited on pre-cleaned glass substrates using electron beam (E-beam) evaporation technique. The thickness of Cr adhesion layer was varied from 2–6 nm keeping the Au layer thickness at 50 nm. The SPR signal was acquired using a low-cost experimental setup prepared in-house employing Kretschmann geometry. The effect of adhesion layer thickness on the angular position and FWHM of the SPR signal was analyzed. As compared to the Au plasmonic structure without adhesion layer, the SPR dip angle shifts within 2% in presence of Cr layer up to 6 nm. Theoretical simulations were also carried out using Fresnel reflection theory for both three-layer (glass–Au–dielectric) and four-layer (glass–Cr–Au–dielectric) systems. Simulation results showed very good agreement with experimental data. The results will help in determining the limiting values of the adhesion layer thickness in order to obtain the SPR signal with acceptable deterioration due to damping.

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Keywords: Surface plasmon resonance; Plasmonic structures; Adhesion layers

Symposium: H

Effect of quenching rate on the electronic properties in Iron Phosphate glass

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Nuclear wastes are hazardous to environment. Especially High level liquid waste (HLW) contains much of the total radioactivity from

the reprocessing of spent nuclear fuel and thus it needs to be immobilized. Vitrification is one of the important methods of immobilization in which the liquid waste elements are mixed with glass melt and then rapidly cooled down to form a solid. Mostly Borosilicate (BS) glasses are used for vitrification all over the world. However there are certain challenges associated such as poor solubility of phosphates, sulphates and heavy metals in BS glasses. Other possibilities like pre-processing or dilution of these waste elements result in increase of volume of the waste form. Thus it is preferable to search for an alternative host matrix which has better solubility of these wastes without compromising other properties that are required for better vitrification. In search of surrogates, studies suggest that iron phosphate glasses are one of the promising candidates for vitrification. It is reported that $60\text{Fe}_2\text{O}_3\text{-}40\text{P}_2\text{O}_5$ has the maximum chemical durability out of all other chemical compositions [2]. Hence in this work we choose to model iron phosphate glasses of composition $60\text{Fe}_2\text{O}_3\text{-}40\text{P}_2\text{O}_5$ as the host glass matrix to explore its properties. For the process of glass forming melt-quench method is one of the most common methods to arrive at the glassy state as it is similar to the experimental procedure. The quenching rate involved in the melt-quench method plays an important role in the microscopic and macroscopic behaviour of glasses. Experimental quench rates range from 1-100 K/s [3] whereas computational methods employ quench rates of the orders of 10^{12} K/s due to time constraints and high computational cost. This significant difference in quench rate necessitates exploring the effect of quench rate on the atomic level properties of the glass. Particularly electronic properties give insights to study the extent of localization of electronic states and also govern many other physical properties of the glass. Thus in this work we aim to understand the effect of quenching rate on the electronic properties of iron phosphate glasses. We use classical Molecular dynamics to generate iron phosphate glass models at different quench rates and we find that some of the Fe-O-P bonds are replaced by Fe-O-Fe bonds at higher quench rates. Also we use DFT to study the effect of quench rate on their electronic properties using the total density of states (DoS), partial DoS, and inverse participation ratio (IPR). Electronic properties of crystal counterpart are also used for comparison with that of glass models. The data analysis will be presented during the conference.

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Keywords: quenching, Iron Phosphate

Orbital Free Density Functional Theory Applied On Solids And Finite Systems

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In the light of recent progress of Orbital-Free Density Functional Theory (OFDFT) based on approximation of non-local (NL) Kinetic Energy Density Functionals (KEDFs), one can foresee the prospects that lies ahead in terms of computational efficiency and dealing with large scale systems. It is important to mention that, accuracy of OFDFT depends on the approximations made for KEDFs. Till now, the most accurate KEDFs are based on NL kernels constructed from the linear response theory of homogeneous electron gas (HEG). In this work, we explore beyond the HEG by employing a more general kernel based on the jellium-with-gap model (JGM). We propose a new NL-KEDF that incorporates several new features¹, such as (i) having the correct low momentum(q) limit of the response function for metals and semiconductors without any modelling term, and most importantly, (iii) parameter-free. The accuracy and efficiency of the proposed JGM NL-KEDF have been demonstrated for several semiconductors and metals. The encouraging results indicate the utility and predictive power of the JGM kernel for NL KEDF developments. We also extend the JGM kernel by making it density-dependent, enabling it to effectively model localized systems such as molecular clusters. Benchmark calculations and the Pauli potential—which satisfies

several critical constraints—demonstrate exceptional agreement with results from the state-of-the-art Orbital-free methods. Additionally, we calculate optical properties using our modified approach. By enhancing the accuracy of NLKEDFs for finite systems, our work advances nanomaterial design and a deeper understanding of nanoscale phenomena.

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Keywords: DFT, finite system, OFDFT, Pauli potential.

Structure, Bonding and Stability of Boron Substituted Tungsten Clusters

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In this study, we investigate effects of boron substitution on the structural, electronic and optical properties of small tungsten clusters using density functional theory (DFT). We construct a series of tungsten boride clusters by replacing tungsten atoms with boron atoms to analyze their stability and other properties. In W_n clusters, structural optimization shows that boron substitution results in geometric distortions. The addition of boron results in shorter bond lengths and a reduction in the cluster's overall symmetry. Within the cluster frameworks, boron atoms preferentially occupy apex or edge positions. The lower atomic radius and stronger electronegativity of boron in comparison to tungsten are the driving forces behind these structural changes. The stability of these clusters has been examined from the systematic analysis of energetics. The average binding energy per atom, HOMO-LUMO gap and chemical hardness increases with boron incorporation, indicating enhanced electronic stability. More negative chemical potentials further confirm greater charge localization and lower reactivity. In the IR spectra, the appearance of high-frequency peaks is attributed to B–B stretching modes, while W–B modes dominate

the mid-frequency region. Fukui functions were also calculated to identify the most reactive sites within each cluster.

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Keywords: Tungsten boride, Clusters, DFT, Stability, IR spectra

Structure-Property Relationship in Triazatruxene Based Donor Materials for Organic Solar Cells: A Computational Study

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In comparison to silicon-based devices, bulk heterojunction organic solar cells (BHJ-OSCs), have gained remarkable attention over the past few years due to their unique features, such as light weight, cheap production costs, mechanical flexibility, and transparency. The advancement of BHJ technology relies heavily on the rational design of donor-acceptor materials that can achieve high power conversion efficiencies (PCE). In this study, we have employed a computational approach to design novel donor molecules for OSCs by incorporating triazatruxene as the electron-rich unit, 2,2-bifuran as the π -spacer, and various

derivatives of (5,6-difluoro-3-oxo-2,3-dihydro-1h-inden-1-ylidene) malononitrile (FCN) as the electron-withdrawing acceptor units.[1] This donor- π -acceptor (D- π -A) molecular framework is selected to achieve optimal intramolecular charge transfer and enhance light-harvesting capability, both of which are crucial for improving photovoltaic properties. Density functional theory (DFT) and time-dependent functional theory (TD-DFT) techniques have been used to study the influence of structural modifications of acceptor units by investigating their geometrical and optical properties. Photovoltaic parameters such as short circuit current density (Jsc), open circuit voltage (Voc), fill factor, and power conversion efficiency (PCE) have also been calculated. Our study reveals that incorporation of 2,2-bifuran as π spacers leads to better planarity and enhanced optical properties. Further, non-covalent interaction (NCI) analysis has been performed for the best-suited donor material and Y6 based non-fullerene acceptor (NFA) to study their interaction and obtain the charge transfer properties.[2] These computational insights not only elucidate structure-property relationships but also lay a rational foundation for experimental synthesis of high-efficiency donor materials tailored for next-generation OSCs.

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Keywords: Triazatruxene; Donor; DFT; Organic Solar Cells (OSCs)

Swarm Intelligence in Quantum Nanorobots for AI-Assisted Detection of Airborne Nanoplastics

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Airborne nanoplastics represent a new category of contaminants, posing significant risks to both the environment and public health. Conventional monitoring techniques are hindered by

inadequate sensitivity, extended analysis duration, and limited spatial coverage. Introducing a swarm-intelligent quantum nanorobot cartridge especially designed for AI-aided detection of airborne nanoplastics can stand as an emerging platform. This nanorobot contains FeO magnetic cores for retrieval, silica/polymer shells for durability, quantum dots for optical signaling, and surface functional groups for selective capture of plastics. They are incorporated into a controlled gel or porous matrix within a sealed cartridge equipped with inlet, outlet, and optical ports. Air from the environment is drawn into the cartridge, allowing the dispersed nanorobot to interact with nanoplastics. The principle of swarm intelligence enhances capture efficiency by experiencing Brownian rotation, airflow-driven tumbling, and density-based clustering. A foraging strategy inspired by honeybees enable dynamic aggregation in areas rich in nanoplastics, resulting in improved interception within sparse three-dimensional airborne environments. The capture of particles is indicated by fluorescence changes by quantum dots, which provide an optical signature for in-situ detection. Followed by sampling, an external magnetic field retrieves the nanorobots into a collection chamber, ensuring total recovery without releasing them back into the environment. Laboratory assessments combine quantum dot fluorescence with single-particle ICP-MS, nano-FTIR, tip-enhanced Raman spectroscopy (TERS), super-resolution fluorescence microscopy, cryo-TEM, and nanoscale XPS to verify the identity and structure of the polymeric residues. AI algorithms also classify the types, quantities, and size distributions of the particles. Informations are normalized to the volume of air sampled and integrated with meteorological data to create detailed spatial maps of nanoplastic pollution. The nanorobots and cartridge can be reused after being cleaned up with solvent and re-functionalized, promoting eco-friendly deployment. This comprehensive workflow merges swarm intelligence, quantum-inspired nanorobotics, and AI-assisted analytics to tackle the persisting issue of detecting airborne nanoplastics. This strategy demonstrates high capture efficiency, reproducibility, and scalability, making it a promising candidate for advanced air quality monitoring solutions.

Keywords: Nanoplastics, Swarm intelligence, Nanorobots, Quantum dots, AI-algorithms.

Role of A cation on the electronic and magnetic properties of the double perovskites A_2TiMnO_6 ($A = Ca, Sr, \text{ and } Ba$): A first principles study

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The unique characteristics of direct bandgap semiconductors make it essential to explore such behavior in perovskite materials. In this study, we present ab initio calculations of the structural, magnetic, and electronic properties of the double perovskite A_2TiMnO_6 by changing divalent cation at A sites with Ca, Sr, Ba. The results show that the antiferromagnetic configuration, with collinear Mn spins aligned along the direction, is energetically preferred. Analysis of the density of states (DOS) and electronic band structure (EBS) confirms that Sr_2TiMnO_6 is a direct bandgap semiconductor with a gap of about 0.98 eV. The material's electronic and magnetic properties are primarily controlled by Mn–O–Mn superexchange interactions.

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Keywords: perovskite materials, DOS, double perovskites

Transition Metal Decorated Boron-Doped Graphene Quantum Dots for Efficient Hydrogen Storage

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The development of efficient hydrogen storage materials remains a critical challenge for enabling hydrogen-based clean energy technologies. In this study, first-principles density functional theory (DFT) is employed to investigate boron (B)-doped di-vacant graphene quantum dots (GQDs) decorated with transition metal (TM = Sc, Co) atoms for hydrogen storage applications. TM decoration strategies are explored to assess the influence of electronic configuration and surface reactivity on hydrogen storage behaviour. B-doping enhances the chemical reactivity of the substrate, while TM decoration facilitates hydrogen adsorption via a combination of Kubas-type interaction and physisorption [1,2]. The TM atoms exhibit strong binding to the B-doped substrate, thereby mitigating metal clustering, a major challenge in TM-based nanostructures. Each system adsorbs up to 12 H_2 molecules, achieving the highest gravimetric capacity for the Sc-decorated GQD system. However, systems containing Co atoms have stronger binding interactions with H_2 compared to those with Sc, due to higher adsorption energies arising from greater d-orbital occupancy and enhanced orbital overlap with H_2 . Among the studied systems, the Co-decorated GQD demonstrates the most promising hydrogen storage behaviour, adsorbing up to 12 H_2 molecules. Thermodynamic analysis and desorption studies further confirm the potential of these materials for reversible hydrogen storage under ambient conditions. These findings suggest the B-doped, TM-decorated GQD as a promising candidate for next-generation hydrogen storage applications.

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Keywords: Hydrogen Storage; DFT; Decoration; Kubas interaction.

Strain-Tunable DMI and Skyrmion Stability in 2D TMDC's

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Two-dimensional (2D) transition metal dichalcogenides (TMDCs) with intrinsic magnetism are emerging as a versatile platform for next-generation spintronic technologies [1,2]. In this work, we explore the influence of biaxial strain on the Dzyaloshinskii-Moriya interaction (DMI) and magnetic anisotropy energy (MAE) in magnetic monolayers of MnTe₂ and FeTe₂ (H phase) using density functional theory (DFT) with Hubbard-U corrections to account for strong electronic correlations. By systematically applying compressive and tensile strains in the range of -6% to +6%, we demonstrate how lattice deformation can significantly tune the magnetic interactions, with dynamic stability verified via phonon dispersion calculations [3]. The modulation of DMI and MAE is primarily driven by the strong spin-orbit coupling (SOC) associated with the heavy Te atoms, which alters the exchange pathways between magnetic ions. Additionally, the coexistence and competition of direct exchange and superexchange interactions lead to complex spin textures, further enriching the system's magnetic behavior. To investigate skyrmion formation and stability, we extract key magnetic parameters from both tight-binding models and first-principles calculations, which are then incorporated into micromagnetic simulations based on the Landau-Lifshitz-Gilbert (LLG) equation [4]. These simulations reveal robust and tunable skyrmions even in the absence of external doping or applied magnetic fields. Our results highlight the pivotal role of strain engineering in controlling topological spin textures in 2D TMDCs, presenting a viable route for the design of low-power, high-density skyrmion-based devices. This study provides fundamental insights into the strain dependent DMI mechanisms and underscores the potential of 2D magnetic TMDCs in strain tunable spintronic applications [5]

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Keywords: DMI, Skyrmion, TMDC.

Orbitronics: Exploiting Orbital Angular Momentum of electrons for Future Spintronic Devices

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As conventional electronics approaches the limits described by Moore's law, new strategies are required. Spintronics, which uses electron's spin rather than its charge, it has been viewed as a possible substitute due to its low-power consumption and non-volatile operation. However, generating and manipulating spin currents typically relies on strong spin-orbit coupling (SOC), which is large in heavy elements. The concept of orbitronics has recently been introduced. Orbitronics uses the orbital angular momentum (OAM) of the electron to transport information rather than spin. Because orbital currents can be produced without the need of heavy metals, lighter and more plentiful materials can be used. In this work, we use first-principles density functional theory (DFT) as implemented in the Vienna ab initio simulation package (VASP)

to investigate the electronic properties of the material. We evaluate the transport properties of the material such as orbital Hall conductivity (OHC) and spin Hall conductivity (SHC) using Kubo formula, with the tight-binding Hamiltonian constructed using maximally localized Wannier functions. The orbital Berry curvature (OBC) and spin Berry curvature (SBC) is also calculated. Our calculations reveal that OHC exceeds the SHC by a significant margin, which shows that the material has a moderate spin Hall effect and a substantial orbital Hall conductivity and strong orbital Berry curvature. These results imply that substantial Hall effects in light-element materials can be achieved without the use of heavy elements. This demonstrates orbitronics' promise as a substitute strategy for upcoming spintronics applications.

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Keywords: Orbitronics, Orbital Hall Conductivity, Spintronics, Density Functional Theory.

Spatial Density of Mayer Bond Order: Distribution of Electrons Shared and Retained by Atoms in Matter

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Total charge in a given system can be partitioned into charges shared among atoms and charges retained by atoms in the basis of atomic orbitals, using the idempotency property of the operator projecting the atomic orbitals on the energy eigen-basis. In this work, we propose an approach to extract the spatial distribution of these partitioned components of the total charge, revealing the spatial extent and shape of the shared and retained charge densities,

thereby opening the possibility of an unambiguous and quantitative association of properties of materials to the ionic and covalent natures of chemical bonding. We demonstrate the effectiveness of the proposed function through three applications: (1) analyzing orbital contributions to the Born effective charge of Ti in BaTiO₃, offering insight into its polarization mechanisms; (2) investigating the evolution of metavalent bonding in GeTe across its rock salt and R-3m phases, revealing how bonding character changes with structure; and (3) analyzing bond breaking through the lens of shared charge, offering a new perspective of bond dissociation. These examples highlight the method's broad applicability for understanding bonding in complex materials.

Keywords: Chemical bonding; Born Effective Charge; Bond dissociation; Metavalent bonding.

Multifunctional properties of alkaline earth-based A₂BTiO₆ (A = Mg, Ca, Sr; B = Hf, Zr) double perovskites: a first-principles investigation for photocatalytic and thermoelectric applications

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This study investigates the multifunctional properties of lead-free alkaline-earth metal-based double perovskites, A₂BTiO₆ (A=Mg, Ca, Sr; B=Hf, Zr). The focus is on evaluating their potential for photocatalytic water splitting, optoelectronic applications, and thermoelectric performance. Structural, mechanical, optoelectronic, water splitting photocatalytic and thermoelectric properties are analyzed. The aim of Hf- and Zr-based double perovskites is to uncover promising candidates that exhibit multifunctional and tunable properties, advancing their integration into next-generation sustainable energy devices. This study employs first principles DFT calculations using the FP-(L)APW+lo method in WIEN2k. Structural and mechanical properties are evaluated using

PBE-GGA, while electronic, optical, photocatalytic properties and thermoelectric properties (BoltzTraP2), including the Seebeck coefficient, electrical conductivity, power factor, and ZT, are computed with TB-mBJ potential. Further, the study confirms the structural and mechanical stability of A_2BTiO_6 ($A=Mg, Ca, Sr$; $B=Hf, Zr$) compounds, supported by negative formation enthalpies, suitable tolerance factors, strong absorption in energy range of 4eV-12eV. Moreover, their bandstructure analysis shows, the valence bands and conduction bands are comprised of O-2p and Ti-3d orbital near Fermi level. Further, A_2HfTiO_6 exhibits wide band gaps (3.39–3.66 eV) and efficient photocatalytic activity (reduction potential < 0 and oxidation potential > 1.23 relative to NHE), while, A_2ZrTiO_6 shows slightly narrower band gaps (3.0–3.3 eV) and excellent thermoelectric performance ($ZT > 3$ at 300K) with chemical potential near Fermi energy. Lastly, the study reveals A_2HfTiO_6 and A_2ZrTiO_6 compounds possess excellent structural stability, wide and tunable band gaps, and strong UV absorption, making them suitable for applications in UV sensors, LEDs, and photocatalytic water splitting. A_2HfTiO_6 shows strong optoelectronic and photocatalytic potential, while A_2ZrTiO_6 exhibits notable thermoelectric performance with high power factors and ZT values. Their lead-free, environmentally friendly nature highlights their promise for sustainable energy technologies, including solar thermal storage and green electronics.

Keywords: Double Perovskites, Photocatalysis, Thermoelectric properties, Wien2k.

Optimization of device parameters in Thermoelectric Generator for Enhanced Waste Heat Recovery in Industrial Systems

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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 modeling (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 150% is achieved with a maximum power output of 10.5W alongside a total potential drop between two ends was observed to be around 14.5V 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.

Keywords: Thermoelectric Generator; waste heat recovery; finite element modelling.

DFT-based computational design of D- π -A- π -D type small molecule electron donors for organic photovoltaic applications

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The performance of organic photovoltaic devices (OPVs) has substantially improved over the past decade, owing to the development of various effective organic electron-acceptor and electron-donor materials, including polymers,

small molecules and fullerenes. The choice of donor (D) and acceptor (A) materials in organic solar cells (OSCs) determines the power conversion efficiency (PCE) and stability of the device.[1] Although PCE improvements in OSCs have been significant, it is essential to deepen our understanding of the structure-property relationships in these organic photovoltaic materials to determine the optimal material combination for the commercialization of OPVs. Density Functional Theory (DFT) is a powerful computational tool that can be effectively used to investigate several functional groups and their molecular arrangements for OPV applications. Small-molecule materials in OPVs offer distinct advantages, including well-defined chemical structures, simple purification, and exceptional batch-to-batch reproducibility.[2] Hence, we have investigated novel small molecule electron donors (SMDs) incorporating amine-based donor units and naphthobisthiadiazole (NTz) acceptor units. DFT and Time Dependent-DFT (TD-DFT) methodologies have been employed to study the light harvesting and charge transfer (CT) characteristics of the designed systems. The molecular orbital energies, band gap, and singlet transition energies, along with their oscillator strengths, have been reported for all studied systems. The qualitative analysis of the CT characteristics for the designed systems have displayed favourable intramolecular charge transfer (ICT) properties for the lowest energy singlet excitation. Our research offers valuable insights into the design and optimization of light-harvesting materials for OSCs.

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Keywords: Small molecule donor (SMD), DFT, TD-DFT, Power conversion efficiency (PCE).

Ultrasonication-Assisted Synthesis of Benzimidazole Derivatives Using Green-Synthesized ZnO Nanocatalyst: Experimental and DFT Insights

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This study effectively synthesized a series of benzimidazole derivatives (S1–S6) by an ultrasonication-assisted approach utilizing ZnO nanoparticles as a catalyst. The ZnO nanoparticles were synthesized using a green method that utilized the leaf extract of *Euphorbia concenensis*, hence promoting an environmentally benign and sustainable process. The generated ZnO nanoparticles were evaluated using X-ray diffraction (XRD) to ascertain their crystalline structure and scanning electron microscopy (SEM) to analyze surface morphology, thereby validating the synthesis of nanostructured ZnO with uniform distribution. The benzimidazole derivatives were further examined by density functional theory (DFT) employing the B3LYP functional, utilizing Gaussian software to analyze their electronic and reactivity properties. Band gap, ionization potential (IP), electron affinity (EA), absolute hardness (η), softness (σ), chemical potential (μ), electronegativity (χ), and electrophilicity index (ω). Among the series, 4-(1H-benzo[d]imidazol-2-yl)-4-phenol exhibited the smallest HOMO–LUMO gap, consistent with enhanced electronic delocalization and increased chemical reactivity relative to its analogues. These theoretical insights enhance comprehension of the structure–property relationship and reactivity trends of the synthesized benzimidazole derivatives, potentially informing their applications in pharmaceuticals, catalysis, and materials science.

Keywords: Benzimidazole derivatives, ZnO nanoparticles, Green synthesis, *Euphorbia concenensis*, DFT.

Dynamical stability of U_3Si : A DFT+U study

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Binary uranium–silicon (U–Si) intermetallic compounds are widely studied as promising accident-tolerant nuclear fuels. They are also valuable systems for investigating 5f-electron correlations, as different U–Si intermetallics exhibit varying U–U distances and correlation strengths. In the present study, USi is studied using Density Functional Theory (DFT). U_3Si exists in three crystallographic phases: orthorhombic (stable below 120 K), tetragonal (stable at room temperature), and cubic (stable above 1038 K). DFT studies have shown that only the orthorhombic phase is dynamically stable, whereas the tetragonal and cubic phases display dynamical instabilities. To understand this behaviour, we examine the connection between 5f electron correlation and dynamical instability. The DFT+U approach, which extends standard DFT by including a Hubbard U correction, is widely employed to account for strong correlation effects in actinide materials at relatively low computational cost [1]. However, the choice of the U value is critical and depends on the strength of the correlation. In this study, we determined the effective U (U_{eff}) values for USi in its three phases using the linear-response method proposed by Cococcioni et al. [2], and these U_{eff} values were then applied within the DFT+U framework to investigate the dynamical stability of U_3Si .

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Keywords: Accident-tolerant nuclear fuel; Hubbard U correction; DFT+U.

Spin-Polarized DFT investigations of Hf-based half-Heusler alloys for Spintronic and Optoelectronic applications

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The continuing advancement of modern high-performance electronic devices is heavily reliant on the discovery and engineering of new materials with superior semiconducting and transport capabilities. Half-Heusler (HH) alloys have lately gained popularity due to their high structure and mechanical stability, tunable electronic characteristics, and good magnetic moment responses, making them potential candidates for spintronic and thermoelectric devices. Among these, Hf-based HH alloys stand out because of their appropriate band gaps, high Seebeck coefficients, and strong electrical conductivities, all required for efficient waste heat recovery and modern electronics. Despite substantial theoretical and practical research into various HH alloys, there is still a great need to develop cost-effective and environmentally friendly materials with improved performance. In this study, we explore the phase stability, elastic-mechanical behavior, thermophysical characteristics, and magnetic response of a Hf-based half-Heusler compound using first-principles calculations within the density functional theory (DFT) framework, which is implemented using the WIEN2k simulation software. The dynamic phase stability of Type-I, Type-II, and Type-III structural configurations is evaluated using total energy optimization. This indicates that Type-III's spin-polarized state is the most energetically advantageous. The electronic structure is half-metallic, estimated with the generalized gradient approximation (GGA) and an additional Hubbard U correction. Elastic constants suggest that the alloys have ductile mechanical behavior. The quasi-harmonic Debye model assesses thermodynamic and thermoelectric stability across a wide temperature range. The computed magnetic moment is consistent with the Slater-Pauling rule. These results demonstrate the potential of the proposed Hf-based half-Heusler alloy for spintronic and optoelectronic applications.

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Keywords: Heusler alloy; Thermoelectric; Optoelectronics.

identification of promising candidate materials. Future directions include incorporating phonon-derived features and exploring generative models to guide the design of new compounds. This framework illustrates the synergy between ab initio methods and ML for efficient thermoelectric materials discovery.

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Keywords: Thermoelectric, Seebeck coefficient, conductivity.

Data-Driven Identification of High-Performance Thermoelectric Materials Using Supervised Learning

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Machine learning (ML) is used to accelerate the discovery of novel functional materials by learning structure–property relationships from large datasets. This poster presents an ML-based approach for predicting and screening thermoelectric materials, with emphasis on systems containing lighter nuclei and low-dimensional compounds. Both regression models (to predict quantitative transport properties such as Seebeck coefficient and conductivity) and classification models (to distinguish high-performance from low-performance candidates) are employed. Feature engineering is performed using Matminer and ASE (Magpie, ElementProperty, Stoichiometry) and DScribe^[1] descriptors (structural-property), with several training datasets drawn from density functional theory (DFT) calculations and open repositories. Early results indicate that regression models successfully reproduce trends in transport properties, while classification enables rapid

Ground state of classical Heisenberg model with DMI and Anisotropy

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Research interests in Heisenberg model systems in 2D are of renewed interest in understanding how reduced dimensionality, spin–orbit coupling, anisotropy, and Dzyaloshinskii–Moriya interaction (DMI) give rise to exotic ground states and non-collinear spin textures. These studies are of great interest for discovering novel magnetic phases and enabling future applications in spintronics and quantum materials.^[1–3] We explore the ground state of the classical 1D Heisenberg model in the presence of DMI and crystal field anisotropy. Beginning with an overview of ordered and disordered magnetic states in materials in the context of Ising, XY, and Heisenberg models, the work focuses on one and two dimensional Heisenberg models where spin–orbit coupling and anisotropic interactions play a crucial role. The study examines ground states under different limiting cases: only anisotropy, only DMI, and the combined effect of both interactions. By formulating and solving the governing equations, the numerical results are compared with experimental data, particularly in layered magnetic compounds such as (C₇H₉NBr)₂CuCl₄.^[4] The findings highlight

the significance of ground state analysis in understanding low-temperature magnetic phases and provide insights into non-collinear spin orders and lay the foundation for studying finite-temperature phase diagrams in these systems.

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Keywords: DMI; Anisotropy; Layered magnetic compound.

Computational Insights into the Adsorption and Detection of SF₆ Decomposition Gases on Ruthenium-Decorated Silicon-Doped Graphene Quantum Dots

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The gas-insulated switchgear (GIS) systems require reliable protection by detecting and removing toxic by-products generated from SF₆ decomposition. In this work, the adsorption and detection behaviours of five representative SF₆ decomposition gases H₂S, HF, SO₂, SO₂F₂, and SOF₂ along with background SF₆, were systematically studied on ruthenium-decorated, silicon-doped 555–777 divacancy graphene quantum dots (Ru@3Si-GQD) using density functional theory (DFT) and the quantum theory of atoms in molecules (QTAIM). Significant parameters, including adsorption energy, charge transfer, band gap, density of states (DOS), work function, sensitivity, and recovery time, were evaluated. The Ru@3Si-GQD surface exhibited chemisorption with high adsorption energies, showing excellent sensitivity and selectivity toward SO₂ and SOF₂ gases at room temperature

(298 K). These findings highlight Ru@3Si-GQD as a highly promising, biocompatible material for advanced gas sensing applications[1,2].

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Keywords: Graphene Quantum Dots (GQD), SF₆ decomposition Gases, DFT Detection.

Biaxial Strain Induced Modulation of Rashba Splitting and Hydrogen Evolution Reaction in AgBiP₂Se₆ Monolayer

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Spin orbit coupling (SOC) with broken inversion symmetry gives rise to Rashba/ Dresselhaus splitting in non-centrosymmetric crystals^{1–5}. Compressive and tensile biaxial strain modulates the crystal's interatomic bond distance and bond angle which affects electronic structure and SOC phenomena in crystals. Rashba spin splitting and hydrogen evolution reaction (HER) modulation in AgBiP₂Se₆ monolayer have been studied under the biaxial strain by utilizing density functional theory (DFT) based computations. Effect of biaxial strain decreased the band gap of AgBiP₂Se₆ monolayer in both tensile and compressive conditions. Moreover, Rashba splitting parameter was found increased with tensile strain while decreased for compressive strain. In addition, an electrocatalytic hydrogen evolution reaction (HER)⁶ mechanism was studied over AgBiP₂Se₆ monolayer. Pristine monolayer is not a HER active catalyst while strain effect makes it a good HER catalyst with adsorption free energy 0.32 eV for 6% tensile strain. Further, correlation was found that with increase of Rashba parameter increases

HER activity by lowering the H adsorption free energy of AgBiP₂Se₆ monolayer. This computational study will guide and motivate to design experiments for tunable Rashba splitting spintronics and HER catalyst applications.

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Keywords: Biaxial Strain, Rashba Splitting, HER

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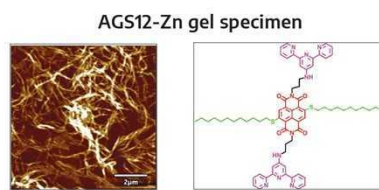
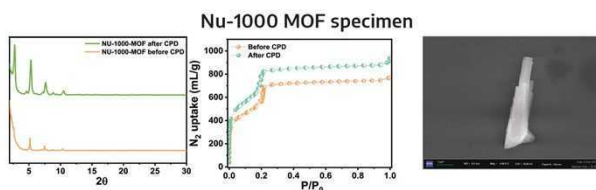
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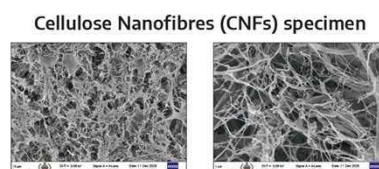
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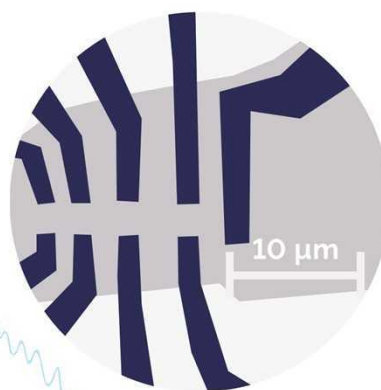
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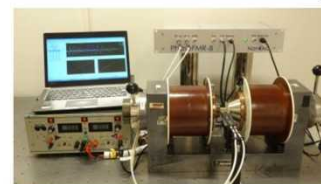
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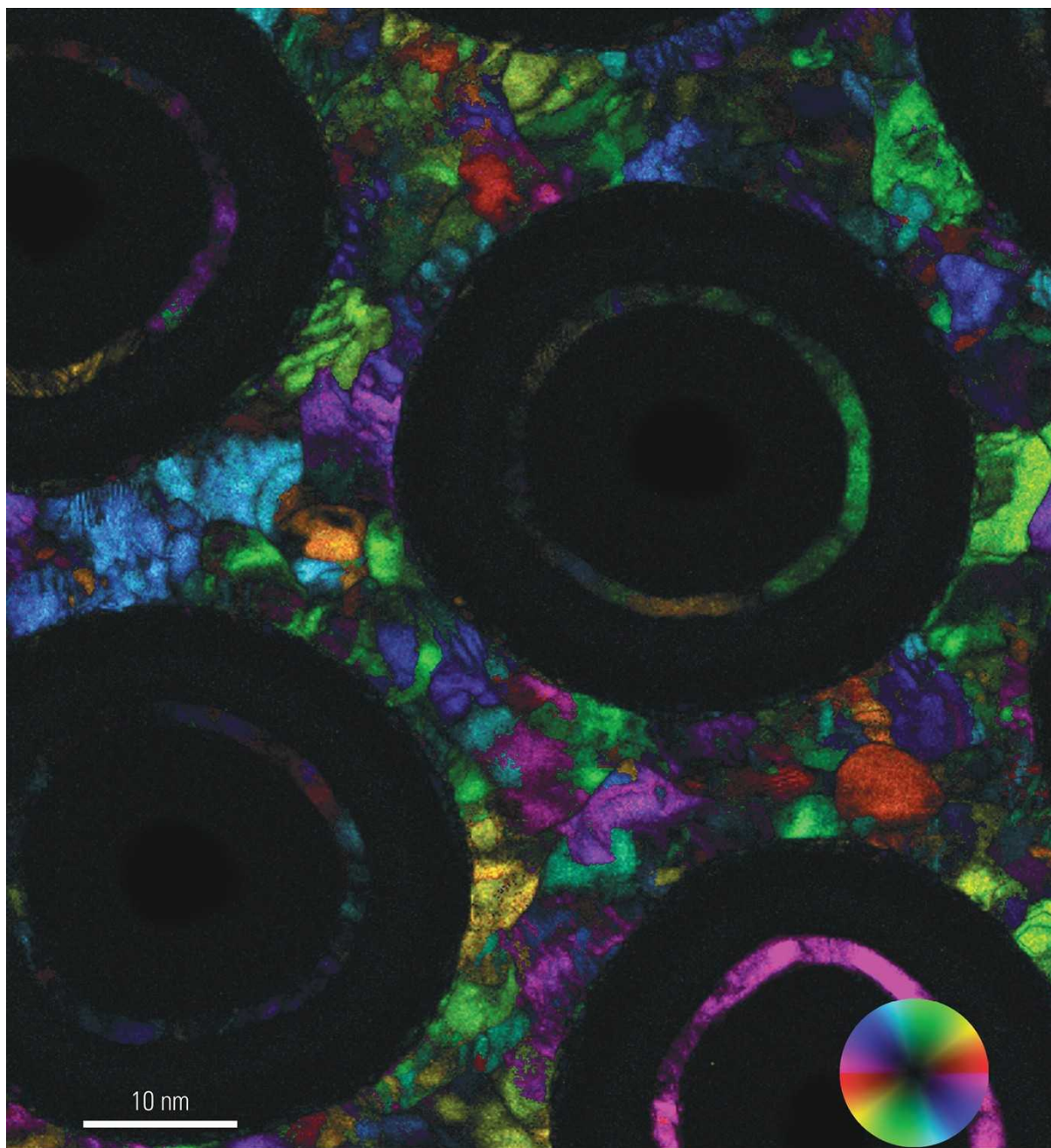
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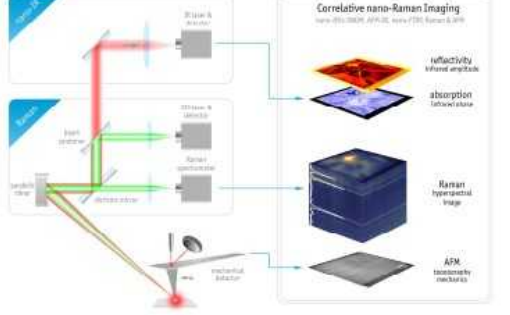
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Author Index

- A Chitharanjan Hegde, 96
A Kathirvel, 210
A. K Sahu, 264
A. Mishra, 82
A. P. Srivastava, 256
A. Sree Rama Murthy, 112
A. Sunderasen, 152
A. Sunil, 86, 200
A. Sunil , 171, 202
A.Sunil , 179
Aabhaas Vineet Mallik, 35
Aarti Jaiswal, 87
Abhinash Maharana, 162
Abhinav Agarwal, 72
Abhinav K P, 264
Abhiprayas Sahoo , 202
Abhiram Senapati, 163
Abhirup Chatterjee, 164, 226
Abhirup Mukherjee, 158
Abhisek Mishra, 136, 138, 149, 155, 156, 161
Abhisek Sahoo, 259, 265
Abhishek Bhattacharjee, 267
Abhishek Das, 152
Abhishek Hazarika, 169
Abhishek Kumar Pandey, 125
Abhishek Misra, 140
Abhishek Ranna, 34
Abhishek Singh, 140
Abinash Dalai, 165
Abinash Mishra, 126
Abir De Sarkar, 59
Abirami R, 88, 97
Achchhe Lal Sharma, 193
Adithyan Puthukkudi, 184
Aditya Ashutosh Dash, 165
Aditya Jadhav, 122
Aditya Mehta, 126
Aishwarya K, 266
Aishwarya S Suvarna, 96
Aiswarya Abhisek Mohapatra, 111, 198
Aiswarya Rath, 101
Ajay Kumar, 233
Ajay Kumar Mishra, 125
Ajay Tripathi, 91
Akhilesh Kumar, 153
Akkiraju Sai Santosh Sri Narayana Raju, 171
Akshata M. Waghmare, 267
Akshaya Kumar Palai, 42
Akshitha, 200
Alagarsamy Pandikumar, 173, 184, 188
Alagarsamy Pandikumar , 228
Aloke Kanjila, 34
Aloke Kanjilal , 155
Aman Kumar, 268
Aman Kumar Singh, 128
Amanpreet Kaur, 77
Amar Dev, 260
Amar K Mohanty, 22
Amba Sankar K N, 171
Amin Doostmohammadi, 248
Amit Bijlwan, 172
Amit Halder, 102
Amit Ranjan, 50
Amit Soni , 272
Amod Kumar, 128
Amreen A. Hussain, 171
Amrita Bhattacharya , 269
Amritpal, 128, 150
Amruta A, 129
Amrutanshu Praharaj, 180
Amul Jain, 242
Anamitra Mukherjee, 143
Ananay Sharma, 72
Anannya Bordoloi, 251
Anant Kumar Gupta, 261
Ananya Kumar, 252
Ananya Mohanty, 173
Andrew P. Mackenzie, 34
Anees Pazhedath, 98
Anik Biswas, 116
Anisha Sainandini Panda, 268
Anita, 130
Anitha Christy A, 254
Anitha Christy Antonysamy, 196, 212
Anjali Maheshwari, 262
Anjeli Sunny, 173, 184
Ankita Agrawal, 182

- Ankita Dey, 159, 262
Ankita Ghosh, 102, 122
Ankur Verma, 174
Ankush Kumar , 244
Anouska Dash , 268
Anshuman Dalvi, 207
Anshumika Mishra, 166
Antarjami Sahoo, 161
Antonio Abate, 88
Anu Bala, 78
Anuj Kanti Nath, 167
Anup Kumar Bera, 129
Anupama Swain, 138
Anuradha M Ashok, 78
Anurag Pritam, 141
Anurup Das, 68
Anushka Das, 265
Anwesha Dutta, 167
Aparajita Mandal, 69, 102, 118, 121, 122
Apoorva, 168
Archana Sagdeo, 157
Archana Tiwari, 92, 257
Arghya Saha, 103
Arijit Sengupta, 17
Arindam Chakraborty, 175
Arjun Behera, 104
Arka Bhowmick, 130
Arpit Patnaik, 252
Arpita Dutta, 131
Arshad Ahamed A, 175
Arumugam Thamizhavel, 143
Arun Rajan, 70, 120
Arun Sam Varghese, 85
Arup Ratan Pal, 108, 116, 251
Arvind Kumar, 262
Arvind Kumar Yogi, 146, 157
Arvind Pandey, 199
Ashis K. Nandy, 146
Ashis Kumar Nandy, 143
Ashish Anand, 111, 198
Ashish Kumar Kar, 79
Ashok K Ganguli, 24
Ashok K. Ganguli, 213
Ashok K. Sahu, 68
Ashok Kumar, 62, 207
Ashok Kumar Ganguli, 217
Ashok Kumar Ganguli , 226
Ashok Kumar., 130
Ashutosh K. Singh, 40
Ashutosh K. Singha, 194
Ashutosh Kumar, 75
Ashutosh Kumar Singh, 174
Ashutosh Mohanty, 42
Ashutosh Srivastava, 140
Ashutosh Thakur, 69
Ashwani Tyagi, 176
Asim Roy, 188
Aswathi P K, 176
Aswin Kumar Burma, 132
Aswini Pradhan, 28
Atal Swathi Patra, 235
Athirai Chelladurai, 240
Atiar Rahaman Mollaa, 167
Atindra Nath Pal, 33, 152
Avala Ramesh, 83
Awadhesh Mani, 76
Awadhesh Mani , 153
Axel Hoffmann, 138
Ayan Datta, 13
Ayash Kanto Mukherjee, 114
B. Dandasena, 177
B. Geffroy, 52
B. Neppolian, 47
B. R. K. Nanda, 270
B. Sanyal, 264
B. Samantray, 134
Babaji Charan Sahoo, 160
Babasaheb R. Sankapal, 211, 230, 231
Bahadur Singh, 56
Bai Yang Wang, 34
Baidyanath Sahu, 76
Baisali Ghadai, 126
Balasaheb J. Nagare , 267
Barnali Dasgupta Ghosh, 80
Barnali Saha, 105
Basanta Roul, 109
Basudeb Dutta, 105, 250, 259
Bebina Swain, 105
Benadict Rakesh, 112
Benedikt Sochor, 129
Berit H. Goodge, 34
Bhagwat S. Chouhan, 102
Bhagyalaxmi Pothal, 119
Bhanu Ranjan, 210, 221
Bharat Kale, 4
Bhargava Nithin T, 179
Bhumika Sharma, 222
Bhuvneshwari Sharma, 132
Bibhudutta Rout, 53
Binoy K Saikia, 169, 263
Binoy K. Saikia , 69
Binud Attry, 263
Biplab K. Patra, 122
Biplab Kumar Manna, 180
Bishnu P. Biswal, 184
Bishnu P. Biswal, 117
Biswajit Chowdhury, 113
Biswajit Maharana, 133
Bitopan Boro, 236
Bivas Saha, 114
Boby Joseph, 48

- Brindaban Ojha, 132
 Brintha T A, 169
- C. Sudakar, 210
 C.K. Suman, 110
 C.K.Suman, 214
 C.N. Anumol, 76
 Chaithanya Purushottam Bhat, 59
 Chandan Kumar Ghosh, 108, 217
 Chandan Upadhyay, 51
 Chandana Mondal, 248
 Chandana Rath, 54, 170
 Chandra Shekhar Pati Tripathi, 81
 Chandrima Chakravarty, 271
 Chetandipta Mahanta, 235
 Chia-Jung Yang, 143
 Chinmayee Patra, 238
 Chithra Lekha P , 240
 Chitra Gurnani, 122
 Christian Hess, 90
 Christian Serre, 79
 Christian Tzschaschel, 131
- D. Das, 145
 D. Samal , 146
 D. Sahoo, 134
 D. Samal, 134
 Dalip Saini, 66, 203
 Darshpreet Kaur Saini, 53
 David E Motaung, 89
 David Willock, 78
 Davinder Kaur, 210, 221
 Dayana Joy, 84
 Dayana Peter, 255
 Dayasindhu Dey, 135
 Deb Kumar Rath, 253
 Debabrata Chakraborty, 238
 Debabrata Sarkar, 196, 212, 254
 Debadutta Samal, 250
 Debakanta Samal, 126, 132
 Debalaya Sarker, 182
 Debanjan Guin, 81
 Debankit Priyadarshi, 131
 Debarghya Dutta, 269
 Debashis Bandyopadhyay, 59
 Debashis Sarmah, 169
 Debashree Nayak, 133
 Debashrita Mahana, 171
 Debdutta Ray, 103
 Debendra Prasad Panda, 88, 132
 Debidatta Mohanty, 170
 Debmalaya Roy, 15
 Debraj Koiri, 238
 Deepa Devapal, 99
 Deepa Ghosh, 46
 Deepak Kumar Palai, 269
- Deepankar Das, 170
 Deepjyoti Kalita, 237
 Deodatta Shinde, 48
 Devasish Chowdhury, 113
 Devasish Chowdhury , 236
 Devendra Singh Negi, 193
 Devendra Singh Negia, 205
 Devi M, 240
 Dheeraj Kumar, 220
 Dheeraj Kumar , 172
 Dibyendu Ghosh, 81
 Digbijaya Palai, 134
 Diksha Arora, 221
 Diksha Srivastava , 106
 Dileep Kumar, 129, 147
 Dillip K. Pradhan, 16
 Dimple Rani, 270
 Dinesh Topwal, 122, 152, 170
 Dinesh Topwal , 201
 Dipak Samanta, 198, 209
 Dipankar Mandal, 66, 203, 229, 233
 Dipti P. Das and K. Kamali, 187
 Dipti Prava Sahoo, 180
 Dipti Ranjan Panigrahi, 181
 Diptikanta Swain, 111, 132, 146, 198
 Dirtha Sanyal, 113
 Divya Choudhary, 182
 Dona Deb, 237
 Dongxin Zhang, 34
 Dr. Sumit Saha, 182
 Durgamadhab Mishra, 94
- E mila Panda, 110
 E. Panda, 208
 Edgar Abarca Morales, 34
 Edouard V`ogtli, 79
 Edward Prabu Amaladass, 76, 153
 Efrat Lifshitz, 90
 Emila Panda , 245
 Esita Pandey, 135, 149
 Evelyn Sharon S, 240
- Florian Theuss, 34
 Fouran Singh, 54
- G S Vinod Kumar, 255
 G. S. Vinod Kumar, 255
 G. Tripathy, 146
 G.S Vinod Kumar, 258
 G. Tripathy, 134
 Gagan Kumar, 102
 Gajiram Murmu, 182
 Gary A. Glass, 53
 Gary Lee, 138
 Gaurav Chouhan, 135
 Geetanjali Vashisht, 73
 Georges Mouchahamv, 79

- Gopal K. Pradhan, 111, 198
 Gopal Pradhan, 154
 Gopinath Shit, 97
 Gourav Manik, 244
 Gracy Nag, 187
 Gunjan Verma, 241
 Gurpreet Kaur, 274
 Gurumeet C. Wadhawa, 273
 Gurvinder Singh, 119
 Gyana Ranjan Kar, 135
 Gyanti Prakash Moharana, 132
- H. S. S. Ramakrishna Matte, 145
 Habeebur Rahman, 221
 Haimyapriya Buragohain, 113
 Hanuma Kumar Dara, 132
 Harekrishna Panigrahi, 254
 Hari Krishna Mishra, 233
 Hari Narayanan Vasavan, 64
 Hari Srikanth, 36
 Haripriya T R, 264
 Harisankar S, 126
 Harold Y. Hwang, 34
 Harsha K, 255
 Harshavardhan Reddy Kalluru, 253
 Heena B. Choudhary, 238
 Heena Bholaram Choudhary, 247
 Hemant Lohumi, 136
 Hemant Singh, 137
 Hermenegildo Garcí'a, 79
 Himanshu Bhatt, 235
 Himansu S. Biswal, 117
 Hirashri Pathak, 271
 Hirendra N. Ghosh, 235
 Hirendra Nath Ghosh, 85
 Hrudananda Jena, 162
- Inderjeet Singh, 107
 Ipsita Parichha, 235
- Jagrati Sahariya, 272
 Jaisri Sanwal, 96
 Jasneet Kaur, 206
 Jaspreet Singh, 130
 Jatis Kumar Dash, 41, 175
 Jayant K. Singh, 106
 Jayanta Vishnu Bharati1b, 254
 Jayita Paul, 136, 155
 Jeebanjyoti Mohapatra, 184
 Jegadeesan P, 153
 Jinho Lim, 138
 Jinsu Mariya Sam, 87
 John Paul and Sagar Agrawal, 107
 Jonas Fransson, 141
 Joydeep Bhaattachajee , 275
 Joydeep Bhattacharjee, 136, 141
 Joydeep Bhattacharjee , 271
- Joyeta Saha, 271
 Joyoti Ghosh, 238
 Jyoti Ranjan Mohanty, 30
 Jyoti Sharma, 137, 150
 Jyotirban Dey, 106
- K. Gurunathana , 183
 K. K. Nanda, 109
 K. N. Uttam, 87
 K. P. Vijayalakshmi, 99
 K. Suresh, 258
 K. U. Akshay, 127
 K. Yadav, 140
 K.V. Mani Krishna, 84
 K. Lal, 134
 Kai Rosnagel, 137
 Kailash C. Jena , 50
 Kajol Sahoo, 185
 Kakali Maiti, 223
 Kalyan Ghosh, 264
 Kalyan Kumar Chattopadhyay, 164, 226
 Kamatchi Jothiramalingam Sankaran, 112
 Kamatchi Sankaranarayanan , 237
 Kanagaraj Rithanya, 173, 184
 Kanchan Rawat, 272
 Kanha Ram Khator, 102
 Kanhai Kumar, 187
 Karabi Kanchan Borgohain, 188
 Kartik Senapati, 133
 Kartikey Chaturvedi, 245
 Karuna Kar Nanda, 187
 Kaushik Mallick, 31
 Kaushik PARIDA, 256
 Kaushik Parida, 38
 Kaustav Jit Bora, 189
 Kavya Bodhi T K , 190
 Keerthi Valsalan, 191
 Ketan S Navale, 126
 Khomdram Bijoykumar Singh, 108
 Kiran Kumar Padhi, 192
 Kiran Manjappa, 119
 Kirti Kirti, 126
 Kishore K. Madapu, 153
 KM Archana Yadav, 232
 Km Sakshi, 192
 Konstant Katin, 141
 Koteswara Rao Peta, 70
 Kouki Mikuni, 131
 Koushik Mahata, 242
 Koushik Pal, 60
 Krishnendu Roy, 81
 Kristian Thijssen. , 248
 Krushna R Mavani, 126
 Kshitij Singh Rathore, 136, 138, 155
 Kshitij V. Goyal, 102

- Kulamani Parida, 166, 180, 195, 208, 214, 224, 230, 232
 Kulamani Parida , 234, 242
 Kuldeep Kumar Kushwaha, 193
 Kuldeep Kumar Kushwahaa, 205
 Kulwant Singh and Pranesh Sengupta, 96
 Kumar Haunsbhavi, 89
 Kumar Kaushlendra, 221
 Kumar Riddhiman Sahoo, 108
 Kumar Shubham, 194
 Kunaal Dhingra, 89
 Kunal Kishore, 272
 Kunchanapalli Ramya, 100
 Kundan Kumar Das, 195
 Kuntala Bhattacharjee, 30
 Kyuho Lee, 34
- L Avilés-Félix, 161
 Lakkimsetti Lakshmi Praveen, 119
 Latika, 185
 Latika Juneja, 186
 Laura N. Serkovic-Loli, 161
 Lavudya Devendr, 119
 Laxman Singh, 108
 Leon C., 71
 Logamithrai D, 196, 212, 254
 Loganathan Kanishga, 188
 Lokanath Patra, 225
 Lucia Iglesias, 34
- M K Padmanabhan, 240
 M. Chithra, 76
 M. Kim, 52
 M. Kumar, 211, 212
 M. Sathish, 183, 215
 M. Sathisha, 178
 M. Yadav, 140
 M. Yadav and S. Patnaik, 145
 M.C. Rathb, 211
 Madhan Jeyaraman, 240
 Madhushree Sarkar, 207
 Madhusmita Nanda, 187
 Madhvesh Pathak, 249
 Mahalakshmi P, 197, 233
 Mahesh Kumar, 62
 Malti Kumari, 109
 Mamata Mohapatra, 196
 Mamata Sahoo , 249
 Manabendra Chandra, 106
 Manan Dholakia, 266
 Manaswini Karsharmaa, 196
 Manfred Fiebig, 143
 Manik Kuila, 155, 156
 Manikantha Panda, 139
 Manju Saraswathy, 87
 Manjunatha Kempasiddaiah, 180
- Manjusri Misra, 38
 Manobalan S., 93
 Manoj Kumar Nayak, 45
 Manoj Varma, 200
 Manoranjan Kar, 43, 204, 260
 Manoranjan Kar1, 160
 Manu Jaiswal, 119
 Manuel Bibes, 34
 Marcin Konczykowski, 34
 Mareeshwari Paramasivan, 240
 Martin Cramer Pedersen, 248
 Martin Gonzalez, 34
 Mathivarsini P, 197
 Mayank Dotiyal, 110
 Md Amira, 167
 Md. Shahid Jamal, 147
 Megha Rana, 110, 214
 Michal Moravec, 34
 Mitali Swain, 161
 Modhurima Bhuiya, 273
 Mohan S, 171
 Mohd Ali, 81
 Mohin Sharma, 53
 Mojibur R. Khan, 237
 Moloy Sarkar , 238
 Monalisa Pradhan, 111, 198
 Monica Chingchuilin Gonmei, 240
 Monotosh Dalapati, 198
 Montek Mohapatra, 199
 Mrinal Deka, 140
 Mrinmoy De , 45, 243
 Mritunjaya Parashar, 53
 Muhammed Ali A V, 145
 Mukesh Kr Dasoundhi, 128
 Mukesh Kumar, 200
 Mukhesh K. Ganesha, 194
 Mukul Gupta, 147, 216
 Munima B Sahariah , 271
 Mutch Shanmukha Rao, 112
- N. Kumar, 41
 N.L. Parthasarathi, 244
 N. Ganguli, 134
 Nabendu Mondal, 141
 Nagendra Singh, 240
 Nainish Tickoo, 143
 Nakshatra Ranjan Pal, 216
 Namitha N.N, 112
 Narayan Ch. Jana, 228
 Narayan Chandra Das, 6
 Navya John, 78
 Nawaz Sarif, 132
 Neelam K, 241
 Neelkamal Das, 240
 Neethu K M, 241
 Neha, 207

- Neha Agnihotri , 268, 269, 273, 276
 Neha Shukla, 95
 Neha Singh, 63, 141
 Nehal Telange, 273
 Nemallapalli Madhusudhan, 171, 179, 200
 Netra Prova Baruah, 113
 Nevin Noble, 201
 Newmoon Priyadarshini, 242
 Niharendu Choudhury, 175
 Nikhil RAM PATRA, 256
 Nikhitha Rajan, 114
 Nikita Ahlawat, 201
 Nikita Choudhary, 114
 Nilakantha Tripathy, 100
 Nilja George, 29, 142
 Nilofar Kurawle, 143
 Nirman Chakraborty, 90
 Nisha T. Padmanabhan, 82
 Nishtha Vats, 94
 Nita Dilawar Sharma , 207
 Nithya Davis, 78
 Nithyanandan Kanagaraj , 275
 Nitika Kharbanda , 235

 O. Plantevin, 52
 Omkar , 273
 Onkar Nath, 242

 P Murugavel and Somnath C Roy , 117
 P. Biswal, 146
 P. Das, 140, 145
 P. Hemani, 208
 P. Kour, 260
 P. Kumar, 145
 P. Nandi , 264
 P. Sharma, 134
 Pachaiyappan Rajamalli, 120
 Palash Jyoti Medhi, 113
 Pankaj Bhalla, 84
 Pankaj Kandwal, 168
 Parasmani Rajput, 157
 Paresh Mohanty, 241
 Paresh S. Gaikar , 273
 Parikshit Moitra, 44
 Parikshit Moitra , 241
 Partha Pratim Ray, 230
 Partha Sarathi Ghosh, 175
 Partha Sarathi Mondal, 199
 Parthasarathi Bera, 7
 Parul, 203
 Parvathy Ravindranath, 203
 Parveen Saini, 8
 Payel Shee, 143
 Perez L., 71
 Peter Berg, 206
 Piyali Biswas, 204, 260

 Pooja Gupta, 129, 147
 Pooja Kumari, 211, 212
 Pounomi Bera, 167, 205
 Prabhakar Lalchand Yadav, 115
 Prabhajan Pradhan, 122
 Prabhat Kumar Chaudhari, 88, 97
 Prabhu Prasad Tripathy, 244
 Prabhukrupa Chinmay Kumar, 144
 Prabuddha Kant Mishra, 139
 Prachi A. Patil, 273
 Pradipta Behera, 243
 Prag Ranjan Das, 116
 Prahallad Padhan, 128, 148
 Prahallad Padhan , 150, 219
 Prahlad Kanti Barman, 140
 Prajnashree Panda, 223
 Prakash Chandra Mondal, 63, 141
 Prakriti Mishra, 145
 Pramoda K. Nayak, 32, 200
 Pranab Kumar Sarkar, 167
 Pranab Kumar Sarkar , 153
 Pranati Nayak, 245
 Pranati Nayak , 154
 Pranava Bhamidipati, 122
 Pranay Ranjan, 193
 Pranay Ranjana, 205
 Prasanjit Samal, 225, 267
 Prasanjit Samal , 270
 Prasanna Das, 114
 Prasanta Kumar Maharna, 274
 Prasanta Kumar Mudulli, 140
 Prasenjit Sen, 57, 275
 Pratap K. Sahoo, 121, 159, 225, 262, 264, 265
 Pratap Kumar Sahoo, 101, 148, 259, 265
 Pratik Deshmukh, 222
 Pratiksha Meena, 275
 Pratiksha Singh, 193
 Pratiksha Singha , 205
 Pratyay Mukherjee, 131
 Pravansu Panda, 228
 Praveen Garg, 114
 Praveen Kumar, 81
 Prem B Bisht, 119
 Pritha Dutta, 174
 Pritish Kumar Behura, 206
 Priya Choudhary, 207
 Priya Mahato, 245
 Priyanka Bhardwaj, 207
 Priyanka Gogoi, 69
 Priyanka Priyadarshini, 208
 Pukhraj Prajapat, 165
 Pulak Pal, 164, 226
 Pulickel M. Ajayan, 2
 Punithavelan N, 197, 233
 Pushpendra Gupta, 138

- Q.-P. Ding, 127
- R J Choudhary , 157
- R. Justin Joseyphus, 157
- R. N. Singh, 84
- R. Naik, 177
- R. Nath, 127
- R. Robin, 215
- R. S. Patel, 35
- R. Vijay, 5
- R.Venkatesh1 and Mukul Gupta, 114
- R. Soni, 134
- Radhika Panickar, 37
- Radhika S. Patil, 66
- Raghunath Singha, 209
- Rahul Ghosh, 275
- Rahul Ravi, 87
- Rahul Vishvkarma, 147
- Raj Saha, 66
- Rajamani Nagarajan, 107
- Rajamani Raghunathan, 135
- Rajan Kumar Pandey, 57
- Rajat Kumar Tripathy, 210
- Rajeeb Rawat, 157
- Rajeev Ahuja , 100
- Rajeev Rawat, 216
- Rajesh Kumar, 31, 210, 221, 253
- Rajesh Kumar , 201
- Rajeshwari Hari, 240
- Raju Kumar Gupta, 87
- Rajulal Sahu , 211
- Rakesh Kumar Behera, 235
- Rakesh Kumar Behera¹, 85
- Ram Kumar, 211, 212
- Ramakanta Naik, 123, 185
- Ramakanta Naik , 144
- Raman Sankar and Sanjoy Kr Mahatha1 , 150
- Ramanathan Mahendiran, 138
- Ramanathaswamy Pandian, 153
- Ramasamy Sakthivel, 112
- Ramendra K Pal , 247
- Ramendra Kishor Pal , 238
- Ramesh Chandra Deka, 113
- Ramesh Chandra Nath, 36
- Ramesh L. Gardas, 16
- Ranbir Singh, 218
- Rashmi R. Das, 159
- Rashmi Ranjan Das, 148, 262
- Rasik Manve, 175
- Rasmi Ranjan Mohapatra, 148, 150, 219
- Raveena P V, 196, 212, 254
- Ravi K. Kunchala, 213
- Ravi Kumar Kunchala, 217, 226
- Ravichandran Shivanna , 116
- Ravindra Naik Bukke, 72
- Reddi Jagadeesh, 179
- Reema Nayak, 124
- Renjith S. Pillai, 99
- Renuka Singh, 81
- Richa Mishra, 264
- Rijo Rajeev, 241
- Riju Paria, 116
- Rishi Verma, 63
- Rita Ghosh, 243
- Ritesh Halder, 41, 232
- Ritik Mohanty, 214
- Ritu Srivastava, 214
- Ritu Srivastava , 110
- RituDuggal, 88, 97
- Ritwik Mondal, 131
- Riya Malik, 110, 214
- Rohini Garg, 96
- Rohit Kumar Meena, 216
- Rohit Ranjan Raut Ray, 213, 217
- Rojalin Sahu, 105, 250, 259
- Romain Grasset, 34
- Romera M. , 71
- Roop L Mahajan, 240
- Roshna S H, 128
- Roshni Begum, 217
- Ruiz B. G., 71
- Ruma Khatun , 276
- Rumu H Banerjee, 96
- Rupalipriyadarshini Chhatoi, 135
- Rupalipriyadarsini Chhatoi, 149
- Rupam Mandal, 69, 102
- Rupesh S. Devan, 18
- Ruta Kulkarni, 143
- Ruturaj V. Puranik, 102
- Rwiddhi Chakraborty, 228
- S M Yusuf, 2
- S. Abhaya, 258
- S. Amirthapandian, 153
- S. B. Krupanidhi, 109
- S. Balakrishnan, 163
- S. Biswas, 82
- S. K. Srivastava , 41
- S. N. Sarangi, 146
- S. Neogy , 256
- S. Ningshen, 97
- S. Patnaik, 140
- S. Porwal, 73
- S. Vinitha, 258
- S. Wazed Alib, 167
- S.K. Gautam, 52
- S.K.Pradhan, 260
- Sabyasachi Chakarabortty, 142
- Sabyasachi Chakrabortty, 29
- Sabyasachi Mukhopadhyay, 100
- Sachin Pal, 107

- Sachindranath Sarangi, 132
 Sagar Sarkar, 146
 Sagarika Padhan, 254
 Sahu M. C., 71
 Saikat Bhaumik, 185, 186, 224
 Saiprakash Rout, 117
 Saira Bano, 218
 Sajeev S. Chacko, 267
 Sajesh P. Thomas, 49
 Salaman Ahamad, 244, 246
 Sambit Choudhury, 137, 150
 Sambit Kumar Prusty, 219
 Samim Hossain, 117
 Samir Kumar Biswas , 240
 Sampat Raj Vadera, 94
 Samriddhi Kushwaha, 200
 Sandeep Sekhar Pradhan, 254
 Sandip Kumar Padhi, 148, 150, 219
 Sangeeta J. Keny, 211
 Sanjay Saini, 256
 Sanjeev Aggarwal, 53
 Sanjeev Kumar, 132
 Sanjeev Kumar Gupta, 211, 212
 Sanjib Banerjee , 242
 Sanjib Kar , 228
 Sanjoy Kr Mahatha, 128
 Sanjoy Kr. Mahatha, 137
 Sankalpa N. Panda, 184
 Sannu Kumar Nayak, 265
 Santamaria J., 71
 Santosh K. Singh, 181
 Santosh Kumar Sahu, 148, 150, 219
 Saralasrita Mohanty , 244
 Sarathi Kundu , 247
 Sarathlal Koyiloth Vayalil, 129
 Sarmistha Bhattacharjee, 245
 Saroj Kumar Nayak, 203
 Sarojini Prusty, 245
 Sasanka Deka, 12
 Saswati Mishra, 184
 Sathasivam Pratheep Kumar, 115, 169
 Satinath Mukhopadhyay, 241
 Satyabrata Sahoo, 184, 220
 Satyajit Rath, 203
 Satyam Shankhdhar, 221
 Satyaprakash Sahoo, 97
 Satyaprasad P. Senanayak, 102
 Satyapriya Nath, 117
 Saumen Mandal, 119
 Saumya Prasad Jena, 151
 Saurabh S. Shiwankar, 221
 Saurav Kumar, 276
 Sawan Kumar Bhakar, 222
 Sayak Roy, 223
 Sayali S. Harke, 122
 Sayari Ghatak, 152
 Sebin J. Sebastian, 127
 Sergio Naval'on, 79
 Shailesh K. Khamari, 73
 Shaista Fatima, 244, 246
 Shaktiranjana Mohanty, 132
 Sham Sundar Ravindranath , 246
 Shamili Bandaru, 29, 142
 Shanu Bandyopadhyay, 118, 121
 Sharanjeet Singh, 129
 Sharat Chandra, 266
 Sharat Chandra , 274
 Sharin Jaswa, 95
 Shaunak Sarkar, 140
 Sher Singh Meena, 160
 Shilendra Kumar Sharma, 277
 Shilpa Pradeesh, 264
 Shilpa Sharma, 76
 Shishir Kumar Pandey, 143
 Shiv P. Patel, 55
 Shivaji B. Sadale, 66
 Shivam Kumar, 247
 Shivam Rakhoulia, 240
 Shivani Soni, 153
 Shovan Kumar Majumder, 222
 Shovon Pal, 102, 131, 143
 Showkat H. Mir, 106
 Shrabanee Sen, 205
 Shrabanee Senc, 167
 Shraboni Ray, 153
 Shradha Bhatt, 257
 Shradha Suman, 112
 Shriganesh Prabhu, 102
 Shriganesh S. Prabhu, 117
 Shruti Narayanan, 119
 Shubham B. Upadhye, 154
 Shubhansu Sahoo, 136, 149, 155, 156
 Shweta G Bhat, 126
 Siddhartha Ghosh, 142
 Siddhartha Ghosh1, 29
 Siddhartha Lal, 158
 Silpa Subhalaxmi, 223
 Simanta Ranjan Barik, 224, 234
 Simantini Nayak, 184
 Simma Shiv Prasad, 119
 Simran Nasa, 200
 Sitharaman Uma, 107
 Smarak Islam Chaudhury, 120
 Smaranika Ray, 224
 Smita A. Acharya, 221
 Smita Borole, 143
 Smrutirekha Mishra, 254
 Sohini Das, 247
 Somasree Bhattacharjee, 131
 Sonali Patajoshi, 155
 Sonali S. Pradhan, 139
 Sonil Nanda, 40

- Sonu Gandhi, 13
 Soubhagya Dash, 149, 155, 156
 Soumen Maiti, 164, 226
 Soumendra Kumar Das, 225
 Soumya S. Sahoo, 53
 Soumya Shephalika Behera, 157
 Soumyajit Maitra, 81
 Soumyaranjan Das, 132
 Soumyendu Roy, 182, 192
 Sourav Mukherjee, 248
 Srabanti Ghosh, 83
 Sreekanth G, 70, 120
 Sreekanth M. S., 85
 Sreelakshmi M. Nair, 35
 Sreelakshmi N, 118
 Sreeraj Puravankara, 176, 252
 Sreya Das, 164, 226
 Sridhar Sahu, 58, 225
 Srijan Maity, 102
 Srijoti Mukherjee, 213, 226
 Srinibas Satapathy, 222
 Srinivasa K. Prasad, 238
 Srinivasa Prasad K, 247
 Srinivasan Nedunchezian, 261
 Srinivasan Nedunchezian , 227
 Sriram Jeyaram, 157
 Stephan Reitzenstein, 25
 Subasa C. Sahoo., 76
 Subash Cherumannil Karumuthil, 174, 190
 Subhadeep Moulick, 152
 Subhajeet Sen, 227, 261
 Subhajit Kar, 228
 Subhajit Nandy, 210
 Subham Kumar Subudhi, 228
 Subhankar Bedanta, 132, 135, 136, 138, 149, 151
 Subhankar Bedanta , 156
 Subhankar Bedanta1, 155, 161
 Subhashis Ghosh, 102
 Subhashree Praharaj , 249
 Subhashree Sahoo, 121
 Subhendra D. Mahanti, 146
 Subinoy Rana, 46
 Subramanian Rajalekshmi, 188
 Subrat Swain, 259
 Subrata Jana, 267
 Sucheta Mondal, 126
 Sudakshina Prusty, 265
 Sudeshna Das Chakraborty, 39
 Sudeshna Maity, 122
 Sudhanshu Gautam, 262
 Sudharsan J, 197
 Sudharsan J B, 233, 275
 Sudhindra Rayaprol , 143
 Sudip Barman, 180, 223
 Sudip Chakraborty, 19
 Sudip Chakraborty , 277
 Sudip Ghosh, 152
 Sudip Naskar, 229
 Sudipta Chakraborty, 124
 Sudipto Chakraborti, 161
 Sugam Kumar, 241
 Sugandh Sirohi, 119
 Sujit K. Ghosh, 4
 Sujit Kumar Ghosh, 105
 Sujith Nedungattil Subrahmanian, 271
 Sukalyan Deb, 158
 Sukanti Behera, 83
 Sumangala T. P., 93
 Sumanth Sekhar Samal, 200
 Sumit Kumar Chaudhary, 193
 Sumit Kumar Choudharya, 205
 Sumit Kumar Pradhan, 238
 Sunetra Mondal, 241
 Sunil S. Kushvaha, 262
 Superb Misra, 245
 Suprabha S. Dixit, 122
 Supravat Ghosh, 230
 Supreet Kaur, 189
 Suraj P. Khanna, 214
 Suraj P. Khanna , 110
 Surajit Ghosh, 73
 Surender Kumar Sharma, 252
 Suresh Kumar Kailasa, 14
 Surjit Sahoo, 203
 Surjyakant Mangaraj, 159
 Surya Prakash Singh, 8
 Susanginee Nayak, 230
 Sushree Nibedita Rout, 160
 Susmita Kundu, 205
 Suswapna Mukherjee, 161
 Swagata Banerjee, 167
 Swapan K Pati, 56
 Swapna Rout, 230
 Swarup Kundu, 192
 Swayang Priya Mahanta, 135, 149, 161
 Swikruti Supriya, 123
 Swosti P. Sarangi, 131
 Syed Minhaz Hossain, 124
 T. K. Sharma , 73
 T. Kedara Shivasharma, 231
 Takuya Satoh, 131
 Tanaya Halder, 143
 Tanmoy Basu, 36
 Tanmoy Maiti , 272
 Tanmoy Pain, 228
 Tanuja Mohanty, 29, 262
 Tapan Kumar Rout, 254
 Tapas Paramanik, 139
 Tapobrata Som, 102, 118, 121, 122
 Tapobrata Som , 69

- Teresa Dong, 206
 Tharamani C. Nagaiah, 9
 Thiruvancheril G. Gopakumar, 106
 Tilottama Baisakhi, 232
 Todd A. Byers, 53
 Tornos J., 71
 Trilochan Mishra, 39
 Triveni Rajashekhar Mandlimath, 191
 Tufan Paul, 164
 Tumpa Gorai, 165

 Udai P. Singh, 66
 Uday Deshpande2 Mukul Gupta, 182
 Uday Deshpandey, 114
 Ujjwal Pal, 51
 Uma Shankari M , 249
 Umesh Kumar Sinha, 148, 150
 Umesh V Waghmare, 23
 Upali Aparajita Mohanty, 232
 Urmimala Naha, 73
 Utsa Sarkar, 233

 V R Rao Medicherla, 157
 V. Bharathi Mohan, 178
 V. Bharathi Mohana, 183
 V. K. Dixit, 73
 V. Kanchana, 130, 139

 V.L.R. Jacques, 52
 V.P.S. Awana, 3
 Vaishnavi S, 233
 Vaivhab Kandwal, 165
 Vanessa Pimenta, 79
 Vanshaj Vidyan, 234
 Vasant Sathe, 157
 Veerababu N , 202
 Venkata Krishnan, 11
 Vidya Unnikrishnan Geetha, 87
 Vijay Kumar, 155
 Vijaya Rangari, 37
 Vikram Singh, 141
 Vipin Mishra, 106
 Vivek Dwij, 102

 Wenjie Sun, 34

 Y. Furukawa, 127
 Y. Pushpalatha Devi, 84
 Yadu Krishnan K T , 258
 Yuefeng Nie, 34
 Yuvraj SINGH NEGI, 256

 Z. Hossain, 134
 Zuzanna H. Filipiak, 34

Keyword Index

BiOBrO₃ , 196
Bi₂Mo₃O₁₂, 191
CoNb₂O₆/Nb₂C, 183
CoWO₄, 191
Fe₂O₃ nanorod, 173
H₂O₂ production, 195
NiCo₂O₄, 171
V₂O₅doping, 192
 π -bonded Organic molecules, 161
operando spectroscopy; surface-analyte
 hybridization; van der Waals
 materials; heterogeneous catalysis,
 90
1D-Tellurium, 233
2-D materials, 161
2D, 83
2D Materials, 4, 13, 183, 215
2D Materials , 252
2D Materials., 100
2D halide perovskite; tunable
 piezoelectricity; spacer cation;
 piezoelectric nanogenerator., 164
2D halide; Vacancy-assisted
 pseudo-capacitance; asymmetric
 supercapacitor; charge transport,
 226
2D materials, 145
absorption, 253
Accident-tolerant nuclear fuel; Hubbard U
 correction; DFT+ U. , 274
Acid Etching (AE), 217
Acid-etching, 213
acid-etching, 226
activated carbon; nanocomposite hydrogel;
 dye adsorption; rice straw., 242
Active Matter, 248
Active Ornstein-Uhlenbeck particle;
 Stochastic Resetting; Viscoelastic
 medium, 249
Additive engineering; stabilization;
 black-phase of FAPbI₃ , 116
Additive Manufacturing Collaboration., 88
AFM, 264
AG, 205
age hardenability, 255
Aggregation caused quenching, 105
AI-algorithms. , 268
Alkali doping, 107
Alkali metal-ion batteries, 59
Alkaline hydrolysis, 37
alloys, 255
Altermagnetism; extended Hubbard model;
 mean-field approach. , 135
Altermagnets. , 151
Alumina composites; Artificial saliva;
 Coefficient of friction; Tribology.,
 244
ammonia detection., 119
Ammonia sensing, 259
Analyzing bending magnet; Electromagnetic
 Quadrupoles; COMSOL
 Multiphysics, 265
and random number generation., 97
angles, 125
Anisotropy, 135, 149
anisotropy, 257
Anomalous Nernst, 36
anoporous membrane, 41
antiferromagnet, 36
Antiferromagnet; Magnon; Magnetization
 Dynamics; Nonlinear 2D
 THz-Spectroscopy. , 131
Antiferromagnet; Spin-Orbit torque;
 Spin-torque ferromagnetic
 resonance. , 155
Antiferromagnetism , 127
antimicrobial, 249
antimicrobial-biofilm therapy, 242
APCVD; Solid-state dewetting, 159
Aptasensor., 13
aqueous interfaces, 50
artificial synapse, 122
Aryl diazonium; CoFe₂O₄ NPs; covalent
 functionalization; paramagnetic to
 ferromagnetic transition , 141
ashba Splitting, 277
asymmetric supercapacitor., 214

- asymmetric supercapacitors, 210
- ATCC, 70
- Atomic layer deposition, 176
- ATR-FTIR; Raman spectroscopy, 87
- autoencoder. , 57

- Band edge engineering, 51
- Band Gap Engineering, 197, 198
- Barium titanate, 199
- basal plane , 154
- BaTiO₃, 81
- batteries (LIBs), 5
- BCN., 2
- BCS and Hydride superconductors., 3
- Benzimidazole derivatives, 273
- Berry phase, 141
- Bi-functional catalyst, 232
- Biaxial Strain, 277
- Bifunctional electrocatalysis, 206
- binary -ternary compositions, 2
- biobased materials, 22
- BiOBr, 196
- Biocarbon, 38
- Bioceramic composite, 249
- biocompatible, 238
- Biodegradable composite, 37
- biodegradable plastics, 22
- biodegradable polymers, 87
- Biomarker, 232
- Biomaterial, 247
- Biomedical, 236
- Biomedical device, 244
- biomineralization, 249
- Biopolymer, 244
- bipolar materials, 252
- Bismuth silver oxytelluride; Microwave synthesis; Nanosheet; Photodetection. , 144
- Black phosphorus, 190
- blowing agent, 258
- Blown Films, 37
- BN, 2
- BNT–BT–KNN, 192
- Borophene, 29
- Bulk heterojunction, 103

- C, 2
- C-H arylation, 42
- Ca²⁺/Ga³⁺ substitution, 160
- cAFM, 69
- Calcination, 261
- Carbon, 179
- Carbon nanomaterials, 6
- Carbon nanotubes., 6
- Carbon Quantum Dots, 259
- Carbonate substitution, 96
- catalytic activity , 245
- CBD, 231
- CdSe, 29
- CDT, 242
- cellulose-based electrode, 205
- cerium, 68
- Chalcogenide, 233
- Chalcogenide thermoelectric materials, 170
- Charge carrier dynamics., 85
- Charge-Carrier Dynamics, 51
- Charge-transfer emission., 103
- Chemical Bath Deposition , 173
- Chemical bonding; Born Effective Charge; Bond dissociation; Metavalent bonding., 271
- Chemical recycling, 11
- Chemical straining , 110
- Chemical vapor deposition, 175
- chemoembolisation, 87
- chiral induction., 209
- Chitosan, 41
- Chlorhexidine, 89
- chromatography. , 243
- CIE lab spectrophotometry, 255
- circular bioeconomy, 22
- Circular economy., 11
- Clear Aligner Materials, 88
- Clinical Diagnosis, 44
- Close space sublimation, 108
- Closed cell silver foam, 258
- Clusters, 267
- CMOS, 57
- CN, 2
- CO₂ reduction, 176
- CO₂ reduction , 50
- Co-doped LAMOX; Ionic Conductivity; Impedance Spectroscopy; Distribution of Relaxation Time , 221
- Co-electrolysis, 173
- coal-derived CQDs, 69
- coal., 169
- Cocatalyst; Rh_{2-y}Cr_yO₃, 212
- coin cell supercapacitors, 232
- Cold sintering process, 199
- Collagen, 236
- Colloidal gels, 248
- combustion, 196
- Complementary Oligonucleotides, 44
- Composite polymer electrolytes (CPEs), 207, 208
- Composites, 80
- conducting filaments, 34
- Conducting Gels; Carbon;Superparamagnetic Iron Oxide Nanoparticles Composites

- (SPION); Triboelectric
 Nanogenerator (TENG);
 Self-Powered Sensor; , 218
 Conducting Polymer, 247
 Conductive Hydrogel, 244
 Conductive Nanocomposites, 15
 Conductivity, 259
 conductivity., 275
 Conjugated polymer nanostructures, 83
 contact resistance, 110
 coordination cages, 198, 209
 Core shell Structure, 142
 core-shell nanostructures, 29
 Core-Shell, 41
 Correlated electronic states, 56
 Corrosion, 97
 Corrosion study., 96
 Coupling Cathode, 64
 Covalent Organic Framework, 44
 Covalent Organic Framework (COFs), 207,
 208
 Covalent Organic Frameworks (COFs), 117
 Crystal violet degradation., 195
 crystallinity, 264
 CsPbX₃ nanocrystals; metal-organic
 frameworks; polymeric fibers;
 WLEDs. , 224
 Cu₂OSeO₃; EXAFS; Dielectric anomaly;
 Magneto-structural coupling , 152
 Cu₂WS₄ nanocomposite, 205
 Cu₂ZnSnS₄, 107
 Cubic anisotropy, 135
 CuO, 81, 110
 Curie temperature, 216
 Current–phase relation asymmetry , 133
 cytotoxicity, 249

 Defect engineering, 213
 defect engineering, 107
 Defects , 107
 Delocalization, 161
 Density Functional Theory, 56, 150, 219
 Density functional theory, 59
 Density functional theory (DFT), 233
 Density functional theory (DFT)., 202
 Density Functional Theory., 271
 designer solvents, 17
 detectivity, 123
 DFT, 30, 60, 83, 259, 267, 273
 DFT Detection., 276
 DFT., 273
 DFT. , 225
 Dielectric properties, 199
 dielectric properties, 192
 Dielectric property, 207
 digital switching, 122

 Diketopyrrolopyrrole, 42
 Direct 3D Printing, 88
 disorder-induced scattering, 153
 Disordered solids, 98
 Display, 72
 DMI, 270
 DMI; Anisotropy; Layered magnetic
 compound. , 276
 DMSO-free, 88
 DNA, 40
 DNAzym, 46
 Doping, 80
 DOS, 269
 Double Perovskites, 272
 double perovskites, 269
 Double Perovskites; Griffiths-like Phase;
 Spin-phonon coupling; Exchange
 Bias , 132
 Drosophila , 250
 drug eluting, 87
 dsDNA., 41
 dye-sensitized solar cells, 8
 dynamic adsorption, 198
 dynamical excitations, 23

 E-waste., 8
 ECD , 31
 ECM-mimicking, 46
 economic potential, 263
 edge plane, 154
 EDX, 230
 Elastomer Matrix, 15
 Electric field, 161
 Electric vehicles (EVs), 5
 Electrical Conductivity, 63
 electrical conductivity., 170
 Electro-mechanical properties., 207
 Electrocatalysis, 179, 181, 182
 Electrocatalyst, 171
 electrocatalyst, 9, 226
 Electrocatalysts, 82
 electrochemical, 176
 Electrochemical biosensors, 100
 Electrochemical energy storage, 217
 Electrochemical sensing, 45
 Electrochemical sensor., 205
 Electrochemical stability., 207, 208
 Electrochemistry, 214
 Electrochromism., 179
 electroluminescence, 124
 electrolyte, 231
 Electromagnetic Absorption Bandwidth.,
 262
 Electromagnetic interference shielding, 93
 Electron irradiation, 96
 electron paramagnetic resonance (EPR), 107

- Electron Phonon interaction, 253
electronic conductivity, 168
electronic structure, 128
Electronic synapse., 118
Electrophoretic deposition, 145
Electroplex, 103
Electrospinning; PM particles; Air filtration;
Anti-bacterial activity, 254
Electrospinning; Porous nanofibers; N-doped
carbon; Supercapacitor. , 223
Electrospun scaffold, 89
Emerging pollutants, 45
emerging pollutants, 81
Endurance, 130
Energy conversion, 18
Energy Density., 214
Energy devices, 42
Energy efficiency, 5
energy generation., 208
Energy Harvest, 66
energy harvesting, 256
Energy harvesting , 80
Energy Storage, 18
Energy storage, 8
Energy storage ceramics, 199
Energy storage device; Perovskite oxide;
Energy density; Thermistor., 204
Energy storage performance, 199
Energy storage., 41
Environmental remediation, 45
Epitaxial Heterostructure, 85
Euphorbia concenensis, 273
ex-situ XRD, 252
exchange bias, 2
Exchange bias. , 142
Exciplex, 103
Exciton binding energy, 101, 162
Exciton binding energy; Photoluminescence;
Non-linear optical properties, 124
Exciton-phonon coupling, 73
Excitonic Radiative Lifetime, 19

f single-QD device, 25
Facile hydrothermal Synthesis, 211, 212
FeCoB/Pt, 147
Fermi level pinning; Integer charge transfer
model; Perovskite; SAM., 169
ferrimagnetic, 30
Ferrite composites, 203
Ferrite; Substitution; Nanoparticles;
Magnetization. , 76
ferroelectric, 222
Ferroelectric materials, 234
Ferroelectric oxides, 16
Ferroelectricit, 100
ferroelectricity, 192

ferroelectrics, 111
Ferromagnetic resonance, 161
Ferromagnetic resonance (FMR), 126, 134,
138
Ferromagnetism, 75
ferromagnetism, 257
FESEM, 230
FET., 66
Figure of merit, 170
finite system, 267
first-principles calculations, 139
Flexible , 221
flexible nanofabrication. , 25
Flexible sensor for Glutathione detection. ,
217
Flexible spintronics, 149
flexible; biomass, 214
Flexible; Carbon Black; EMI Shielding;
Tensile Strength, 260
floral, 231
Fluorapatite, 96
Fluorescence, 41
fluorescence sensing, 105
Fluorescent Biosensor, 40
fluorescent probe, 250
foam stabilization, 258
Food quality analysis., 87
Food safety , 45
Food toxins, 45
Freeze-Thaw ; Gelatin ; Hydrogel ; Piperine
, 246
Frenkel Exciton, 19
Fruit juice interaction, 87
frustrated antiferromagnetism, 24
Functional Materials, 66
functional materials, 31
Functional Materials., 19
functionalized ILs., 17
Fused cyclic energetic materials;
Coumarin;oxygen rich; reduced
sensitivity. , 220

gamma-ray detectors, 28
Gas sensing, 100
gas sensor, 62, 119
Gd-doped In₂S₃, 89
Generative AI, 57
Germanene, 4, 13
GFRP, 7
GHGs, 7
Gilbert damping, 161
GISAXS. , 129
Glass-Ceramics; Ion-Exchange; Piezoelectric;
Energy Harvesting; dielectric
capacitor, 167
Glucose, 205

- glucose, 245
 Gold Nanoparticles, 44, 105
 Gold Nanowires, 13
 Gold(III) corrole; NIR-phosphorescence;
 Singlet oxygen sensitization. , 228
 Gold-Ni Photocatalyst, 63
 grain boundaries, 116
 Graphene, 4, 13
 graphene, 112
 Graphene Quantum Dots (GQD), 276
 Green chemistry, 11
 green hydrogen , 173
 Green synthesis, 87
 Green synthesis , 273
 growth, 125
 guanidium, 46

 Half metal, 136
 Halide perovskite; Polymer; Composites;
 Resistive switching., 188
 Hall Effects, 36
 halloysite, 171
 hard gold, 255
 hase segregation., 52
 Healthcare monitoring. , 233
 Heat Capacity, 143
 Heat loss, 157
 Heavy metal ions; Metal Chalcogenides;
 portable device; IoT-enabled., 122
 Helicity-resolved Raman spectroscopy, 140
 HER, 9
 HER , 277
 Heterojunction, 235
 Heterojunction and S-scheme photocatalyst,
 51
 Heterostructure, 63
 Heterostructures, 83
 HeterostructuresIT-B01, 33
 Heusler alloy, 149
 Heusler alloy; Thermoelectric;
 Optoelectronics. , 275
 Heuslers, 36
 Hexagonal Boron Nitride, 236
 High Density Glasses, 264
 High entropy alloys; Cu nano precipitates;
 He bubbles; positron annihilation
 spectroscopy., 258
 high entropy oxide, 119
 High figure of merit, 202
 High-Entropy Alloys, 91, 92
 High-frequency applications, 157
 High-pressure; Diffraction; Raman
 spectroscopy; Superconductivity.,
 48
 Hikami–Larkin–Nagaoka (HLN) model, 153
 Hofmeister Series, 105

 hole-transport materials, 8
 Hot Electrons, 63
 hybrid, 119
 Hybrid composite, 215
 Hybrid Composites, 183
 hybrid energy storage material., 205
 hybrid materials . , 31
 Hybrid Memristor, 66
 Hybrid modes , 136
 Hybrid nanogenerator, 203, 233
 hydrazine oxidation, 173
 Hydride embrittlement., 84
 hydrogen bonding, 50
 Hydrogen Evolution, 235
 hydrogen evolution, 12, 39
 Hydrogen evolution reaction, 179, 182
 Hydrogen evolution reaction., 184
 Hydrogen evolution reaction; Nickel cobalt
 phosphate; Graphite sheet;
 Electrodeposition., 188
 Hydrogen evolution. , 212
 Hydrogen Generation, 51
 Hydrogen generation, 179, 182
 Hydrogen gettering, 84
 Hydrogen production, 82
 Hydrogen Storage; DFT; Decoration; Kubas
 interaction., 269
 Hydrogen sulfide (H₂S) detection, 100
 hydrometallurgical, 196
 hydrothermal, 123
 Hydrothermal Method, 121
 Hydrothermal Synthesis, 142
 Hydrothermal synthesis, 199
 Hydrovoltaic effect; water evaporation;
 electrical double layer;
 hydrovoltaics , 228
 Hydroxyapatite, 37
 Hyperbolic optical metamaterials., 28
 Hysteresis, 160

 iEBL, 25
 illumination, 124
 Impedance spectroscopy, 160
 In-sensor, 121
 Indium sulfide thin films, 89
 inherent electrochemistry, 154
 Interfacial magnetism, 134
 Interlayer Excitons, 32
 Inverse spin Hall effect (ISHE) , 138
 iodine, 198
 Ion beam nanopatterning, 129
 ion implanation, 259
 Ion implantation, 97
 Ionic liquids, 17
 Ionic Liquids; Deep Eutectic Solvents;
 Sustainable Materials Chemistry;

- Sorption and Extraction Processes., 16
- IPSC, 167
- IR spectra, 267
- Iron Phosphate , 266
- Iron-pnictides, 3
- Jahn-Teller distortions; orbital ordering; spin-phonon coupling; orbital glass, 157
- Kane-Mele model, 141
- LaNiO₃, 206
- Lanthanum carbonate, 261
- large area device., 194
- Laser Ablation, 91, 92
- Laser Processing, 91, 92
- laser-scribed graphene, 245
- Lattice Thermal Conductivity, 219
- Layered double hydroxide, 187
- layered double hydroxide, 173
- Layered double hydroxides; Substrate effect; Electrodeposition., 184
- LDL, 243
- Lead free halide perovskite, 167
- Lead-free piezoelectric ceramics, 192
- Lead-Free Semiconductors., 197, 198
- Leaky integrate and fire, 71
- lectric Field, 63
- lectrochromic materials, 31
- LEDs, 70
- LEE, 7
- LEED, 30
- Li-ion Batteries, 19
- LIBs, 168
- ligand, 176
- Light–Matter Interactions, 33
- Liquid phase exfoliation, 145
- Lithium-ion, 5
- Lithium-ion hybrid capacitor., 183
- lithography, 25
- Local drug delivery., 89
- Localized surface plasmon resonance (LSPR), 87
- LOD, 250
- loss mechanism, 93
- Low-dimensional, 128
- LSPR, 105, 119
- LSPR Effect , 224
- LSPR Effect., 234
- LSPR., 63
- luminescence, 108
- Machine Learning. , 219
- Magnetic Anisotropy, 94, 150
- Magnetic anisotropy, 129
- magnetic behaviour, 216
- Magnetic damping , 134
- Magnetic materials, 2
- Magnetic phase transition , 140
- Magnetic properties, 142
- magnetic proximity effect, 2
- Magnetism, 143
- Magnetism , 63
- Magnetization dynamics, 161
- magnetization reversal, 2
- Magneto-elastic Coupling, 149
- Magneto-electrodeposition, 96
- magnetocaloric effect, 2
- Magnetoelectric, 203, 222
- Magnetoresistance, 148
- magnetoresistance, 259
- Magnetoresistance. , 140
- Magnetostriction; Strain mediated; Composite; Magnetodielectric., 211
- magnetostrictive, 222
- magnetotransport, 139
- magnetron sputtering, 194
- Magnon–magnon coupling, 138
- Material stability., 155
- materials engineering, 57
- MAX, 18
- MD simulation , 175
- Mechanical Integrity, 15
- Mechanical Properties, 99
- mechanism, 179
- melt route., 258
- membrane electrode, 184
- membranes, 17
- mesoporous, 180
- Metal halide perovskite; Photolithography; Anticounterfeiting; Reversibility., 186
- Metal nanoparticles, 184
- Metal organic framework, 217
- Metal organic frameworks, 262
- metal oxide composite; pulse reverse potential; supercapacitor; specific capacitance., 201
- metal oxide gas sensors, 173
- Metal phthalocyanine, 122
- metal-free catalyst, 181, 182
- Metal-organic framework; Single crystal structure; Electrochemical NO₃RR; Density functional theory , 180
- metal-organic frameworks (MOF), 79
- Metal-Organic-Frameworks, 208
- Metal–insulator transition; Unitary renormalization group; Spin liquid ; Strange metal ; Quantum criticality. , 158
- Metal–organic frameworks (MOFs), 45

-
- methacrylation, 238
 Micro-cavity, 73
 Micro-sampling, 232
 microbeads, 87
 Microelectrode, 245
 microfabrication, 238
 micromagnetic., 30
 Microplastics, 187
 microplastics, 22
 Microwave Absorbing Materials, 262
 Microwave absorption, 8
 Minerals Extraction, 4
 miniaturized, 210
 Minor actinides, 175
 mixed pollutant., 196
 ML models, 57
 ML., 83
 Mn doped BiFeO₃, 210
 Modified Curie-Weiss law, 170
 MOF, 259
 MOFs, 4, 196
 molecular memristor, 122
 molecular separation, 209
 Molecular simulations, 99
 Molybdenum disulphide, 85
 monoclinic, 110
 monolayer , 125
 Monte Carlo Simulation, 56
 Morphology, 94
 MOS devices, 57
 MoS₂, 4, 13, 81, 108, 125
 MoS₂ hybrids, 82
 MoS₂ monolayer, 119
 MoS₂ membrane, 200
 Mott transition, 71
 MRI, 29
 multi-bit, 122
 multibit operation, 102
 multiferroics, 2
 MWCNTs, 85
 MXene, 39, 119, 153, 173
 Mxene, 206, 214
 Mxene , 252
 MXene; Photoacoustic Imaging;
 High-frequency; Broad-Bandwidth;
 Transducers., 240
 MXenes, 4, 13, 14, 18, 100, 154, 183, 215
 Mycotoxins; Ochratoxin A; Wine;
 Electrochemical Biosensors; Food
 Safety., 66
 Mössbauer spectroscopy, 160

 N-doped graphene, 181, 182
 n-i-p heterojunction, 194
 Na-ion batteries, 252
 nanoclusters, 14

 Nanocomposite, 85
 Nanocomposite; Heterojunction; Dye
 Removal; CO₂ adsorption , 247
 nanocomposites, 171, 174
 nanocrystals, 185
 Nanofiber, 233
 Nanofiller Networks, 15
 nanoflakes, 110
 Nanogenerator, 221
 Nanogenerators, 38
 nanohybrids, 112
 Nanomaterials, 13
 Nanoparticle, 91, 92
 Nanoparticle organic network, 184
 Nanoparticles, 214
 nanoparticles, 14
 Nanoplastics, 268
 Nanopore density, 200
 Nanorobots, 268
 NASA, 40
 NCS, 24
 Negative differential resistance (NDR), 118
 Nematic superconductivity, 140
 Neural networks. , 153
 Neural Stimulating Probe, 247
 Neuromorphic Computing, 34
 Neuromorphic computing, 71
 neuromorphic computing, 102
 Neuromorphic Computing., 121
 neuromorphic devices, 234
 Neutron Diffraction , 143
 Ni₂P-SiO₂, 11
 Ni-Mn-In, 221
 Ni-V alloy, 96
 Nickelates, 34
 C/Nb₂C, 215
 NiO. , 117
 Nitric Acid, 97
 Nitrofurantoin, 191
 NLO, 70
 NLO; ATCC; Z Scan. , 120
 NMR relaxation, 127
 non-Centrosymmetric, 196
 non-centrosymmetric, 139
 Non-enzymatic, 205
 Non-linear optical properties, 101, 162
 Non-linear optics, 29
 Non-Volatile Memory, 153
 Nonlinear optics, 105
 Novel Materials, 60
 NRR, 224, 234
 Nuclear fuels, 175
 Nudged elastic band., 59

 Oblique angle deposition, 129
 ODMR, 36

- OER, 171, 180
OFDFT, 267
OLEDs, 8
Open-circuit voltage, 59
operating temperature, 173
Optical detection, 45
Optical Properties, 264
opto-electronic properties, 42
optoelectronic, 264
Optoelectronic Materials, 117
optoelectronics, 111
Orbital Current, 156
Orbital Hall Conductivity, 271
Orbital Hall Effect, 156
Orbital Hall effect, 84
Orbitronics, 271
Organic Electronics; Memristors; Capacitive Coupling , 165
organic field-effect transistors, 234
Organic memristor; Write-Once-Read-Many memory; Flexible device; Interfacial dipole modulation , 114
Organic molecules, 8
organic photovoltaics, 8
organic solar cell, 108
organic; Thin film; Charge transport; Optoelectronic materials, 106
ORR, 9
ORR catalyst, 41
ORR mechanism. , 181, 182
overall water splitting, 79
Overburden, 263
overpotential. , 226
oxide mixed phase, 97
Oxide perovskite, 210
Oxide semiconductor, 50
Oxygen evolution reaction, 213
Oxygen Evolution Reaction (OER), 226
Oxygen evolution reaction (OER). , 217
oxygen reduction reaction., 12
Oxygen reduction reaction; Core-shell nanocatalyst; Catalytic activity and stability enrichment; Morphological engineering; Electrocatalyst optimization , 223
oxygen vacancies, 69
Oxygen vacancies., 210
Oxygen vacancy, 166

p-n heterojunction, 117
p-n junction, 39
p-n junction , 232
P-vacancy, 180
pair-breaking defect, 34
Palladium quenching., 259
parkerite, 128

Pauli potential., 267
PdSeTe, 140
PDT, 242
PEDOT: PSS, 247
PEG, 243
Percolation Threshold, 15
Periodontal therapy, 89
perosvkite, 185
Perovskite, 16
perovskite materials, 52, 269
Perovskite oxide, 213
perovskite quantum dots., 14
Perovskite solar cells, 88
perovskite solar cells, 8
Perovskites, 19
perovskites, 78, 176
Peroxymonosulfate, 191
Perpendicular Magnetic Anisotropy, 147
Persistent Homology , 248
PET, 11
phase coherence length, 153
phase evolution, 256
phase transition, 252
Phonon, 98
phonon, 111
Phonon dispersion, 130
Phonon stability, 59
Phosphate glass, 163, 165, 178
phosphate glass, 68
phosphor converted LED, 108
Phosphorene, 4, 13
Photocatalysis, 208, 224, 234, 272
photocatalysis, 12, 70, 79, 232
Photocatalyst, 212
photocatalyst, 39
Photocatalysts: , 78
photocatalytic, 50
Photocatalytic activity, 225
Photocatalytic degradation, 187
Photocatalytic degradation; Fukui function; charge carrier dynamics. , 113
Photocatalytic water splitting., 83
photocharging, 41
photodegradation, 120
Photodetection, 108
photodetection, 109, 116
Photodetectors., 89
Photoelectrochemical water splitting, 194
Photoelectrochemical; Water splitting; Cu SPR; Plasmonic heterostructure., 230
photoemission spectroscopy , 128
photolithography, 238
Photoluminescence, 101, 162
photoluminescence, 52, 68
Photopolymer Resin, 88

-
- PHT, 255
 Phytochemicals, 87
 PI-STENG, 38
 Piezo-electric ceramic, 207
 piezocatalysis, 81
 Piezochromism, 19
 Piezoelectric, 80
 piezoelectric etc. , 222
 Piezoelectric properties. , 16
 Piezoelectricity, 174, 190
 piezopolarization, 224, 234
 PL, 124
 PLA, 11
 Plasmonic Damping , 105
 plastic waste management, 256
 PMN-PT, 221
 polarisation, 108
 pollutant, 112
 poly(ionic liquids), 17
 Polyaniline, 259
 Polyaniline; composites; In-situ
 polymerization; Anticorrosion. ,
 254
 Polylactic Acid, 37
 Polymer composite, 37
 polymer composite, 93
 Polymer Composites; Bent Core Liquid
 Crystals; Piezoelectricity; Density
 Functional Theory., 189
 Polymeric waste, 8
 polymerization, 31
 Polymer-carbon nanocomposites, 6
 Polynitroarenes; tetrazole; methylene bridge;
 tricationic energetic salt., 172
 Polyol synthesis, 157
 Polystyrene, 187
 polyurethane , 38
 Porous hierarchical materials, 45
 Potential Dual Imaging Probe, 29
 Power conversion efficiency (PCE). , 273
 Predictive descriptors, 56
 pressure sensors, 174
 Pressure sensors., 190
 Propellant; Viscosity, 99
 Proton Irradiation, 97
 Prussian blue, 217
 Pseudo Jahn-Teller, 4, 13
 pseudocapacitive, 210
 Punica granatum, 87
 Purcell enhancement, 73
 PUREX, 97
 PVDF nanofibers, 203
 Pyroelectric, 203
 Pyroelectricity, 207
 pyrolysis, 89
 QDs, 25
 QSL., 36
 Quantitative approach, 135
 Quantum dot, 161
 Quantum Dots, 136
 Quantum dots, 268
 Quantum fluctuations, 127
 Quantum kinetic approach, 84
 quantum magnetism, 2
 Quantum materials, 56, 84
 Quantum Spin Liquid, 56
 Quasicrystals, 257
 qubit., 36
 quenching, 266

 radiation, 171
 Radiation Effects, 264
 Radiation shielding materials, 6
 Radiation stability, 96
 Radioactive waste, 163, 165, 178
 Raman , 252
 Raman spectroscopy, 219
 Rare earth doping; Langbeinite; Inorganic
 Phosphors; NIR-Emission , 115
 rare earth elements, 255, 263
 Rare earth free permanent magnets, 94
 Rare earth nickelates, 71
 Rare earth oxides; REEs; E-waste; LEDs, 95
 Rare Genetic Disorders. , 44
 Rare-Earth, 132
 rare-earth, 30
 Rare-earth doping, 89
 Rare-earth oxides; dye degradation;
 hydrogen production. , 227
 Rashba Splitting, 19
 rate equation, 69
 Recyclable and reprocessable composites, 6
 recyclable polymers, 22
 Recycling, 256
 reduction products., 176
 refractive index, 253
 regenerative potential. , 46
 renewable energy, 7
 renewable energy., 8
 ReRAM, 66, 102
 Resistive Switching, 130
 Resistive switching, 102, 161
 resistive switching, 69
 Resistive switching , 145
 Resistive switching (RS), 118
 Resistivity, 140
 Resonant Fano, 253
 Retention , 130
 Reticular Materials, 117
 Return Loss, 262

- RF Sputtering; Thin Films;
 Magnetoresistance; Binary
 Transition Metal Alloy , 128
rGO wrapped Fe_2O_3 nanorod, 173
rGO- Cr_2O_3 composite; solution combustion
 synthesis; ethanol sensing. , 112
Rietveld refinement, 199
Ruddlesden-Popper perovskite, 170
rutile phase, 109

S-Scheme, 166
S-scheme, 235
S-scheme heterojunction, 83, 195
S-scheme pathway, 242
Salinity gradient energy, 200
Scalable Osmotic Power., 200
Scanning electron microscopy (SEM), 87
Scheelite-type material, 108
Schiff base, 250
scintillator detector, 68
Se doping, 180
SECM., 9
Seebeck coefficient, 275
selectivity., 62
self-assembly, 209
Self-healing, 244
Semiconductors, 72
Sensing, 62
Sensing , 232
Sensing Applications , 66
sensitivity, 245
separation science, 17
Sericin; Polyethylene glycol; Progesterone;
 Drug delivery system, 237
 SF_6 decomposition Gases, 276
SHI, 16
Si-based photoanode, 194
Silicene, 4, 13
silicon nanorods, 124
silk fibroin, 238
Silk Fibroin , 247
Silver nanoparticles (AgNPs); Zingiber
 officinale, 87
Single Defect Spectroscopy., 33
Single perovskites, 197, 198
single-atom catalysts, 12
sintering kinetics., 192
Skyrmion, 132, 270
Small molecule donor (SMD), 273
smart windows, 110
Sodium-Ion Batteries, 64
Soft magnetic composites, 157
sol-gel combustion, 249
Solar cells, 107
Solid particle erosion., 85
solid-state phosphor, 69
solution processing, 234
Sono-Photo-Fenton degradation, 166
Specific Capacitance, 214
specific ion effect. , 50
Spin Current, 156
Spin Filters. , 136
Spin Hall angle, 155
Spin Hall conductivity , 130
Spin polarization, 126
Spin Pumping, 151
spin reorientation , 139
Spin-Orbit Coupling, 148
Spin-orbit torque, 136
Spin-Orbital Coupling, 4, 13
Spin-reorientation transition, 147
Spin-torque ferromagnetic resonance, 136
Spinel ferrites, 41
Spintronics, 75, 155, 271
Spintronics , 132
spintronics., 2
Spin-orbit coupling (SOC), 133
SRIM, 36
Stability, 267
Stainless Steel, 97
STM , 30
Stoner-Wohlfarth Model, 150
STP, 167
Stretchable Devices, 15
Strongly correlated systems; CEF
 transitions; THz spectroscopy;
 Kondo lattice. , 143
Strontium Hexaferrites, 94
structural modulation; magnetic anisotropy;
 proximity effect; spin-state
 transition , 126
Structural phase transition, 140
Sulphur-doped g- C_3N_4 , 195
Sum Frequency Generation Vibrational
 Spectroscopy, 50
Supercapacitor, 175, 179
supercapacitor, 169
supercapacitor performance, 205
Supercapacitor., 211, 212
Supercapacitor; nickel antimony oxide;
 symmetric device; cyclic stability.,
 203
Supercapacitor; Wheat Bran; Lemon
 Extract; Green Synthesis., 193
Supercapacitors, 41
Superconducting diode effect, 133
Superconducting Diode Effect; Time reversal
 Symmetry; Inversion symmetry;
 Spin orbit coupling. , 133
Superconductivity, 3
superconductivity, 34
superlattice, 157

- supramolecular, 46
 Surface engineering, 83
 Surface modified nanostructured materials, 14
 Surface plasmon resonance (SPR), 87
 Surface plasmon resonance; Plasmonic structures; Adhesion layers, 265
 Surface-enhanced Raman spectroscopy (SERS), 187
 Sustainability., 18
 Sustainable Ammonia production; Magnesium single atom catalysts (Mg-SACs)., 187
 sustainable polymers, 22
 sustainable recovery, 263
 Swarm intelligence, 268
 Switchable NLO, 119
 Synaptic learning process, 167
 synaptic plasticity , 234
 Synaptic properties, 153
 synaptic properties., 34
 Synchrotron, 75
 Synchrotron X-ray Scattering., 15
 Synergistic effect, 148
 Synergistic effect., 215
 Synthetic ferrimagnets, 132

 Tactile sensor, 221
 TADF, 120
 Tantalum pentoxide (Ta_2O_5); Titanium dioxide (TiO_2); sol-gel; cost-effective., 245
 TCOs, 28
 TD-DFT, 273
 TENG, 38
 Terahertz (THz) Spectroscopy, 117
 Terahertz Metamaterials; Strong Coupling; Phonon-Polariton; Electromagnetically Induced Transparency, 102
 thermal instability, 216
 Thermal phonon, 253
 Thermal stability, 165
 Thermal stability , 178
 Thermal stability., 163
 Thermal transport, 98
 thermochromic, 110
 thermodynamic properties , 233
 Thermoelectric, 275
 Thermoelectric Generator; waste heat recovery; finite element modelling. , 272
 Thermoelectric material, 236
 Thermoelectric materials, 197, 198, 202, 233
 Thermoelectric materials; XPS; XRD; LFA., 201
 Thermoelectric properties, 272
 Thermoelectric; Raman spectroscopy; BOLS theory; lattice thermal conductivity. , 219
 thermoelectricity., 257
 Thin Film , 148
 Thin Film Transistors, 72
 Thin Films , 150
 threshold switching, 97
 Tin perovskite, 88
 TiO_2 , 121, 176
 TiO_2 nanoflakes, 117
 tissue repair, 46
 Titanium Nitride, 118
 TMD, 83
 TMDC. , 270
 TMDC; CDW. , 137
 TMDCs , 252
 TMDs; Hydrothermal method; Green energy; Hydrogen. , 177
 Topological defects, 136
 Topological insulator; Anharmonic phonon decay, 262
 Topological Insulators, 4, 13, 141
 topological insulators, 148
 Topological materials, 140
 Topological phonons, 130
 Topological quasicrystal approximants, 56
 topological semimetal; Magnetoresistance; Shubnikov-de Haas oscillations; Berry phase. , 145
 Topological Superconductivity, 3
 TR-MOKE, 151
 transition metal, 109
 Transition metal chalcogenides, 175
 Transition metal nitrides; nanoparticles; LSPR; plasmonics., 114
 Transition metal Oxides, 211, 212
 Transition metal oxides (TMOs), 217
 Triazatruxene; Donor; DFT; Organic Solar Cells (OSCs), 268
 triboelectric nanogenerator, 256
 MoSSe2D nanofiber; Braille; Auditory feedback;, 230
 tunable photodetectors , 148
 Tungsten boride, 267
 turbostratic graphene, 169
 Twist angles, 32
 twisted bilayer graphene, 169

 Ultrafast Dynamics, 32
 Ultrafast Spin Dynamics, 151
 Ultrahigh Seebeck coefficient, 202
 ultrasound, 81
 uninterrupted foaming, 258
 Upcycling, 11

- supercapacitive, 31
- UV sensor, 117
- UV-Vis spectroscopy, 87

- V_2O_3 , 75
- V_2O_5 , 253
- Vacancy Engineering, 224, 234
- van der Waals magnets; magnetic anomalies;
Raman Spectroscopy., 35
- vanadium dioxide, 110
- vdW Heterostructures, 32
- Vibrating Sample Magnetometry (VSM),
126
- vibrational spectroscopy, 23
- Visible light photocatalysis., 187
- Vitrification, 163, 165, 178
- VO_2 , 75
- VOC alternatives, 17

- Wannier center , 141
- Wannier-Mott Exciton, 19
- Waste valorisation; wastewater;
Polyhydroxybutyrate (PHB);
Bacillus strain., 250
- Water dissociation, 179, 182
- water purification, 198
- Water Splitting, 225
- Water splitting, 82, 166, 182
- water splitting, 173
- water splitting , 171
- Water splitting., 179, 206
- Weak Antilocalisation, 148
- Wearable Devices, 15
- Weyl semimetal. , 84
- Weyl semimetals; Magnetoresistance;
Topological surface states; Residual
resistivity ratio, 150
- Wien2k. , 272
- Wigner Formulation, 98
- Wigner transport equation, 56
- WLED, 69, 185
- Wound Healing; Bacterial Nanocellulose
(BNC); Coal-derived graphene
oxide(C-GO); Hydrogel; In vivo
studies., 240
- WS_2 , 13

- X-ray diffraction, 256
- X-ray diffraction (XRD), 87
- XPS, 170, 261
- XPS spectroscopy. , 235
- XRD, 170, 261, 264
- XRR , 147

- Yttria-stabilized zirconia; Graphitic-carbon;
UV absorption; Photocatalysis., 82
- Yttrium, 84

- Z Scan. , 70
- Z-scheme; mixed-phase TiO_2 ; B-doped
g- C_3N_4 ; ciprofloxacin (CIP). , 104
- ZFC-FC, 24
- ZIBs, 40
- ZIFs, 232
- zinc phthalocyanine, 108
- Zinc-Tin-Oxide, 72
- Zn based batteries, 9
- Zn-Ion Batteries, 40
- ZnO nanoparticles, 273
- ZnO nanostructures, 70
- ZnV_3O_8 . , 40
- Zr-Nb alloys, 84

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