SPARC
Scheme for Promotion of Academic and Research Collaboration

INTERNATIONAL SYMPOSIUM ON ADVANCED MATERIALS
ISAM 2026

MARCH 6-7, 2026

Outreach Auditorium,
Indian Institute of Technology Kanpur, Kanpur,
Uttar Pradesh, India - 208016

ORGANIZED BY DEPARTMENT OF CHEMISTRY AND SUSTAINABLE ENERGY ENGINEERING

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PROGRAM

ISAM2026
International Symposium on Advanced Materials

DAY 1 - 6TH MARCH

Friday, Session I-IV, 9h30 - 18h30

International Symposium on Advanced Materials – 2026

Session	Time	Session Description
	08h30 – 09h00	Registration
	09h10 – 09h30	Inauguration
Session I	**Session Chair: Prof. R. Gurunath, CHM, IIT Kanpur**	
	09h30 – 10h00	**Lecture 1 – Prof. Sebastian C. Peter, JNCASR, Bengaluru** Title: **Deciphering C-C Coupling in CO_2 Reduction: Advanced Nanomaterial Design Strategies**
	10h00 – 10h30	**Lecture 2 – Prof. Uttam Manna, IIT Guwahati** Title: **Design of Interfaces for Functional Liquid Wettability**
	10h30 – 11h00	**Lecture 3 – Prof. Tanmoy Maiti, IIT Kanpur** Title: **High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene**
	11h00 – 11h30	**Tea Break**
Session II	**Session Chair: Dr. Nagaraju Barsu, NCL Pune**	
	11h30 – 12h00	**Lecture 4 – Dr. Jagabandhu Kole, JSW, Mumbai** Title: **Advance Materials and Means of CCUS in Building Materials Sector**
	12h00 – 12h30	**Lecture 5 – Prof. Samir Chikkali, NCL Pune** Title: **Waste Plastic Depolymerization and Upcycling**
	12h30 – 13h00	**Lecture 6 – Prof. Venkata Krishnan, IIT Mandi** Title: **Non-Noble Metal based Sustainable Heterogeneous Catalysts for Chemical Recycling and Upcycling of Plastic Waste**
	13h00 – 14h15	**Lunch**

Session III	**Session Chair: Prof. Santosh Misra, BSBE, IIT Kanpur**	
	14h15 – 14h45	**Lecture 7 – Prof. Sujit Ghosh, IISER Pune** Title: **Critical Minerals Extraction by Pore-engineered MOFs+ for A Sustainable Future**
	14h45 – 15h15	**Lecture 8 – Prof. Pradip Pachfule, SN BOSE Institute** Title: **Harnessing Sunlight for Photocatalytic Water Splitting**
	15h15 – 15h45	**Lecture 9 – Prof. Peter Budd, The University of Manchester** Title: **Polymers of Intrinsic Microporosity (PIMs) and their Applications**
	15h45 – 16h45	**Tea Break and Poster Session**
Session IV	**Session Chair: Prof. Anand Singh, CHM, IIT Kanpur**	
	16h45 – 17h15	**Lecture 10 – Prof. R. Kothandaraman, IIT Madras** Title: **When Mn Helps – and When It Hurts: Covalency Enhancement vs Antisite Defects in Ni-Rich Layered Cathodes**
	17h15 – 17h45	**Lecture 11 – Dr. Mohana Sundararam, IOCL** Title: **Advanced Materials for Energy Storage Applications – Indian/Oil Perspective**
	17h45 – 18h15	**Lecture 12 – Dr. Anantharaj Sengeni, IIT Kanpur** Title: **Mechanistic Origins of Enhanced OER Activity in NiFe Metal Organic Frameworks**
	19h30	**Dinner**
DAY 2 - 7TH MARCH		***Saturday, Session V-VIII, 9h00 - 18h30***
Session V	**Session Chair: Prof. Kantesh Balani, MSE, IIT Kanpur**	
	09h00 – 9h30	**Lecture 13 – Prof. Ashish Garg, IIT Kanpur** Title: **Performance and Stability of Perovskite Solar Cells**
	9h30 – 10h00	**Lecture 14 – Dr. Koustuv Ray, IIT Kharagpur** Title: **In Search of Cost-effective Catalysts for the Chemical Value Chain: Examples on CO_2 Conversion, DRM and PDH**
	10h00 – 10h30	**Lecture 15 – Prof. Santhosh B. Sukumaran, NCL Pune** Title: **Molecular Architecture of Curved Nanographenes and Graphene Nanoribbons**
	10h30 – 11h00	**Lecture 16 – Dr. Nilesh Badwe, IIT Kanpur** Title: **Next Generation Materials in Semiconductor Packaging**
	11h00 – 11h30	**Tea Break**

Session VI	**Session Chair: Prof. Pratik Sen, CHM, IIT Kanpur**	
	11h30 – 12h00	**Lecture 17 – Prof. Santosh Misra, IIT Kanpur** Title: **Nanocarbon-Enforced Polymer Composites Generate Triggerable Biomaterials for Advanced Therapeutics (TrigBioD-Therapeutics)**
	12h00 – 12h30	**Lecture 18 – Prof. Nirmalya Ballav, IISER Pune** Title: **Facing the Interface: Hetero-Structured Thin Films of Coordination Polymers**
	12h30 – 13h00	**Lecture 19 – Dr. Pratyush Sinha, LOHUM** Title: **Scaling Advanced Materials from Lab to Factory**
	13h00 – 14h15	**Lunch**
Session VII	**Session Chair: Prof. M. L. N. Rao, CHM, IIT Kanpur**	
	14h15 – 14h45	**Lecture 21 – Prof. K. Muralidharan, University of Hyderabad** Title: **Main Group Materials for Health, Energy, Environment, and Defense (HEED) Applications**
	14h45 – 15h15	**Lecture 20 – Prof. Radha Boya, The University of Manchester** Title: **Monolayer Water and Ionic Memory in Angstrom-Scale Channels made from 2D materials**
	15h15 – 16h30	**Flash Presentation** **Chairs: Profs. Apparao Draksharapu & Soumyabrata Roy**
	16h30 – 17h00	**Tea Break**
Session VIII	**Session Chair: Dr. Deepti Kalsi, IIT Bombay**	
	17h00 – 17h30	**Lecture 22 – Dr. Suresh Mothika, IIT Kanpur** Title: **Functional Porous Organic Polymers (POPs) for Clean Fuel Production and Uranium Extraction**
	17h30 – 18h00	**Lecture 23 – Prof. Ashok Keerthi, The University of Manchester** Title: **Heteroatom-rich Framework Materials: Why Are They Exciting?**
	18h00 – 18h30	**Lecture 24 – Dr. Abhishek Aggarwal, IIT Indore** Title: **Designing High-Performance Energy Storage Systems for Decarbonization**
	18h30 – 18h45	**Valedictory Session**
	19h30	**Dinner**

IL–01

Deciphering C-C Coupling in CO_2 Reduction: Advanced Nanomaterial Design Strategies

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As a notorious greenhouse gas and a potential carbon feedstock, the transformation of carbon dioxide (CO_2) into high value-added fuels or chemicals has been recognized as a promising way to mitigate energy shortages and problems caused by the greenhouse effect. The greenest solution for making fuel from anthropogenic CO_2 is by utilizing abundant solar energy. To make this process economically viable, C_{2+} products are desired. The challenging multi-electron transfer and kinetically high energy barrier of C-C coupling reaction are the primary reasons for low selectivity of C_{2+} products. Starting from the fundamental aspects, this talk highlights the discovery of novel catalysts for the efficient photocatalytic CO_2 reduction C_{2+} products. It will discuss about catalyst design, in-situ techniques for the detection of intermediates and mechanistic insights through experimental and theoretical analysis for the selective photoreduction of CO_2 to C_{2+} product.

Keywords: CO_2 reduction; C-C Coupling, Advanced Material, Mechanism

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Dr. Sebastian C. Peter received his MSc (2000) from St. Thomas College, Thrissur, Calicut University and MTech (2002) from Cochin University of Science and Technology. He received his Ph. D. in chemistry from the University of Münster, Germany (2006). He was a post-doctoral fellow at Max Plank Institute for Chemical Physics of Solids, Dresden, Germany (2006-07) and Northwestern University, USA (2007-10). Dr. Peter joined as a faculty fellow at New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore in 2010. His broad research interests include the development of solid-state inorganic materials for various applications ranging fuel cell, CO_2 reduction and in condensed matter physics. He has more than 210 peer reviewed publications and five patents. He was invited and attended around 100 national and international conferences. He is the recipient of Young Investigator awards from ACS (2013), RSC (2017) and IOP (2016). He was awarded Ramanujan fellowship (2010), MRSI medal (2016), SwarnaJayanti Fellowship in the category of Chemical Science (2018) and CRSI medal (2020), SMC Medal (2022) and IAAM fellow (2022). He is a member of American Chemical Society, Royal Society of Chemistry, ASM international, Chemical Research Society of India, Material Research Society of India, International Union of Crystallography, Indian National Young Academy of Science and Society for Material Chemistry of India. He is the founder and director of the start-up “Breathe Applied Sciences Pvt Ltd” and entered into the final round of the NRG-COSIA XPRIZE 20 million USD prize on waste CO_2 utilization. His team is the only one team in final round of the competition earning half a million USD as milestone prize. Breathe Applied Sciences Pvt Ltd has been selected as one of the best 100 start-ups by Karnataka state Government in 2017 through ELEVATE-100. CleanEquity, Monaco (2019) selected CO_2 reduction technology as the second best in the global level. His team scaled-up the technology CO_2 to methanol from the lab to pilot level with a capacity of 300 kg CO_2 per day. In 2021, Technology Development Board of the DST awarded National Technology Award for this development. In Dec 2021, his start-up has been selected as the winner of the KPMG ENRich21 on the theme The Global Corporation: preparing for the Low-Carbon World. He also received National Prize on CO_2 reduction and green hydrogen production instituted by CNR Rao foundation and ETU of JNCASR in 2022. Dr. Peter is also featured in the “75 under 50: Scientists Shaping Today's India” by the DST and selected for J C Bose Diamond Jubilee Lecture Award by IAAM. In 2023, Dr. Peter led Breathe to win the competition MaterialsNext 4.0 hosted by Tata Steel. Dr. Peter Received Research Partnerships and Industry Translation Medal from Chirantan Rasayan Sanstha and Materials Science Annual Prize from MRSI in 2023. Dr. Peter is also part of the Editorial Advisory Board of Journal of the American Chemical Society, Chemical Science, ChemSusChem and Journal of Solid State Chemistry. He has received the scientist Medal in 2024 from IAAM. He also elected as the fellow of Indian Academy of Science in 2024. His startup Breathe became the winner of National Startup Award in the category of “Sustainability Champion” from Government of India in 2024. He has been selected for the Rajib Goyal Prize in 2024. Dr. Peter is currently a visiting Professor at IIT Roorkee and Adjunct Professor at Shiv Nadar University. In 2026, he received the VAVIK industrial research award on his contribution to applied research in India.

IL–02

Design of Interfaces for Functional Liquid Wettability

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The nature-inspired wettabilities that either extremely repelled or allowed effortless sliding of different liquids (oil/water) in air or underwater are with immense potential for various prospective applications. In common practice, essential chemistry and appropriate topography that conferred the special liquid wettabilities were mostly and generally achieved by associating delicate chemistry. Eventually, the synthesized materials suffered from poor durability issues. In the literature, very few designs are capable of providing durable bio-inspired wettability—but fabrication processes remain generally complex. Moreover, the integration of various other relevant physical properties with such durable liquid wettability is highly challenging to achieve. Hence, design of robust bio-inspired liquid wettability following a simple fabrication process that would allow to integrate different and relevant physical properties is utmost important for various fundamental and applied contexts. Related to this, recently, our research group has extended 1,4-conjugate addition reactions between amine and acrylates at ambient conditions for systematic and orthogonal tailoring of topography and surface free energy to derive a range of functional materials embedded with a wide range of bio-inspired wettability having immense potential in a wide range of applications related to environment, health and energy.[1-10] In this lecture, I will reveal fundamental parameters that control slippery property on solid surface and strategy for developing smart polymeric surfaces with rewritable and liquid-selective wettability.[2]

Keywords: Polymeric material, liquid wettability, 1,4-conjugate addition reaction, rewritable, reactive coating

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Prof. Uttam Manna, Fellow of the Royal Society of Chemistry (FRSC), is a professor in the Department of Chemistry and also affiliated with the Centre for Nanotechnology at the Indian Institute Technology Guwahati (IITG). He obtained his Integrated Ph.D. from the Indian Institute of Science (IISc), Bangalore, in 2011, followed by postdoctoral research at the University of Wisconsin–Madison, USA from 2011 to 2015.

Prof. Manna has been recognized internationally as an emerging and pioneering investigator by *Journal of Materials Chemistry A* (2018), *Chemical Communications* (2020, 2023), *Nanoscale* (2021), and *Chemical Society Reviews* (2022). His accolades include the CRSI Bronze Medal (2023), the Humboldt research Fellowship for experienced researchers (2021) and the International Excellent Fellowship from KIT, Germany (2024). The Society for Polymer Science, India (SPSI), has recognized him with the Prof. K. Kishore Award for year 2023-24.

IL–03

High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene

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

Tanmoy Maiti

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Dr. Tanmoy Maiti is Rahul and Namita Gautam Chair Professor in the Department of Material Science and Engineering at the Indian Institute of Technology Kanpur, India. Prior to joining IIT Kanpur, he did his post-doctoral research in Lawrence Berkeley National Laboratory, USA. Dr. Maiti received his Ph.D. in Materials Science and Engineering from The Pennsylvania State University, USA. His research interests span the areas of Thermoelectrics, Plasmonics, and Oxide electronic materials and devices.

IL–04

Advance Materials & Means of CCUS in Building Materials Sector

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Portland cement is one of the most common building materials used worldwide. However, its production contributes approximately 7% of global CO_2 emissions, with India's average emissions estimated at approximately 529 kg of CO_2 per tonne of cement. Regardless of its significant carbon footprint, Portland cement is expected to continue dominating the construction market due to its proven performance, versatility, durability, and strong customer acceptance. A common strategy to reduce CO_2 emissions in the cement industry involves partially replacing clinker with supplementary cementitious materials (SCMs) such as fly ash and slag. Nevertheless, these measures cannot completely eliminate emissions, as a substantial amount of CO_2 is released during the limestone calcination in the clinker production process.

As India undertakes the commitment to attain net-zero emissions by the year 2070, Carbon Capture and Utilization (CCU) has become one of the key approaches that would be employed to control the CO_2 emission. In this context, several industrial-scale technologies are emerging that enable the capture of CO_2 and its utilization through various strategies to produce advanced materials, which can subsequently be incorporated into the construction value chain.

Several CO_2 sequestration strategies are currently being worked out, including carbonation curing, mineral carbonation, and carbonation of recycled aggregates. In carbonation curing, high-purity captured CO_2 is injected into freshly mixed concrete at an early age, where it reacts with calcium hydroxide ($Ca(OH)_2$) and calcium silicate hydrate (C-S-H) to form nanoscale calcium carbonate ($CaCO_3$). This reaction produces stable hydration products that enhance the performance of concrete. Mineral carbonation is another circular economy practice can be used as well, in which industrial solid wastes such as steel slags (LD and EAF slag), mining and mineral processing wastes, and incinerator residues are carbonated using accelerated carbonation technology (ACT). Through ACT, these materials can be converted into value-added products such as SCM and raw material for cement and concrete production. Similarly, construction and demolition waste can undergo carbonation treatment and be reused as recycled aggregates within the construction value chain. In addition, some advanced binders enable CO_2 storage during the hardening process, such as calcium silicate–based cement (CSC) and carbon-activated steel slag used for masonry and precast applications.

In parallel, advanced low-carbon binders are also emerging to further reduce the clinker content and overall CO_2 footprint. These include geopolymer-based binders, slag cement, iron ore slime-based binders, and graphene-based binders. Hence, advancements in these technologies collectively contribute to building a more sustainable construction ecosystem by valorizing industrial waste, reducing CO_2 emissions, and supporting the transition toward net-zero emission targets.

Keywords: Cement, Carbon Capture and Utilization (CCU), Construction value chain, binders

Dr. Jagabandhu Kole

Senior V. P. & Head, - R & D, JSW Cements Limited.

Dr. Jagabandhu Kole is an experienced and seasoned researcher with over 35 years of expertise in building materials, including cement and cement-based products (such as grouts, floor hardeners, tile adhesives, cementitious waterproofing and repair products, ready-mix plaster, concrete, micro-concrete, and many more). His work also extents to construction chemicals and sustainable structural materials. Last one decade working in circular economy space specially in the field slag utilizations in various building products and particularly conversion into cement and cementitious materials. The Carbon capture & utilization to de-carb the Cement Industry is another area of his passion for work on national & Global interest.

Dr Kole earned his Ph.D. in Chemical Technology from the University of Calcutta, with a focus on raw materials mobilization in cement manufacturing. With more than 25 patents, Dr. Kole has developed 150-200 products across the building and construction sectors, with a strong emphasis on waste utilization. His innovations include cement additives, admixtures, grinding aids, and various construction chemicals, covering a wide range of water proofing systems, performance based coatings, flooring products etc. based the materials like bitumen, SBR latex, acrylics, epoxy, polyurethane, poly-aspartic, polyester, poly-urea, and PCE.

Currently his work mostly focuses on advancing circular economy initiatives aimed at achieving ultra-low and zero-carbon products in cement manufacturing. He has worked extensively on utilizing various slags (such as GGBS, BOF, AOD, EAF, LHF, KR, etc.) in cement production, improving their reactivity both mechanically and throug h chemical transformations into cementitious materials, like GGBS. His efforts contribute to the circular economy by addressing disposal challenges and conserving natural resources. In his present endeavour, he is working closely with 10-12 IIT’s to resolve the current burning problems of building and structural sectors, Cement & allied Industries with respect to delocalisation of process, energy uses & sources, alternative materials etc.

Dr.Kole has recently secured six patent grants, which serve as critical tools in the cement industry's transformative journey toward de-carbonization. His contributions have earned him several accolades, including the "Excellence in Research and Development – Corporate" award by World of Concrete recently.

Having visited countries like Germany, the USA, the UK, Belgium, Austria, Dubai, Thailand, Taiwan, Singapore, Malaysia and Bangladesh, Dr Kole has immensely contributed to research, participated in conferences, and evaluated various technologies in cement and allied products. Currently across globe he is well recognised and very famous scientist in decarbonisation, circular economy and sustainability space.

He is an active member of several organizations, including BIS, CMA, the Indian Chemical Society, the Indian Ceramic Society, the Faculty of Dr Fixit Institute, and the ISO certification body.

IL–05

Waste plastic depolymerization and upcycling

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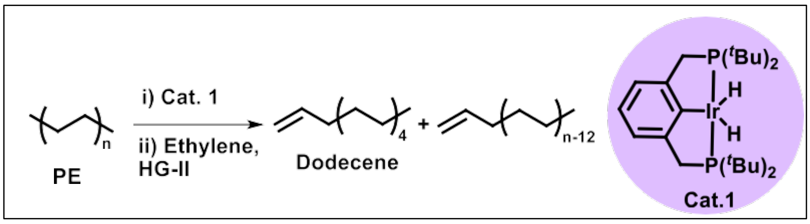
India produces approximately 20 million tons of plastic every year, yet only a meager 15-20% of this plastic is recycled, presenting a significant challenge to plastic waste management. The remaining waste predominantly ends up into landfills or leaks into water bodies, causing severe environmental pollution. Thus, the current linear model of plastic utilization, that is, take, make, use, and throw is not sustainable. To address this critical issue, we have undertaken in-depth investigation about plastic depolymerization and upcycling. A brief overview of segregation, plastic to fuel and downstream processing will be presented.

The second part of the talk will deal with depolymerization of waste plastic to value added long-chain alkenes. The PCP-iridium complex Cat.1 (Fig. 1) catalyzes the dehydrogenation of commercial, as well as post-consumer polyethylene waste to produce dehydrogenated polyethylene (DHP). The DHP was subjected to an ethylene cross-metathesis reaction in the presence of suitable catalysts. Through meticulous optimization of reaction parameters, 63% selectivity toward dodecene was achieved. The practical significance of our method has been demonstrated by subjecting the plastic waste to dehydrogenation followed by ethylene metathesis to produce dodecene as a major product, together with long-chain alkenes.[1,2]



***Scheme 1:** Schematic representation of PE depolymerization to long-chain alkenes.*

Keywords: Waste Plastic, Polyethylene, Depolymerization,Upcycling

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Samir Chikkali earned his Ph.D. under the supervision of Prof. Dietrich Gudat from the University of Stuttgart, Germany. Subsequently, he did postdoctoral research with Prof. Joost Reek at the University of Amsterdam, the Netherlands and Prof. Stefan Mecking at the University of Konstanz, Germany. In 2012 he returned to India and joined CSIR-National Chemical Laboratory (CSIR-NCL), Pune, to start his independent research career. He has guided 10 Ph.D. students, 6 post-docs and 15 project assistants. Currently he leads a team of 15 highly motivated researchers in organometallics, polyolefins, and renewable/degradable polymers. His scientific interests are- olefin polymerization, renewables to polymers, P-stereogenic phosphines, asymmetric hydrogenation/hydroformylation and depolymerization. His honours and awards include a summer fellowship from the Indian Academy of Science, DPI (Dutch Polymer Institute) postdoctoral fellowship, AvH (Alexander von Humboldt) postdoctoral fellowship, the Ramanujan (DST) Fellowship, Best Scientist Award by North Maharashtra University, Scientist of the Year Award 2016-2017 by NCL-RF, Young Associate of Maharashtra Academy of Sciences 2017, Professor Kaushal Kishore Memorial Award 2020 by Society of Polymer Science, India (SPSI), 10th National Award 2020, by Ministry of Chemicals and Fertilizers, Government of India, Scientist of the Year Award (above 40 years of age) 2021-2022 by NCL-RF and Fellow of Maharashtra Academy of Sciences 2024.

His research in polymers and organometallic catalysis has been rightly recognized by peers with top-quality publications and has been equally applauded by the industry with sponsored/consultancy projects. He has published over ~90 papers in international journals of high repute (including J. Am. Chem. Soc.; Angew. Chem. Int. Ed.; Macromolecules; J. Org. Chem.; Inorg. Chem.; Organometallics, Prog. Polym. Sci. etc), he is an inventor on 11 patents (including, WO, US, EP, JP, DE etc) and has edited a book on metal catalyzed polymerization (https://www.taylorfrancis.com/books/metal-catalyzed-polymerization-samir-chikkali/e/10.1201/9781315153919). He is currently an Associate Editor of “Bulletin of Materials Science” jointly published by Springer Nature and Indian Academy of Science.

Industry Sponsored Projects: RIL, HPCL, GAIL
Consultancy Projects: RIL, HMEL, OICL, CFL
GoI Projects: DST (1), DST-SERB (4), DSIR (1), CSIR (2), DCPC (1) Technical Service Projects: CFL, GARWARE, etc.
Technologies Transferred: 1

Ph.D. Students Guided: 12
Ph.D. students currently working: 8

IL–06

Non-Noble Metal based Sustainable Heterogeneous Catalysts for Chemical Recycling and Upcycling of Plastic Waste

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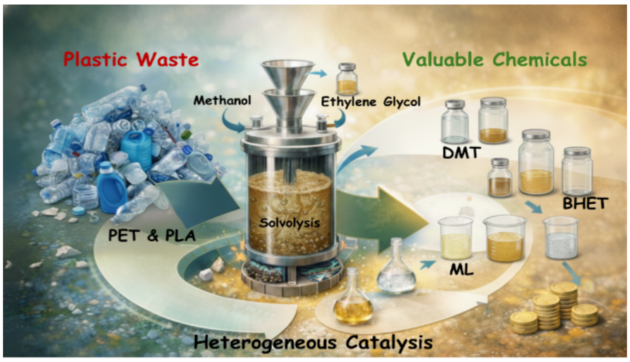
Chemical recycling and upcycling of plastic wastes offer sustainable solutions to mitigate environmental pollution and to enable circular plastic economy. Our research group has developed several non-noble metal based sustainable heterogeneous catalytic strategies for the depolymerization and valorization of widely used plastics, including polylactic acid (PLA) and polyethylene terephthalate (PET), as presented in Scheme 1. PLA waste was selectively depolymerized to methyl lactate (ML) under mild conditions employing Cu-CeO_2 catalysts, achieving complete conversion with high product selectivity. In addition, PET waste bottles were effectively converted into value-added monomers such as bis(2-hydroxyethyl) terephthalate (BHET) and dimethyl terephthalate (DMT) through glycolysis and methanolysis using layered double hydroxides, nickel phosphides, and supported metal-based catalytic systems. In all cases, the reaction parameters were systematically optimized, and excellent catalyst reusability was demonstrated. Green chemistry metrics and life cycle assessment confirmed the environmental and energy advantages of the developed protocols. Overall, these studies highlight sustainable, low chemical input catalytic routes for closed and open-loop recycling of plastic waste into valuable chemicals.



Scheme 1: Representation of the conversion of plastic waste into valuable chemicals (Credit: Google Gemini).

Keywords: Heterogeneous catalysis, nanomaterials, plastic upcycling, value-added products, circular economy

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Prof. Dr. Venkata Krishnan completed his Ph.D. in Chemistry in 2006 from University of Stuttgart, Germany. Subsequently, he worked as a postdoctoral researcher at University of Pennsylvania, U.S.A. from 2006 to 2010 and then as a research associate at National Institute for Materials Science (NIMS), Tsukuba, Japan from 2010 to 2012. He joined as a faculty at the Indian Institute of Technology (IIT) Mandi in April 2012 and is currently a full professor. His research group is mainly working in the field of Green Chemistry and Heterogeneous Catalysis for Energy and Environment Applications. He has successfully guided 13 Ph.D. and 35 M.Sc. students and is currently guiding 1 postdoc, 10 Ph.D. and 5 M.Sc. students, in addition to several short-term research interns. Prof. Krishnan has published more than 200 articles in well reputed international journals, 14 book chapters and has been granted 6 patents. He has an h-index of 65 as per Google Scholar. In addition to being a reviewer for several scientific journals, he serves as an Associate Editor of the New Journal of Chemistry, published by the Royal Society of Chemistry (RSC) and is on the Editorial Advisory Board of ACS ES&T Engineering, published by the American Chemical Society (ACS). He has been bestowed with several awards, including CRSI Bronze Medal, MRSI Medal, DST INSPIRE faculty award, IIT Mandi foundation day award for excellence in teaching, MANA research fellowship, DoE postdoctoral fellowship, DFG doctoral fellowship, DAAD visiting scholar fellowship, etc. Besides teaching and research, he has served IIT Mandi in various administrative positions, such as first warden of the main hostel in permanent campus, founding coordinator of Advanced Materials Research Center (AMRC), Associate Dean Research and Dean of Sponsored Research, Industrial Consultancy, and International Relations (SRIC & IR). He has also served as Director of IIT Mandi Catalyst (a technology business incubator) and Director of IIT Mandi iHub and HCi foundation (a technology innovation hub). He also serves on several scientific and administrative committees at institute, national and international levels. Apart from academics, he likes reading books and is interested in linguistics.

IL–07

Critical Minerals Extraction by Pore-engineered MOFs+ for A Sustainable Future

Sujit K. Ghosh*

Professor, Department of Chemistry, Indian Institute of Science Education and Research (IISER) Pune, Dr. Homi Bhaba Road, Pashan, Pune 411008, India.

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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 (Scheme 1).

Scheme 1: *Advanced porous materials for efficient extraction of various metal ions.*

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Sujit is currently a Professor of Chemistry at IISER Pune, India. Before joining IISER in 2009 he did his postdoctoral work with this year’s one of the Chemistry Nobel prize winners, Prof. Susumu Kitagawa, Japan. His research interest is metal–organic frameworks (MOFs) and related porous materials for extraction of critical minerals, sustainable environment and safe drinking water. He has published >175 papers with average IF ~8, with total citations > 18000 and h-index-68. Recently he got selected for "The Distinguished Lectureship Award" by the Chemical Society of Japan (CSJ), Friedrich Wilhelm Bessel Research Prize by the Humboldt Foundation, Germany.

IL–08

Harnessing Sunlight for Photocatalytic Water Splitting

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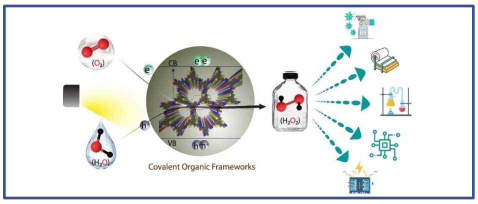
Covalent organic frameworks (COFs) are crystalline, porous, two- and three-dimensional materials distinguished by their tunable topologies and versatile functionalities.[1] Owing to their intrinsic microporosity, adjustable pore dimensions, high surface areas, improved chemical stability, and scalable synthetic routes, COFs have emerged as promising platforms for diverse applications.[2] In particular, imine-linked COFs exhibit notable chemical robustness, enabling their use in gas storage, heterogeneous catalysis, energy storage systems, and proton-conducting membranes.[3] In our efforts to develop efficient, recyclable photocatalysts for solar-driven water splitting and hydrogen evolution, we designed crystalline, porous, heptazine-based COFs that consistently produce hydrogen with high efficiency. To address challenges associated with co-catalysts and sacrificial electron donors for hydrogen generation, we developed hydrazone-linked COFs that directly generate hydrogen peroxide photocatalytically from pure water - highlighting the broad potential of COFs in photochemical transformations.[4,5] Additionally, we have demonstrated that COFs with optimized donor-acceptor architectures and controlled spatial separation exhibit enhanced photocatalytic performance for hydrogen peroxide production.[6]



Scheme 1: *The schematic for photocatalytic hydrogen peroxide generation using covalent organic frameworks.*

Keywords: covalent organic frameworks, photocatalysis, water splitting, hydrogen, hydrogen peroxide

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EXPERIENCE

Associate Professor

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Research on covalent organic frameworks (COFs) for their applications in photocatalytic water splitting, hydrogen peroxide generation, organocatalysis and energy storage.

Assistant Professor

S. N. Bose National Centre for Basic Sciences, Kolkata, India.

08/2021 - 12/2024 Kolkata, India.

Research on covalent organic frameworks (COFs) for water splitting and energy storage.

Postdoctorate Research Fellow

Technische Universität Berlin, Germany.

03/2019 - 08/2021 Berlin, Germany.

Research on covalent organic frameworks (COFs) for their application in photocatalytic water splitting, visible light mediated radical polymerization and electrocatalysis.

Alexander von Humboldt Postdoctorate Fellow

Technische Universität Berlin, Germany.

01/2017 - 02/2019 Berlin, Germany.

Research on covalent organic frameworks (COFs), covalent triazine frameworks (CTFs) and porous carbons for photocatalysis and electrochemical energy storage.

JSPS Postdoctoral Research Fellow

National Institute of Advanced Industrial Science and Technology, Osaka, Japan.

10/2015 - 10/2016 Osaka, Japan.

Research on metal organic frameworks (MOFs) and porous carbons for electrochemical energy storage, catalytic hydrogen evolution from ammonia borane and formic acid, and heterogeneous catalysis.

Postdoctorate Research Fellow

National Institute of Advanced Industrial Science and Technology, Osaka, Japan.

09/2014 - 10/2015 Osaka, Japan

Research on metal organic frameworks (MOFs) and porous carbons for energy storage applications.

FELLOWSHIP AND AWARDS

Thieme Chemistry Journals Award

From: Editorial Boards of Synthesis, Synlett and Synfacts

02/2025

Young Associate of Maharashtra Academy of Sciences

From: Maharashtra Academy of Sciences, India.

12/2018

Alexander von Humboldt Postdoctorate Fellowship

From: Alexander von Humboldt (AvH) Foundation, Germany.

01/2017 - 02/2019

JSPS Postdoctorate Fellowship

From: Japan Society of Promotion of Science (JSPS), Japan.

10/2015 - 09/2017

EDUCATION

Doctor of Philosophy (Ph.D.)

CSIR-National Chemical Laboratory, Pune, India.

01/2009 - 08/2014

GPA
8.14 / 10

Master of Sciences (M.Sc.): Chemistry

Solapur University, Solapur, India.

06/2006 - 05/2008

%
63.5 / 100

Bachelor of Sciences (B.Sc.): Chemistry

Shivaji University, Kolhapur, India.

06/2003 - 05/2006

%
67.3 / 100

PUBLICATIONS

- Published more than 95 papers in international peer-reviewed journals including Nature Chemistry, JACS, Angewandte Chemie, Chemical Science, Chemistry of Materials, ChemComm, etc.
- An US Patent on porous metal organic framework composites for hydrogen (H_2) storage
- A Book Chapter in a book entitled 'Metal-Organic Framework Materials' published by UK: John Wiley & Sons Ltd.

SKILLS

- Synthesis of COFs, MOFs and porous polymers
- Single crystal and powder X-ray diffraction (XRD)
- Refinement of crystal data, structure solution and disorder modeling
- Characterization of porous materials using NMR, FT-IR, mass spectroscopy and elemental analyses
- Handling of water splitting and CO_2 reduction set-up

RESEARCH INTERESTS

Covalent Organic Frameworks
Photocatalysis
Energy Storage
Water Splitting
Metal Organic Frameworks
Hydrogen Storage
Materials Chemistry
Heterogeneous Catalysis

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IL–09

Polymers of Intrinsic Microporosity (PIMs) and their Applications

PETER M. BUDD*

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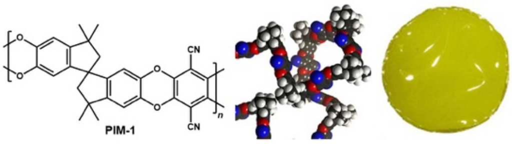
Polymers of intrinsic microporosity (PIMs) exhibit high free volume and behave like microporous materials (pore size <2 nm) because their rigid, contorted macromolecular backbones cannot pack together efficiently in the solid state. Since the first publications on solution-processible PIMs in 2004,[1] there has been considerable research on this class of polymers and a wide variety of applications have been explored, including membranes for molecular separations and sensors. PIMs can be tailored for bespoke applications in various ways, including chemical modification and thermal or photo-oxidative treatment. The development of PIMs will be outlined and recent progress discussed.

Membrane processes have a key role to play in a sustainable future, as they can be compact and energy-efficient compared to conventional separation processes. However, there is scope for improving the sustainability of the materials that are used; greener solvents are being explored for PIM synthesis.[2] Membrane applications of PIMs have been constrained by concerns about the effects of physical ageing and plasticization. One way to improve long-term membrane performance is through the addition of fillers, however, poor compatibility between filler and polymer can be an issue.[3] A key development is the recognition that, depending on the polymerization conditions, a PIM sample may contain a variety of polymer topologies, including branched, cyclic and network structures. The distribution of polymer topologies can have a profound impact on membrane performance and long-term behaviour.[4] Recently the focus of much research has shifted to commercially realistic thin-film composite (TFC) membranes, rather than thick films. TFC membranes have been prepared in hollow-fibre form, as well as flat-sheet form.[5]



Scheme 1: *Chemical structure of the prototypical polymer of intrinsic microporosity PIM-1, molecular model of a fragment of PIM-1, and a self-standing membrane formed of PIM-1*

Keywords: Polymer, Topology, Membrane, Molecular separation

References

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Professor of Polymer Chemistry

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Peter Budd is a Professor of Polymer Chemistry at the University of Manchester. He studied at Manchester for his BSc in Chemistry (1978) and his PhD in Polymer Chemistry (1981). After eight years as a research chemist at the BP Research Centre, Sunbury-on-Thames, he returned to Manchester in 1989. His research involves the development of novel polymers for a variety of applications, including molecular separations by membrane processes. He is a co-inventor of the class of polymers referred to as Polymers of Intrinsic Microporosity (PIMs).

SOME RECENT PUBLICATIONS

Í. Martínez-Visus, L. Carrillo-Sánchez, J. Miguel Luque-Alled, A.B. Foster, P.M. Budd, C. Téllez and J. Coronas, Synergy of Block and Microporous Polymers with Tailored Zeolitic Imidazole Frameworks for Membrane-Based Direct Air Capture, *Adv. Mater.*, 2025 DOI: 10.1002/adma.202510740

B. Qiu, M. Yu, M. Alshurafa, P. López-Porfiri, M. Perez-Page, A.B. Foster, P.M. Budd, X. Fan and P. Gorgojo, GO as gutter layer in superglassy thin film composite membranes for enhanced gas separation, *J. Membr. Sci.*, 2025, **732**, 124245. DOI: 10.1016/j.memsci.2025.124245

C. Rizzuto, F. Nardelli, M. Monteleone, L. Calucci, C.G. Bezzu, M. Carta, E. Tocci, E. Esposito, G. De Luca, B. Comesaña-Gándara, N.B. McKeown, B. Sayginer, P.M. Budd, J.C. Jansen and A. Fuoco, Unravelling the origin of enhanced CO2 selectivity in amine-PIM-1 during mixed gas permeation, *J. Mater. Chem. A*, 2025, **13**, 17865- 17876. DOI: 10.1039/D4TA08839E

M. Pérez-Miana, J.M. Luque-Alled, Á. Mayoral, I. Martínez-Visus, A.B. Foster, P.M. Budd and J. Coronas, Amphiphilic zeolitic imidazolate framework for improved CO2 separation in PIM-1 mixed matrix membranes, *Angew. Chem. Int. Ed.*, 2025, **64**, e202420879. DOI: /10.1002/anie.202420879

X. Yang, Z. Feng, M. Alshurafa, M. Yu, A.B. Foster, H. Zhai, T. Yuan, Y. Xiao, C. D'Agostino, L. Ai, Ma. Perez- Page, K. Smith, F. Foglia, A. Lovett, T.S. Miller, J. Chen, P.M. Budd and S.M. Holmes, Durable Proton Exchange Membrane Based on Polymers of Intrinsic Microporosity for Fuel Cells, *Adv. Mater.*, 2025, **37**, 2419534. DOI: 10.1002/adma.202419534

A.B. Foster, M Yu, M. Alshurafa and P.M. Budd, Impact of polymer topology on physical aging of thin film composite membranes based on PIM-1, cPIM-1, and associated blends, *Macromolecules*, 2025, **58**, 4289- 4299. DOI: 10.1021/acs.macromol.4c02657

A. Ayyaz, A.B. Foster, L. Cseri, G. Szekely and P.M. Budd, Greener synthesis of the polymer of intrinsic microporosity PIM-1 for gas separation, *ACS Sustainable Chem. Eng.*, 2025, **13**, 2784-2792. DOI: 10.1021/acssuschemeng.4c08475

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IL–10

When Mn Helps—and When It Hurts: Covalency Enhancement vs Antisite Defects in Ni-Rich Layered Cathodes

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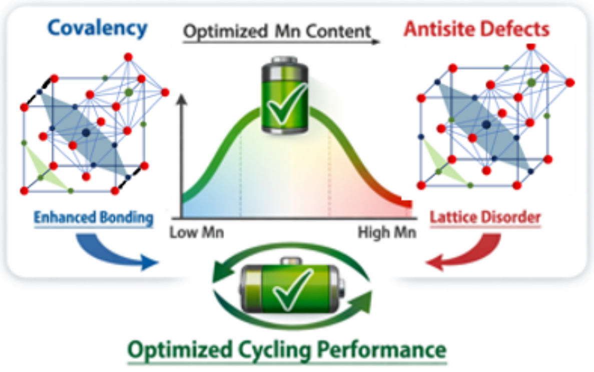
Nickel-rich layered oxide cathodes have emerged as one of the leaders for next-generation lithium-ion batteries (LIBs), offering high energy density and relatively lower cobalt content. However, challenges such as cation mixing, structural degradation, and poor cycle retention persist. In this study, we systematically investigate the effect of controlled manganese (Mn) substitution in NCA cathode materials synthesized via a solid-state route, targeting enhanced structural and electrochemical stability by manipulating the material's covalency and antisite disorder. Mn introduction enhances the hypervalent state of Ni and Co, leading to increased covalency and structural defects. Besides, due to Jahn-Teller distortion, particles undergo pulverization with the introduction of Mn. This talk describes how the enhanced covalency, antisite defects, particle size variation, and Li^+ diffusion kinetics are followed using XRD, XPS, EELS, and GITT to understand the capacity retention and cycling performance of the Mn-substituted NCA series.



Scheme1*: Summarizing the Effect of Enhanced Covalency and Antisite Disorder in Deciding the Battery Performance*

Keywords: Cathode Material, Anti-site disorder, Covalency, Jahn-Teller Distortion, Depth Profiling

References

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Annamalai & Santhi Rajendran Chair Professor

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Professional Appointments:

Jul 2021– current : Professor, Dept. Chemistry, IIT Madras, Chennai, India
Jun 2016 – Jun 2021 : Associate Professor, Dept. Chemistry, IIT Madras, Chennai, India
Mar 2011 – Jun 2016 : Assistant Professor, IIT Madras, Chennai, India
Mar 2009 – Feb 2011 : Research Associate, National Research Council of Canada, Ottawa (Supervisor: Dr Christina Bock)
March 2007 – Feb 2009 : Post Doctoral Researcher, Dept. ChemicalEngineering, Michigan State University, East Lansing, USA (Supervisor: Prof Scott Calabrese Barton)

Awards and Honours:

Name of the Award	**From**
ASC-Masila Vijaya Award -2024 (for innovative patent)	The Academy of Sciences, Chennai
IESA Researcher of the year-2024	India Energy Storage Alliance (IESA)
SMC Bronze Medal – 2023	Society of Materials Chemistry, BARC, India
CRSI Bronze Medal – 2023	Chemical Research Society of India
Australia Awards Fellowships to collaborate with U. Sydney	Department of Foreign Affairs and Trade
Trend Setter Grant Award-2023 (Rs 49 lakhs = $58k)	The Energy Consortium, IIT Madras
CSR Changemaker Award-2023	IIT Madras
Amara Raja Award-2021	Electrochemical Society of India, Bengaluru
Fellow of the Royal Society of Chemistry (2020)	RSC
Fellow of the Academy of Sciences, Chennai	Academy of Sciences, Chennai
Gold Medallist in BSc, University 1st Rank holder	Bharathiar University, Coimbatore

IL–11

Advanced materials for Energy Storage Applications – Indian/Oil perspective

P. Mohana Sundaram*

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The Presentation focusses on method of production of Carbon Nano Tube from Refinery feed stocks and its applications in Lead acid and Li-Ion battery applications and focusses on battery grade graphite from Needle coke / Pet coke for production of Li-Ion battery grade graphite. Further discusses on production of high initial coulombic efficiency (ICE) hard carbon and its properties on Na-Ion battery applications. It will provide a glimpse of Bipolar Lead acid battery performance for SLI and e-Rickshaw applications. It covers detailed knowledge on CNT in advanced polymer composite for thermal conductive and electrically conductive applications also.

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Professional Summary

Twenty-two years' research experience in oil and alternative energy area preferably around Lube processing, process development of carbon nanotube and batteries. Successfully commercialized process for preparing carcinogenic free rubber process oil. Currently working in Alternative energy area including carbon nanotube and battery. Successfully developed MWCNT process and commercial implementation is under progress. Further key contributor in development of CNT additized lead acid battery and completed successful commercial trial at leading battery manufacturer. It has provided the pathway for IOCL to enter the battery business and rolling out of CNT additized lead acid battery in retail outlets. Utilizing innovation and strategic leadership skills expedite SWCNT, hard carbon process development and launching of Sodium-ion battery for sustainable future and battery grade graphite from Petroleum coke.

Experience

Indian Oil Corporation- R&D Centre (2003 to Till Now)

- Steered a team to develop Sodium-Ion battery along with preparation of hard carbon anode for sustainable energy storage
- Key lead role in prototype development of Lead Acid based Electrolyzer (Battolyzer) for Domestic/Industrial/Laboratory applications
- Lead a project for Process development for production of Carbon Nanotube (CNT) Process development for CNT catalyst and Purification process
- Major contributor in product development for CNT additized Li-Ion battery & Lead-acid battery
- Directing strategic commercial roll out of CNT additized LAB in IOCL retail outlet along with Leading battery manufacturer as a vision of IOCL as a key player in energy storage business
- Major contribution in Specialty products development – CNT-Concrete, CNT-Polymer and Bipolar lead acid battery etc.
- Major contribution in development of High thermal conductive and electrical conductive polymer composites
- Major contribution in development of Battery grade graphite from Petroleum coke
- Process development of Carcinogenic free rubber process oil and Bitumen

Technology commercialization Experience

- ✓ Successfully commercialized a process for development of Carcinogenic free rubber process oil in one of IOCL refinery and it has steered IOCL as a major export grade rubber process oil supplier for Indian tyre manufacturers

Under Commercialization Experience

- ✓ MWCNT Process/ Catalyst / MWCNT Purification – To Set up 100 TPA plant in one of IOCL refinery
- ✓ After Successful commercial trial run at leading battery manufacturer , to roll out CNT-LAB in IOCL retail outlet along with leading battery manufacturer under progress

Process Owner/mentor experience for IOCL start-up scheme

- ✓ Graphene based super capacitor development and Integration with battery EV –Hyderabad (India)based Start-up
- ✓ Nano Silicon- Carbon composite for Li-Ion battery Anode – Odisha (India) based Startup successfully mentored for launch a product

Fluid Control Research Institute (2002-2003)

- ✓ Key developer role in CFD development and Oil Flow measurement

Academic Credentials

Total no of Patents: 45 (Indian & International)

No of Publications: 6

IL–12

Mechanistic Origins of Enhanced OER Activity in NiFe Metal–Organic Frameworks

Anantharaj Sengeni*

Laboratory for Electrocatalysis and Energy (LEE), Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India

The enhanced oxygen evolution reaction (OER) activity of Ni–Fe systems in alkaline media is well established, yet the underlying mechanistic origin remains unresolved. Herein, we present a comparative mechanistic study of a bimetallic NiFe metal–organic framework (NiFe MOF) and its monometallic Ni MOF and Fe MOF counterparts, synthesized using 1,4-benzene dicarboxylic acid (H_2BDC) as the organic linker. In 1.0 M KOH, the NiFe MOF delivers markedly improved OER performance, exhibiting lower overpotential and a reduced Tafel slope relative to both monometallic analogues. Interestingly, the trend in electrochemically active surface area, inferred from double-layer capacitance measurements, does not correlate with catalytic activity, indicating an intrinsic, molecular-level enhancement rather than surface-area-driven effects. Mechanistic interrogation through pH-dependent kinetics and chemical probe experiments using methanol and tetramethylammonium hydroxide (TMAH) reveals that the NiFe MOF facilitates a kinetically favored lattice oxygen mechanism (LOM), whereas Ni MOF and Fe MOF primarily operate via the slower adsorbate evolution mechanism (AEM). Notably, despite the emergence of LOM, the rate-determining step in the NiFe MOF remains the $OH^* \rightarrow O^*$ oxidation, challenging conventional mechanistic assumptions. These findings demonstrate that efficient LOM can proceed even under high OH* coverage, highlighting a previously underappreciated aspect of Ni–Fe synergy and emphasizing the need for systematic mechanistic studies to unravel its role in OER electrocatalysis.

ANANTHARAJ SENGENI

Assistant Professor, Department of Chemistry, IIT Kanpur

Email: ananths@iitk.ac.in | Google Scholar: https://scholar.google.com/citations?user=b2mYUxwAAAAJ&hl=en

ORCID: **0000-0002-3265-2455** | Research Group: https://www.ananthsteamlee.com/

ADDRESS

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Department of Chemistry,
IIT Kanpur
+91-9487768836

EDUCATION

Ph.D., Electrochemistry
AcSIR, CSIR-CECRI, India
(2018)

PUBLICATION METRICS

- **110 peer-reviewed publications**
- **14,500+ citations**
- **h-index: 51** (*Google Scholar*)
- Author of **highly cited reviews and perspectives** shaping best practices in electrocatalysis

FUNDED RESEARCH

- **PMECRG from ANRF (72 lakhs)**
- **Several proposals are under review**

RECOGNITIONS

- Rising Star of Chemistry, Research.com *(2025)*
- Associate, Indian Academy of Sciences, Bengaluru *(2023)*
- Waseda Research Award for High-Impact Publication (2022)
- Ramanujan Faculty Fellowship, SERB, India *(2022)*
- ECS India Section S.K. Rangarajan Graduate Student Award *(2017)*

RESEARCH IDENTITY

Electrochemist and electrocatalysis researcher specializing in **energy conversion**, **rigorous catalyst benchmarking**, and **low-/no-Pt catalyst design** for water splitting and related reactions.

ACADEMIC APPOINTMENTS

Assistant Professor (Grade-I) — IIT Kanpur, India *(09/2023–Present)*
Assistant Professor (Research) — SRM Institute of Science & Technology, India *(04/2023–08/2023)*
Assistant Professor (Junior Researcher) — Waseda Research Institute for Science and Engineering, Japan *(04/2021–03/2023)*
JSPS Postdoctoral Fellow — Waseda University, Japan *(01/2019–03/2021)*

SELECTED PUBLICATIONS (Full List)

1. Angewandte Chemie International Edition, 2021, 60 (43), 23051-23067
2. Angewandte Chemie International Edition, 2021, 60 (35), 18981-19006h-index: 51
3. ACS Energy Letters, 2021, 6 (4), 1607-1611
4. Energy & Environmental Science, 2018, 11 (4), 744-771
5. ACS Energy Letters, 2019. 4 (6), 1260-1264

RESEARCH CONTRIBUTIONS (WHAT SETS ME APART)

- **Redefined electrocatalyst screening standards** by identifying artefacts and proposing rigorous benchmarking protocols now widely cited
- Designed **ultra-low Pt and Pt-free electrocatalysts**, including architectures achieving **~200× noble-metal reduction**
- Advanced **self-supported and high-current-density OER electrodes** (≥1000–2000 mA cm^{-2})
- Broad materials expertise: **metal oxides, hydroxides, chalcogenides, precatalysts**, and dealloyed systems
- Active programs in **HER, OER, MOR**, and electrolyzer-relevant electrode architectures

RESEARCH SUPERVISION (Group Page)

- **Ph.D. students:** 11 (ongoing)
- **Postdoctoral fellows:** 2 (ongoing)
- **MSc students:** 7 (1 completed, 5 ongoing)

REFERENCES

- Dr. Subrata Kundu
  CSIR-CECRI, India
- Prof. Suguru Noda
  Waseda University, Japan

IL–13

Improving Performance and Stability of Perovskite Solar Cells

Ashish Garg*
Department of Sustainable Energy Engineering, IIT Kanpur
Email: ashishg@iitk.ac.in

Since their emergence in 2009, perovskite solar cells have come a long way with top efficiencies approaching 27%. Despite all the high-efficiency claims, its commercial implementation has not been possible, primarily because of poor atmospheric stability, driven by multiple factors. This talk will focus on strategies to improve the stability of perovskite solar cells and on detailed investigations of the underlying physical mechanisms.

Ashish Garg

Professor and Head,

Sustainable Energy Engineering
Chandrakanta Kesavan Center for Energy Policy and Climate
Solutions Kotak School of Sustainability
Indian Institute of Technology Kanpur

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Webpage: https://sites.google.com/view/ashish-garg-iitk-group/

Ashish Garg is currently Professor and the Head of Sustainable Energy Engineering at the Indian Institute of Technology (IIT) Kanpur. He played the lead role in founding several sustainability-related entities and actions at IIT Kanpur since 2020, including the Department of Sustainable Energy Engineering, Kesavan Center for Energy Policy and Climate Solutions, and Kotak School of Sustainability, securing a significant amount of external funding. His research, largely funded by the Department of Science and Technology, is on different aspects of clean energy and sustainability, with current interests in solar photovoltaics, energy harvesting, hydrogen, recycling, decarbonization, and NetZero matters. He currently leads the Schmidt Sciences Initiatives for building an academic network on energy modelling and decarbonization. He has coauthored over 200 research publications and has guided/co-guided more than 45 Masters and PhD theses. He is a regular speaker and panellist on several forums related to sustainability. He is a Materials Engineer and Scientist by training and has studied at NIT Nagpur, IISc Bangalore and University of Cambridge for his undergraduate, postgraduate and doctoral degrees.

IL–14

In search of cost-effective catalysts for the chemical value chain: Examples on CO_2 conversion, DRM and PDH

Rahul Kumar, Athira P, Sunil Kumar Sahoo, Koustuv Ray*

Department of Chemical Engineering, IIT Kharagpur, Kharagpur-721302

Detailed abstract

In the present energy and environmental context, conversion of small molecules such as carbon dioxide (CO_2), methane or propane has drawn massive interests into academia and industry. To facilitate converting these molecules, relevant catalytic processes are known but the challenge is to design a cost-effective catalyst. The processes to be discussed in light of heterogeneous catalyst development are thermochemical and photochemical conversion of CO_2, dry reforming of methane (DRM), and Non-oxidative dehydrogenation of Propane (PDH). The activity-property correlations are often found to set design rules by providing rationality to the catalytic activity trend. One such approach is descriptor based catalyst screening which has become popular in the past one decade to heterogeneous catalysis community. We have demonstrated structure-activity relationships and proposed descriptors for thermocatalytic CO_2 conversion to Methane [a, b]. Moreover, combining specific and relevant characterization information we established structure-property-activity relations in photocatalytic CO_2 conversion to methanol [c]. We have explained the intrinsic kinetics and carbon deposition behaviour using Nickel and Nickel based alloy (Ni_3Co, Ni_3Fe, Ni_3Cu) catalysts in DRM, providing a rationalized approach to catalyst development [d, e]. Finally, our recent work is focussing on optimizing the amount of Iron oxide and Vanadium oxide into Chromium oxide to formulate such mixed metal oxides as better alternative catalysts for commercial PDH process.

Keywords: Nickel based alloy, descriptor, catalytic turnover frequency, mixed metal oxide, structure-activity relationship

References

[a] Ray, K.; Deo, G. A potential descriptor for the CO_2 hydrogenation to CH_4 over Al_2O_3 supported Ni and Ni-based alloy catalysts. *Applied Catalysis B: Environmental* **2017,** 218, 525-537.

[b] Kumar, R.; P, A.; Prabhakar, J. K.; Nayek, S. C.; Apte, P. A.; Deo, G. Benchmarking potential catalysts and choice of descriptor for CO_2 methanation using transition metal based catalysts. *Applied Catalysis A: General* **2024**, 687, 119957-119970.

[c] Sahoo, S. K.; P, A.; Ray, K.; Pandey, D. Addition of CuO to form CuO/TiO_2 and CuO/ZnO heterojunctions for photocatalytic CO2 conversion to methanol. *Chemical Physics Letters* **2024**, 856, 141678–141687.

[d] Ray, K.; Sengupta, S.; Deo, G. Reforming and Cracking of CH_4 over Al_2O_3 supported Ni, Ni-Fe and Ni-Co catalysts. *Fuel Processing Technology* **2017**, 156, 195-203.

[e] Ray, K.; Sandupatla, A. S.; Deo, G. Activity and stability descriptors of Ni based alloy catalysts for dry reforming of methane: A density functional theory study. *International Journal of Quantum Chemistry,* **2021**, *121 (e26580)1-7.*

Dr. Koustuv Ray

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Department of Chemical Engineering
Indian Institute of Technology Kharagpur
Kharagpur-721302, West Bengal, India
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Office: +91-3222-284582, Mobile: +91-8004616428

PROFESSIONAL EXPERIENCE

Designation	Year	Department	Institution
Assistant Professor	December 2018 - Present	Chemical Engineering	IIT Kharagpur
Project Engineer	August 2018 - November 2018	Chemical Engineering	IIT Kanpur

EDUCATION

Degree	Specialization	Year	Institution	CGPA/Rank
Doctor of Philosophy	Heterogeneous Catalysis, Density Functional Theory	July 2013 - June 2018	IIT Kanpur	10.00/1
Master of Technology	Chemical Engineering	July 2011 - May 2013	IIT Kanpur	10.00/1
Bachelor of Engineering	Chemical Engineering	July 2007 – May 2011	Jadavpur University	9.09/2

TEACHING RESPONSIBILITIES

Subject as Instructor	Reaction Engineering, Mass Transfer-II, Petroleum Refinery Engineering, Computer Aided Process Engineering
Subject as Tutor	Engineering Thermodynamics (NPTEL)
Laboratory as Instructor	Fuel, Fluid Flow, Process Equipment Design, Reaction Engineering, Instrumentation and Process Control

RESEARCH STUDENTS' GUIDANCE

Curriculum	Number	Graduated	On-going
Postdoctoral fellow	3	n.a.	3
Doctor of Philosophy	5	1	4 (2 are PMRF)
Master of Technology	17	16	1
Bachelor of Technology 5 Yr	16	15	1
Bachelor of Technology 4 Yr	13	11	2

RESEARCH INTERESTS

Heterogeneous catalysis, DFT and Machine Learning, Process modelling and simulation

ACADEMIC ACHIEVEMENTS

PROJECTS as PI/Co-PI: **6** (Submitted -2, Running-2, Completed-2), Funding Agency: (DBT, Ministry of Steel, ISRO, BIRAC, DST/SERB, IIT Kharagpur)

SCIENTIFIC & INDUSTRIAL COLLABORATION: MoU with Ulm University (Germany), Organic Recycling Systems Limited (India)

LIST OF PUBLICATIONS:

- *Total Number of Publications – 26 (After PhD – 21), Total Citations – 762, h-index: 13*
- *Google Scholar Link: Koustuv Ray - Google Scholar*

CONFERENCE/WORKSHOP/SYMPOSIUM (till date) – 32

INVITED LECTURE/PANEL DISCUSSION (till date) - 11

Other Activities: Reviewed journal articles, PMRF Annual Review, various academic and administrative responsibilities

IL–15

Molecular Architecture of Curved Nanographenes and Graphene Nanoribbons

Santhosh Babu Sukumaran[a,b]

[a]Organic Chemistry Division, National Chemical Laboratory (CSIR-NCL), Dr. Homi Bhabha Road, Pune-411008,

[b]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201 002, India.

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Nanographenes (NGs) and graphene nanoribbons (GNRs), molecular cut-outs of graphene sheets, represent an important platform bridging discrete organic molecules and bulk carbon materials.[1,2] NGs broadly encompass subgraphene fragments with lateral dimensions ranging from 1 to 100 nm, offering tunable electronic and optical properties governed by size, edge structure, and functionalization.[2] Although top-down fabrication methods enable large-scale production, they often lack atomic precision, limiting fine control over structure–property relationships. In contrast, bottom-up solution-phase synthesis provides molecular-level precision, enabling rational design of nanographene architectures with tailored functionalities. Among emerging strategies, the introduction of non-planarity into nanographene frameworks has gained significant attention. Structural distortions such as helicity, incorporation of non-benzenoid rings, and heteroatom doping modulate π-conjugation, strain distribution, and intermolecular interactions, thereby tuning electronic, optical, and energy-storage properties. These curved and topologically engineered graphenoid systems open new avenues for advanced functional materials. Inspired by these concepts, we have designed and synthesized a series of hexabenzocoronene-based non-planar NGs and GNRs with precise structural control. Their structural, photophysical, and electrochemical properties were systematically investigated, highlighting their potential applications in energy storage and as luminescent materials.[3]

References

[1] Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A. *Science* **2004**, *306*, 666.

[2] Narita, A.; Wang, X.-Y.; Feng, X.; Müllen, K. *Chem. Soc. Rev.* **2015**, *44*, 6616–6643.

[3] (a) Kumar, V.; Venugopal, G.; Jadhav, A. B.; Dongre, S. D.; Gonnade, R.; Kumar, J.; Babu, S. S. *Angew. Chem. Int. Ed.* **2025**, 202422125.

(b) Dongre, S. D.; Kumar, V.; Jadhav, A. B.; Venugopal, G.; Kumar, J.; Babu, S. S. *Angew. Chem. Int. Ed.* **2024**, e202420767.

(c) Kumar, V.; Bharathkumar, H. J.; Dongre, S. D.; Gonnade, R.; Krishnamoorthy, K.; Babu, S. S. *Angew. Chem. Int. Ed.* **2023**, *62*, e202311657.

(d) Kumar, V.; Dongre, S. D.; Venugopal, G.; Narayanan, A.; Babu, S. S. *Chem. Commun.* **2024**, *60*, 2024-003707.

(e) Venugopal, G.; Kumar, V.; Jadhav, A. B.; Dongre, S. D.; Khan, A.; Gonnade, R.; Kumar, J.; Babu, S. S. *Chem. Eur. J.* **2024**, *30*, e202304169.

SANTHOSH BABU SUKUMARAN

Senior Principal Scientist & Professor
Organic Chemistry Division
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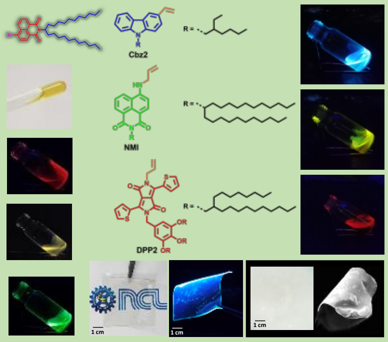
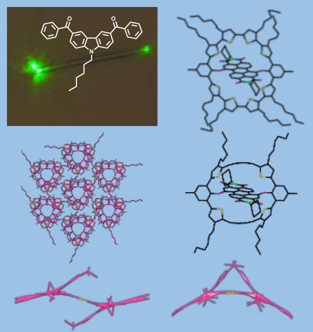
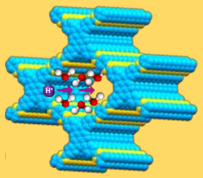
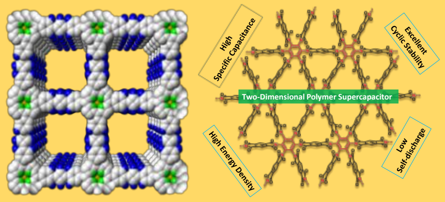
Web: https://sbsukumaran.wixsite.com/ncl-csir

Professional and Research Experience

Oct. 2024-to present	Senior Principal Scientist, CSIR-NCL, Pune, India & Professor, AcSIR
Oct. 2020-Oct. 2024	Principal Scientist, CSIR-NCL, Pune, India & Associate Professor, AcSIR
Oct. 2016-Oct. 2020	Senior Scientist, CSIR-NCL, Pune, India & Assistant Professor, AcSIR
Sep. 2014- Sep. 2016	Adhoc Scientist, CSIR-NCL, Pune, India
Sep. 2012- Aug. 2014	Marie Curie-AUL incoming postdoctoral fellow in the research group of Prof. Davide Bonifazi, University of Namur, Belgium
Nov. 2010-Apr. 2012	Postdoctoral fellow in the research group of Dr. Takashi Nakanishi, National Institute for Materials Science (NIMS), Japan
Sep. 2009-Oct. 2010	Postdoctoral fellow in the research group of Prof. Dr. Helmuth Möhwald and Dr. Takashi Nakanishi, Max Planck Institute of Colloids and Interfaces, Germany
Aug. 2004-Aug. 2009	Ph. D. Mentor: Dr. A. Ajayaghosh, Photosciences and Photonics Group, CSIR-NIIST, Trivandrum, India Thesis Title: "Control on Optical and Morphological Properties of Oligo(*p*-phenylenevinylene) Self-assemblies"

Research Interests

Solvent-free Organic Liquids	**Functional Organic Molecules & π-Extended Nanographenes**	**2D-Polymers for Catalysis and Energy Applications**
 **CT, Phosphorescent, and TADF Liquids** **Polymerizable Liquids for Large-Area Films**	 Phosphorescent & TADF Materials Helical Nanographenes D-A Based Macrocycles	**2D-Polymers for** **H₂ production** **Proton Conduction** **Energy Storage**  

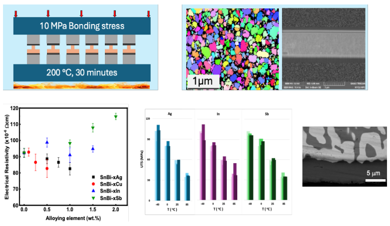
IL–16

Next Generation Materials in Semiconductor Packaging

Gulnaz Parween[a], Ankush Kumar[a,b], Radhakrishnan Sriram[a], Waqar Malik[a], Chih Chen[c],
Nilesh U. Badwe[a]

[a]Department of Materials Science and Engineering, IIT Kanpur, Kanpur, UP 208016.
[b]International College of Semiconductor Technology, NYCU, Hsinchu 300093, Taiwan.
[c]Department of Materials Science and Engineering, NYCU, Hsinchu 300093, Taiwan.
Email: nbadwe@iitk.ac.in

As transistor scaling approaches the limits of Moore's law, system-level performance gains are increasingly driven by "More-than-Moore" strategies centered on advanced packaging. Moore's law for packaging emphasizes heterogeneous integration combining logic, memory, photonics, and specialized chiplets within a single module to deliver functionality beyond monolithic scaling. 2.5D interposers and 3D IC stacking enable high-bandwidth, low-latency interconnects but introduce new manufacturing and reliability challenges. Fine-pitch interconnects necessitate direct Cu–Cu bonding due to limitations of solders at the first level interconnections. Large package sizes and coefficient of thermal expansion mismatch lead to high warpage, driving the need for high reliability low-temperature solders at the second level interconnections. This talk will summarize our efforts to enable the next generation packaging through different interconnect materials technologies.



Keywords: Semiconductor Packaging, Heterogeneous Integration, Interconnects, Cu-Cu bonding, Low Temperature Solders

References

[1] Tummala, R. *Proc. Pan Pacific Symp.* **2019**, *24*, 1.

[2] Kumar, A.; Chen, C.; Badwe, N. *J. Taiwan Inst. Chem. Eng.* **2025**, *182*, 106601.

[3] Parween, G.; Chen, B. Y.; Tran, D. P.; Chen, C.; Badwe, N. *Proc. IEEE EDTM* **2024**, *8*, 1–3.

Nilesh Badwe

Associate Professor
Department of Materials Science and Engineering at IIT Kanpur.

Prof. Nilesh Badwe is currently an Associate Professor in the Department of Materials Science and Engineering at IIT Kanpur. His research primarily focuses on interconnect materials, mechanical behavior of metallic materials and alloy design for various applications through process-structure-property correlations. He has published over 20 journal articles, conference proceedings and book chapters. Prior to joining IIT Kanpur in 2021, he spent ~5.5 years in Intel Corporation where he served as Staff Packaging Engineer and Materials Technologist. Prof. Badwe has obtained his B.Tech. from IIT Bombay in Metallurgical Engineering and Materials Science and Ph.D. from Arizona State University in Materials Science and Engineering. He serves as an Associate Editor for the journal Microelectronics Reliability.

IL–17

Nanocarbon-Enforced Polymer Composites Generate Triggerable Biomaterials for Advanced Therapeutics (TrigBioD-Therapeutics)

Niranjan Chatterjee,[a] Adheeti A. Agarwal,[a] Sandarbh Kumar,[a] Santosh Kumar Misra[a,b,c]*

[a]Department of Biological Sciences & Bioengineering, Indian Institute of Technology Kanpur, UP, India 208016
[b]The Mehta family Centre for Engineering in Medicine, Indian Institute of Technology Kanpur, UP, India 208016
[c]Centre of Excellence in Point-of-care Diagnosis, Gangwal School of Medical Sciences & Technology, Indian Institute of Technology Kanpur, UP, India 208016
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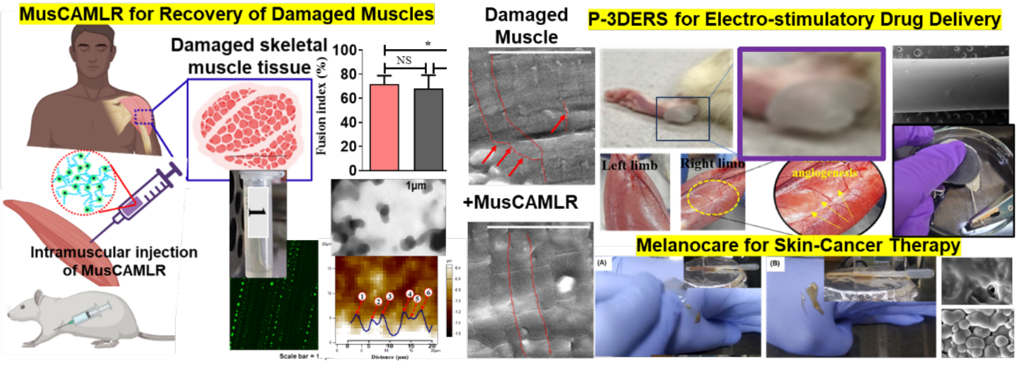
The advancements in the therapeutic methods over the past two decades have greatly played a major role in increasing the longevity of individuals but according to the World Health Organization (WHO), “people are living longer-but with more disability”. Most of the times such sufferings are result of sub-optimal or over-dosing of medication due to uncontrolled availability of therapeutics. To counter this shortcoming, approach of using triggerable biomaterials for advanced therapeutics (TrigBioD-Therapeutics) has taken center stage. TrigBioD-Therapeutics ranges from use of nanotechnology-based solutions, to injectable hydrogels, to lipid-based drug carriers, drug patches, drug delivery grafts etc. To generate such TrigBioD-Therapeutics, we have utilized various forms of nanocarbon-enforced polymer composites and fabricated **MusCAMLR**,[1-3] **Melanocare**,[4] and **P-3DERS**[5] for controlled recovery from muscular injury and cachexia and therapy against melanoma.



Scheme 1: *TrigBioD-Therapeutics for controlled recovery from muscular injury and therapy against melanoma.*

Keywords: Nanocarbon, Polymer, Mechano-stimulation, Hydrogel, Electrostimulation.

References

[1] Chatterjee, N., & Misra, S. K. *ACS Applied Materials & Interfaces*, **2023**, *15*(23), 27533-27547.
[2] ***Granted Indian Patent*** No. 533077,15/04/2024; Santosh Kumar Misra, Niranjan Chatterjee.
[3] Chatterjee, N.; Agarwal, A. & Misra*, S. Repression of the phospho-STAT3 Signaling via Nano-Engineered Delivery of an Inhibitor Prevents Skeletal Muscle Degradation During Doxorubicin-Induced Cancer Cachexia.
[4] ***Granted Indian Patent*** No. 504,008, 2024; Santosh K Misra, Dhirendra S. Katti, Sreyashi Das.
[5] Kumar, S.; Chatterjee, N.; Misra, S. K. *Langmuir* **2024**, *40*, 11858–11872.

1. Name and full correspondence address: **Dr. Santosh Kumar Misra, Ph.D.**
Associate Professor, Prof. T. R. Vishwanathan Young Faculty Fellow for Excellence in Teaching,
BioMeDHs Lab (Laboratory of Biomedical Materials & Devices for Human Sustainability)
Dept. of Biological Sciences & Bioengineering, & Mehta Family Centre for Engineering in Medicine, &
Centre for Excellence in PoC Diagnosis, GSMST, Indian Institute of Technology, Kanpur, Uttar Pradesh,
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Email: skmisra@iitk.ac.in; https://scholar.google.com/citations?user=qP9e2NYAAAAJ&hl=en

2. Email(s) and contact number(s): Email: skmisra@iitk.ac.in; Ph: 512-679-4013

3. Institution: Indian Institute of Technology, Kanpur, Uttar Pradesh, INDIA

4. Date of Birth: August 16, 1983, India

5. Academic Qualification (Undergraduate Onwards)

	Degree	**Year**	**Subject**	**University**	**% Marks**
1	B. Sc.	2002	Botany, Chemistry	DDU, Gorakhpur	67
2	M. Sc.	2005	Organic Chemistry	Lucknow university	64
3	Ph.D.	2013	Bio-organic chemistry	IISc, Bangalore	Gold medal

6. Work experience (in chronological order)

S.N.	**Position held**	**Name of the Institution**	**From**	**To**
1	Associate Professor	IIT Kanpur	Jan, 2023	-
2	Asst. Professor	IIT Kanpur	Oct, 2018	Dec, 2022
3	Research Scientist	UIUC, IL, USA	Aug, 2016	Oct, 2018
4	Postdoctoral Researcher	UIUC, IL, USA	Oct, 2013	Aug, 2016

7. Professional Recognition/ Award/ Prize/ Certificate, Fellowship received by the applicant

S.N.	**Name of the award**	**Award Agency**	**Year**
1	Bronze-Medal-2025	Society for Materials Chemistry (SMC), India	**2025**
2	Prof. T.R. Viswanathan Young Faculty Fellowship in Teaching Excellence	IIT Kanpur	**2023-2026**
3	Ramalingaswami Fellowship	DBT, India	2019-2024
4	Guha Research Gold Medal for Best Thesis	IISc, Bangalore	2013

8. Publications

[**Bibliography**-Total publications: 90+**(Avg. Impact Factor per publication 7.0+)** Total Citations: **3500+**; Total Impact: **700+**; h-index:**36**; i10 index: **65**. **Patents Granted/Applied**: 15 (10+5); Books edited: 1; Book chapters co-authored: 9; **Expert Talks**: 25+; **Oral conference presentations**: 20+; **Conference poster presentations**: 35+; **Research Grants** (completed/being executed): 10+5].

Selected Publications/In Submission/In Review/ Published/Accepted/In Press

1) Niranjan Chatterjee, Adheeti A. Agarwal, **Santosh Kumar Misra**,* Nanoengineered Therapeutics for Repression of the phospho-STAT3 Signaling Prevents Skeletal Muscle Degradation in Chemotherapy-Induced Cancer Cachexia (Manuscript in Review)
2) Niranjan Chatterjee, Urvashi Pandita, **Santosh K Misra**,* Surface Passivated Nanocarbon Generates Phase-Separated Hydrogel Meshwork for Skeletal Muscle Tissue Engineering (In review)
3) **Santosh K. Misra**,1 Ketan Dighe,1 Pranay Saha,1 Teresa Aditya, Muhammad S. Khan, Maha Alafeef, Parikshit Moitra, and Dipanjan Pan, Electro-stimulated Graphene-Polymer Nanocomposites Enable Wearable Patches with Feedback-Controlled Drug Release. ***Adv Healthcare Mater.*** 2025 (Accepted) (**I.F. 9.5**)
4) Aditya Teresa1, Pranay Saha1, **Santosh K. Misra1**, Maha Alafeef, Priyanka Ray, Enrique A. Daza, Aaron S. Schwartz-Duval, Indu Tripathi, Dipanjan Pan, Spatio-temporal nano-biomineralization and pro-antibiotic release for synergistically combatting multidrug-resistant bacteria. *Materials Today*, 2025, 88, 64-77 (**I.F. 21.5**)
5) Kaushal R. Shakya, Niranjan Chatterjee, **Santosh K. Misra**, Vivek Verma, A bacterial cellulose-polydopamine based injectable hydrogel for enhanced hemostasis in acute wounds. *Biomaterials Science*, 2025, 2025, 13, 3307-3324 (**I.F. 5.8**)
6) Niranjan Chatterjee, **Santosh Kumar Misra*,** Nanocarbon-Enforced Anisotropic MusCAMLR for Rapid Rescue of Mechanically Damaged Skeletal Muscles, *ACS Applied Materials & Interfaces,* 2023, 15 (23), 27533–27547. (**IF. 10.2**)
7) Xiangyu Zhang,1 **Santosh Kumar Misra**,1 Parikshit Moitra, Xiuli Zhang, Se-Jin Jeong, Jeremiah Stitham, Astrid Rodriguez-Velez, Arick Park, Yu-Sheng Yeh, William E Gillanders, Daping Fan, Abhinav Diwan, Jaehyung Cho, Slava Epelman, Irfan J Lodhi, Dipanjan Pan, Babak Razani, Use of acidic nanoparticles to rescue macrophage lysosomal dysfunction in atherosclerosis. *Autophagy*, 2022, 1-18. (**IF. 16.2**)
8) Parinaz Fathi, Hailey J Knox, Dinabandhu Sar, Indu Tripathi, Fatemeh Ostadhossein, **Santosh K Misra**, Mandy B Esch, Jefferson Chan, Dipanjan Pan, Biodegradable Biliverdin Nanoparticles for Efficient Photoacoustic Imaging. ***ACS nano*** **2019**, 13 (7), 7690-7704. **(IF: 15.8)**
9) **Santosh K. Misra**, Fatemeh Ostadhossein, Ramya Babu, Joseph Kus, Divya Tankasala, Andre Sutrisno, Corinne R. Bromfield, and Dipanjan Pan, 3D-Printed Multidrug-Eluting Stent from Graphene-Nanoplatelet-Doped Biodegradable Polymer Composite. ***Adv. Healthcare Mater.*****, 2017,** 6 (11), 1700008. **(IF: 11)**
10) **Santosh K. Misra**, Sarwat Naz, Paturu Kondaiah and Santanu Bhattacharya, A Cationic Cholesterol based Nanocarrier for the Delivery of p53-EGFP-C3 Plasmid to Cancer cells. ***Biomaterials***, **2014,** 35, 1334-1346. **(IF: 12.5)**

9. Details of relevant patents.

- Analyte Sensing for Eye Injuries and Conditions, D Pan, SK Misra, MR Gartia, LT Labriola, USA 10,400,262, 2019, Granted
- Transdermal gel for transdermal melanoma therapy and a process thereof, SK Misra, DS Katti, Sreyashi Das, Application No. 202211042880; Patent No. 504,008, 2024, INDIA, Granted
- A Musculo-responsive polymer carbon composite for assisting myotubular regeneration (MusCAMLR) and process thereof, SK Misra, Niranajn Chatterjee, Application No. 202211076408; Patent No. 533,077, 2024, INDIA, Granted
- A Biodegradable Silica Based Therapeutic Carrier and Process of Synthesizing the same, Santosh K. Misra, Dohare, Akanksha, Niranjan Chatterjee, Application No. 202411056645; Patent No. 575844, 2025, INDIA, Granted

IL–18

Facing the Interface: Hetero-Structured Thin Films of Coordination Polymers

Nirmalya Ballav*

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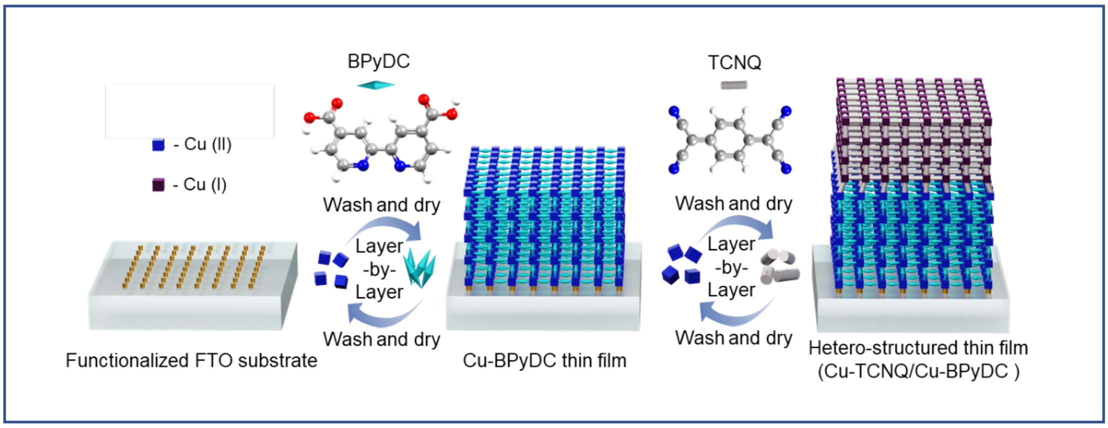
Hetero-structured thin films of electrically insulating transition metal oxides are important research platforms for the realization of interesting interfacial phenomena like emergent magnetism, metallic conduction, high-mobility electron gas, culminating to superconductivity. Here, we have focused on the fabrication of hetero-structured thin films of coordination polymers (CPs) and measurements of electrical conductance across the thin films. CPs are crystalline solids that are constructed upon an extended coordination of metal centers and organic linkers, and are also often found to be electrical insulators. Using Cu-based CPs, we have designed various distinctive hetero-structures with different organic ligands and respective thin films were grown on functionalized Au and FTO (fluorine doped tin oxide) substrates by employing the layer-by-layer (LbL) technique. Electrical transport measurements across the thin films revealed emergence of p-n junction interface and an unusual metallic conduction was identified which was attributed to be due to charge-transfer across the interface. Also, light-induced reversible perturbation of the p-n junction interface was observed. Overall, the results obtained open up new avenues for the design and development of functional materials in thin film configurations for various electronic and electrochemical device applications.



Keywords: thin film, hetero-structure, interface, coordination polymers, electrical conductivity

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Nirmalya Ballav completed MSc in Organic Chemistry (2000) and PhD in Physical Chemistry (2005) from University of Calcutta, India. Before joining IISER Pune as an Assistant Professor in 2011, he was a postdoctoral fellow at Applied Physical Chemistry, University of Heidelberg, Germany (2005-2008) and a senior postdoctoral fellow at the Laboratory for Micro and Nanotechnology, Paul Scherrer Institute (ETH Domain), Switzerland (2008-2011). His primary research focuses on interfacial materials chemistry – from fundamental to applications – and research platforms include coordination polymers, low-dimensional materials, and magnetic semiconductors. He was a visiting scientist at Paul Scherrer Institute, Switzerland during 2011-2016. He has published 140 research papers in international journals of repute and 2 Indian patents. He is currently a full Professor and HoD in the Department of Chemistry, IISER Pune.

IL–20

Main group materials for Health, Energy, Environment, and Defense (HEED) applications

Krishnamurthi Muralidharan* and all my students

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The research activity of our group revolves around the concept of Health, Energy, Environment, and Defense (HEED). The primary focus of the research is the design of materials aimed at addressing fundamental issues about the efficiencies of devices related to Energy Harvesting (solar energy and hydrogen production), Energy Storage (battery and capacitors), and Energy Release (propellant and explosives). For these applications, we have been involved in producing nanomaterials, small molecules, and polymer materials and their application studies. In this talk, I will cover some of our research in the topic listed below.

- Small molecules: Nitrogen and boron rich molecules and salts as high-energy materials;
- Polymers: Polymers having phosphorus with intrinsic disordered framework for Li-ion mobility; Solid polymer electrolytes for batteries.
- Nano materials: Production of organic surfactant free nanoparticles for various applications; High-energy materials for spontaneous and controlled energy release.

Keywords: metal chalcogenides, Li-ion batteries, Aluminium nanaopartcilces, boranes

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Academic Qualifications

Ph.D. Chemistry, Indian Institute of technology (IIT) Kanpur (2003)
M.Sc. Applied Chemistry, Anna University (1997)
PG diploma in Applied Chemistry, Loyola College, Chennai (1995)
B.Sc. Chemistry, University of Madras (1993)

Fellowship/Membership

Fellow of the Telangana Academy of Sciences (FTAS) (2021)
Editorial Board Member of the journal “Energetic Materials Frontiers” (2019)
Elected member of The National Academy of Sciences, Allahabad (from 2016) Associate member of AP Akedemi of Sciences (2015)
Centenary Postdoctoral Fellowship, Indian Institute of Science (2007)

IL–21

Monolayer Water and ionic memory in Angstrom-Scale Channels made from 2D materials

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Condensed Matter Physics Group, National Graphene Institute and Photon Science Institute
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Angstrom-scale confinement fundamentally alters the structure, dynamics, and transport of liquids, giving rise to phenomena that are absent in bulk systems. Two-dimensional material-based angstrom-scale fluidic channels provide a uniquely well-defined platform to explore these effects, combining atomic-scale control of channel height, with tunable channel walls and their dimensions. Using such angstrom-scale channels, we have revealed highly selective ionic and molecular transport, enhanced ordering of confined water, and non-linear ionic conduction emerging from strong confinement and interfacial interactions.[1-8] These behaviours enable functional nanofluidic devices, including ionic memory elements, neuromorphic response, quantum emitters with implications for fluidic computing,[4-6] and sensing applications.[7]

Beyond transport, angstrom-scale nanofluidics offers new opportunities to probe the fundamentals of confined liquids. In this talk, I will also discuss advances in spectroscopy of confined water, outlining our experimental approaches to directly access molecular structure, and interactions under extreme confinement. Together, these studies highlight angstrom-scale confinement as a powerful framework for both discovery science and functional device engineering.

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Professor Radha Boya FRSC

Royal Society University Research Fellow **and** ***Kathleen Ollerenshaw Fellow***

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URL: Webpage (https://www.research.manchester.ac.uk/portal/radha.boya.html)

• EDUCATION AND TRAINING

Ph.D., 2012	Materials Science	Jawaharlal Nehru Centre for Advanced Scientific Research, India
M.Sc., 2007	Chemistry	Sri Krishnadevaraya University, India
B.Sc.,2005	Maths, physics, chemistry	Sri Krishnadevaraya University, India

• PROFESSIONAL APPOINTMENTS

2020-now	Professor (Chair) in Nanoscience,The University of Manchester (UoM), UK
2018-now	Royal Society University Research Fellow & Kathleen Ollerenshaw Fellow, UoM, UK
2016-2017	Leverhulme Early Career Fellow, UoM, UK
2014-2016	Marie Curie International Incoming Fellow, UoM, UK
2012-2013	Indo-US Postdoctoral Fellow, Northwestern University, USA
2011	Visiting A-STAR Research Fellow, IMRE A-STAR, Singapore
2009	Visiting scholar, NEST, CNR-INFM and Scuola Normale Superiore, Pisa, **Italy**

• AWARDS, RECOGNITIONS & INVITED TALKS

Radha has been invited to deliver >85 research presentations, including Plenary/Keynote/ Invited talks in international research conferences (Nanofluidics, Gordon Research conference, MRS, APS, Liquid Matter, World Laureates Forum China {2x}, microTAS) and departmental seminars in reputed Universities/Industry (Oxford, Cambridge, MIT, Max Planck, Cornell, Stuttgart, EPFL, Bristol, IBM). She has won several highly competitive awards as below.

2026 – Blavatnik Award (UK) finalist in the Physical Sciences theme
2025 – Distinguished Achievement Medal, Researcher of the Year, Faculty of Sci & Eng, UoM
2024 – ChemSocRev Pioneering Lectureship by Royal Society of Chemistry
2022 – Analytical Chemistry Young Innovator award
2021 – Philip Leverhulme Prize in Physics
2020 – Royal Society of Chemistry Marlow Award
2019 – European Research Council (ERC) starting grant
2018 – UNESCO-L'Oréal International Rising Talent
2018 – Royal society University Research Fellowship & Kathleen Ollerenshaw fellowship
2017 – MIT Technology Review's"Innovators under 35" global list;
2017 – UNESCO L'Oréal UK & Ireland women in science fellow
2016 – Leverhulme Early Career Fellowship; 2014 – Marie-Sklowdoska Curie Fellowship

Research Grants - Total grant amount **>£8 million**, selected grants awarded as PI

2026 – 2031: ERC Consolidator grant, Angel **£2.67M**
2024 – 2027: MSCA Doctoral Network, credit share **£260K;**
2024 – 2027: Royal Society URF renewal, **£665K**
2022–2025: EPSRC Strategic equipment grant**, £0.97M; 2023 – 2025:** New Horizons Award **£200K**
2020–2025: European Research Council (ERC) starting grant, £**1.3 million**
2018–2023: Royal Society university research fellowship, £**520K**

• RESEARCH CONTRIBUTIONS - PEER-REVIEWED PUBLICATIONS

Radha has **83 refereed publications and** has published her research in highly reputed international journals such as *Nature (3 papers) and Science* (5 papers). Radha's 36, and she has 3 patents (1 US and 2 international patents), and has written two book chapters.

A core strand of Radha's work is the development of Å-capillaries and pores as platform to probe intriguing molecular-scale phenomena experimentally, including: fast water flow under atomic-scale confinement (*Nature* 2019, *Nature* 2016), ion exclusion and ionic memory (Science 2023, *Nature Nanotechnology* 2023, *Science* 2019, *Science* 2017), quantum effects in molecular interactions off a surface (*Nature Materials* 2023, *Nature* 2018, *Science Advances* 2020).

• SERVICE AND LEADERSHIP

2022 – 2023 Faraday Division ***Diversity Committee Chair***, 2020–2022 RSC ***Awards Committee***
2023 - Scientific Advisory Board for MIT-CENT centre for nanofluidics
2023 – International Advisory Committee for 12th Liquid Matter Conference
2022 – Subcommittee member & International advisory, 6th IEEE ICEE conference, India

Grant Reviewer: EPSRC, ERC starting, consolidator and Advanced grant Reviewer; Newton Prize; L'Oreal women in science awards; Lindau Young scientists awards.

Reviewer for various reputed science journals (Nature, Science, ACS, Wiley, RSC, IOP)

IL–22

Functional Porous Organic Polymers (POPs) for Clean Fuel Production and Uranium Extraction

Dr. Venkata Suresh Mothika*
Assistant Professor, Department chemistry, Indian Institute Technology Kanpur, Kanpur,
Uttar Pradesh, India – 208016.
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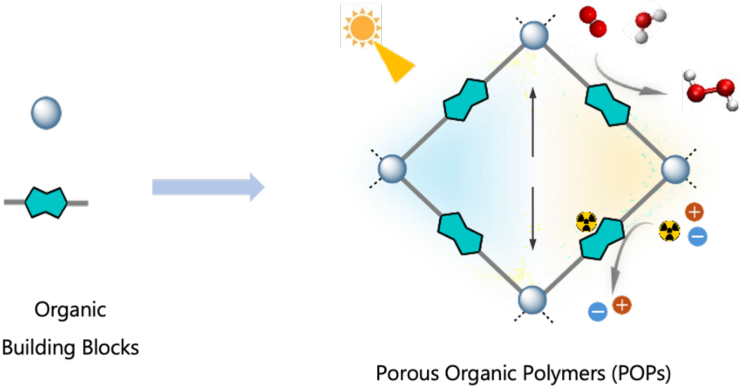
The efficient utilization of solar energy and Earth's abundant resources, such as natural seawater, for chemical synthesis or energy production minimizes the challenges posed by current industrial chemical methods, enables on-site production, and greatly reduces the generation of toxic chemical waste.[1] Porous organic polymers (POPs) have recently emerged as functional porous materials for a wide range of applications, including chemical sensing, energy storage/conversion etc.[2-4] In this talk, I discuss our recent results on porous organic polymer (POP)- based photocatalysts for tunable hydrogen peroxide (H2O2) applications, with an emphasis on understanding the underlying photophysical/chemical processes involved in the photolytic generation of H2O2. As a highlight, the POP design enabled an unconventional pathway for ^{1}O2 generation via interfacial electron transfer, as confirmed by EPR analysis. In the second part of my talk, I discuss the development of uranium (UO $^{2+}$) extraction (an alternative clean energy fuel) and release using *o-hydroxyimine-based POPs as* self-indicating POPs for efficient uranium extraction from seawater and their potential in practical applications.



Scheme 1. *POPs for Photocatalytic Hydrogen Peroxide Production and Uranium Capture*

Keywords: Porosity, polymers, H_2O_2 production, photocatalysis, uranium extraction

References

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[2] Li, R.; Byun, J.; Huang, W.; Ayed, C.; Wang, L.; Zhang, K. A. I. *ACS Catal.* **2018**, *8*, 4735-4750.
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Curriculum Vitae

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EDUCATION

2016	Ph.D.(Materials Science), Chemistry & Physics of Materials Unit (CPMU), JNCASR Bangalore, India, in the group of Prof. Tapas K Maji Thesis title: *Investigation on photophysical properties of nanoscale metal organic frameworks and conjugated microporous polymers*
2009	M.Sc. (Chemistry) from National Institute of Technology (NIT-Trichy), India
2007	B.Sc.(Mathematics, Physics & Chemistry) from Andhra Loyola College, Acharya Nagarjuna University, Andhra Pradesh, India

CURRENT POSITION

Sep 2022-	**Assistant Professor, Department of Chemistry**, **IIT Kanpur**, India

PREVIOUS POSITIONS

2020-2022	**Postdoc**, Department of Chemistry, University of York, UK
2018-2019	**Postdoc**, Department of Chemistry, Weizmann Institute of Science, Israel
2016-2018	**Postdoc**, School of Mathematical & Natural Sciences, Bergische Universität Wuppertal, Germany
2011	JRF Assistant, Department of Chemistry, Indian Institute of Technology-Chennai, India

RESEARCH AWARDS & ACHIEVEMENTS

2024	Member of the Royal Society of Chemistry (MRSC)
2019	The Royal Society Newton International Postdoctoral Fellowship, UK
2019	PBC Postdoctoral Fellowship, Israel
2017	AvH Foundation nomination for 67th Lindau Nobel Laureates Meeting
2016	Alexander von Humboldt (AvH) Foundation Postdoctoral Research Fellowship
2016	Irish Research Council (IRC) Postdoctoral Research Fellowship (declined)

CONFERENCES/WORKSHOPS

2026	MOFES 26, JNCASR, Bangalore, India (Invited)
2025	National Organic Symposium Trust (NOST-ECR), IISER Bhopal, India (Invited)
2024	Chemical Frontier, IISER Bhopal, India (Invited)

IL–23

Heteroatom-rich Framework Materials: Why Are They Exciting?

Ashok Keerthi*

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Heteroatom-rich framework materials offer a powerful molecular platform for tuning electronic structure, redox activity, and charge transport in extended π-conjugated systems. Incorporation of heteroatoms such as nitrogen and oxygen enables precise control over spin density, orbital alignment, and ion–electron coupling, opening new opportunities in energy storage and quantum-enabled materials.

In this talk, I will discuss our recent work on heteroatom-engineered covalent organic frameworks (COFs), metal-organic polymers (MOFs), and nanographene-based architectures, highlighting how molecular design principles translate into macroscopic function. Using hexaazatriphenylene- and quinone-based building blocks, we demonstrate that strategic heteroatom placement produces chemically robust, redox-active, and spin-active frameworks. These materials can be accessed through complementary solution-phase and mechanochemical synthesis, enabling scalable fabrication while maintaining extended electronic communication. Electrochemical and spectroscopic studies reveal synergistic charge-storage mechanisms, where fast, reversible redox processes couple with delocalized spin states and efficient ion transport through intrinsic porosity. Beyond performance metrics, combined experimental and electronic-structure analyses uncover how heteroatoms govern spin delocalization, redox potentials, and charge localization.

Overall, heteroatom-rich framework materials provide a unifying chemistry-driven strategy for connecting molecular design with emergent electronic, spintronic, and energy-relevant functionalities.

Keywords: Nanographenes, Graphene Nanoribbons, Covalent Organic Frameworks, Metal-Organic Frameworks

References

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EDUCATION

2009 – 2014	**PhD in Materials Chemistry** Department of Chemistry, National University of Singapore Thesis title "Design and Synthesis of Novel Perylene and Carbazole based Conjugated Materials for Electronic and Photovoltaic Applications". Supervisor: Prof. Suresh Valiyaveettil
2007 – 2009	**MSc in Chemistry** School of Chemistry, University of Hyderabad, India Thesis Title: Synthesis of Pyridine based Polybenzimidazole for the use in Fuel Cell

PROFESSIONAL MEMBERSHIPS

Member, EPSRC Quantum Technologies Early Career Forum since September 2025 onwards
Member, IUPAC Committee on Chemistry and Industry from September 2024 onwards
Member, IUPAC Polymer division from August 2023 onwards
Member, Royal Society of Chemistry (RSC) from 2019 onwards
Member, Society of Chemical Industry (SCI) from 2019 onwards
Member, Materials Research Society (USA) from 2013 onwards
Member, Materials Research Society (MRS-Singapore) from 2011 onwards

CURRENT AND PREVIOUS APPOINTMENTS

- March 2022 – present: Presidential Academic Fellow, Department of Chemistry, The University of Manchester, Manchester, **UK**.
- June 2019 – March 2022: Ramsay Memorial Fellow, Department of Chemistry, The University of Manchester, Manchester, **UK**.
- April 2016 – May 2019: Research Associate, School of Physics & Astronomy, The University of Manchester, Manchester, **UK**.
- September 2013 – March 2016: Max Planck Institute Postdoctoral Fellow, Max Planck Institute for Polymer Research, Mainz, **Germany**.
- August 2009 – August 2013: Graduate Research Assistant in Department of Chemistry, National University of Singapore, **Singapore**.
- June 2006 – July 2007: Senior Executive, Analytical Research and Development, Dr. Reddy's Laboratories, Hyderabad, Telangana, **India**.

RESEARCH CONTRIBUTIONS - PUBLICATIONS

Ashok has published 65 peer-reviewed papers (including **ten** in ***Nature*** and **three** in ***Science*** journals) in internationally leading journals (H-index 26). Six of his publications are mentioned by ISI web of knowledge as top 1% cited papers of the academic field of Chemistry/Physics based on a highly cited threshold for the field and publication year.

1. A. Thanai, V. Sharma, L. Minion, H. Khan, H. Abbas, G. F. S. Whitehead, A. Hasija, J. Wade, M. J. Fuchter, **Ashok Keerthi***, "Bay-functionalized [7]Helicene Bilayer Nanographenes", **Advanced Optical Materials**, 2026, e02564 (10.1002/adom.202502564).

2. Y. Liu, S. Rahaman, H. Jyotilal, T. Dumpala, K. Kar, B. Duff, B. Radha, **Ashok Keerthi***, "Hexaazatriphenylene-Quinone-Based Covalent Organic Frameworks with Unprecedented Areal Capacitance", **Journal of Americal Chemical Sciences**, 2026 (major revision)

3. H. Jyothilal, S. Rahaman, V. Sharma, K. Pandey, **Ashok Keerthi***, B. Radha*, "Two-dimensional Metal Organic Framework for Supercapacitors: Thickness-Dependent Charge Storage Mechanisms", **Nano Letters**, 2026 (accepted).

IL–24

Designing High-Performance Energy Storage Systems for Decarbonization

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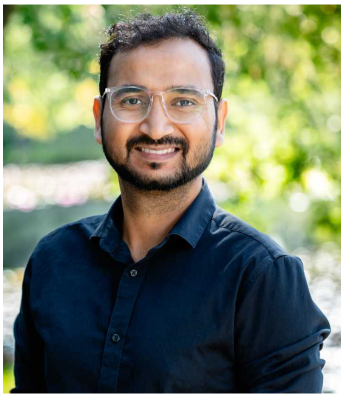
There is an urgent need to reduce our global carbon dioxide emissions to mitigate climate change. While low-cost electricity from solar and wind sources provides exciting opportunities to reduce emissions, the transition to decarbonization is only possible once energy storage devices with higher energy densities, longer lifespans, and faster charging capabilities are available. In this seminar, I will present a computational approach to establishing design guidelines for high-performance energy storage devices. I will discuss the driving forces and thermodynamic barriers of Li^+ ion adsorption onto commercial electrode materials in different salt electrolytes using insights from state-of-the-art computational techniques, like molecular dynamics (MD), machine learning (ML), and density functional theory (DFT) simulations. I will show that the weaker cation-anion pairing enhances the driving force for adsorption for an electrode-electrolyte interface with zero cation coverage but is also accompanied by an increased thermodynamic barrier at an equilibrium surface coverage of Li^+ ions. Focusing on designing liquid electrolytes where the Li^+ ion diffuses independently of its solvation shell to enhance the transference number, I will also elaborate on the different transport mechanisms of ions in an electrolyte solution.

Abhishek Aggarwal



Assistant Professor

Mehta Family School of Sustainability at the Indian Institute of Technology, Indore

Dr. Abhishek Aggarwal is an Assistant Professor at the Mehta Family School of Sustainability at the Indian Institute of Technology, Indore (IIT Indore) since January 2026. He got his Ph.D. from Indian Institute of Science (IISc) in 2022 and had two postdoctoral stints at Massachusetts Institute of Technology (MIT) and the University of Illinois Chicago (UIC) from 2022-2025. He uses various state-of-the-art computational tools, such as Molecular Dynamics (MD), Density Functional Theory (DFT), and Machine Learning (ML) techniques to understand the fundamental physical and chemical properties of various material systems, including Li-ion batteries, biomaterials, rocket fuels and polymer membranes. His current research focuses on modeling the energy storage systems, and water properties near polymers and other surfaces in extreme conditions.

Flash Presentation Schedule

Guidelines:

1. The flash presentations will begin at 15:15 on 7th March 2026.
2. Each presenter will be given 4 minutes (strictly) to present. At the end of the presentation, only short questions will be entertained, and the speaker is expected to provide brief answers.
3. Every second used beyond the allotted 4 minutes will lead to negative marking. Hence, we request that you plan your presentation within the 4-minute limit.

Flash Presentation order	Name of Presenter	Title of Presentation
F01	Sadhan Dey	Porous Co-SAC Catalysed Cyclopropanation via Carbenoid C-C Bond Formation
F02	Ayusie Goyal	M^{3+} or $M^{4+?}$ Identifying the Active Sites for IOR and OER
F03	Shivani Gupta	Enhanced Photocatalysis via Perovskite-Molecular Synergy and Surface Engineering
F04	Vatsalya Gupta	Benzyl Thioether : A Dynamic Covalent Motif for Covalent Adaptable Networks
F05	Parvathy Jayan	CO_2 Electroreduction to CO over Silver Nanoclusters: The Impact of Nuclearity on Synergistic Activity Modulation
F06	Dr. Grace Kaul	Customizable Microfluidic Platforms for Analyte and Pathogen Detection
F07	Madhulika Madhu	Mixed-Viologens enabling Multichromic Phenomena: A Sum is Better than the Individuals
F08	J. Manojkumar	Next-Gen Energetic 3D MOFs for High Energy Density Materials and Iodine Encapsulation
F09	Joseph Nishanth	Fabrication of high-loading SPAN cathodes for alkali metal-sulfur batteries via electrospinning
F10	Shailesh Kumar Sah	Enhancing efficiency of semi-transparent perovskite solar cells via additive engineering
F11	Anurag Sharma	Helper lipids accelerate the mass transfer of cationic lipid nanoparticles, resulting in an efficient gene delivery
F12	Diksha Srivastava	Molecule Based 2D-Materials for Electronic Applications

FP–01

Porous Co-SAC Catalysed Cyclopropanation via Carbenoid C-C Bond Formation

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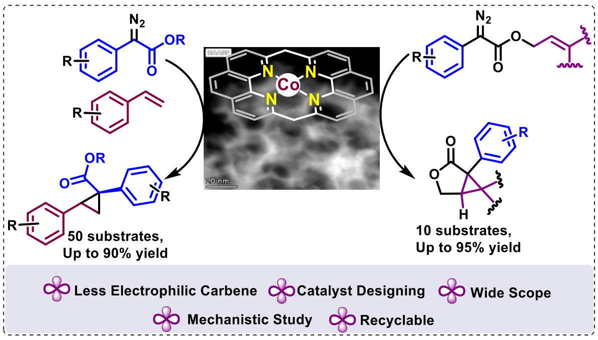
Single-atom catalysts (SACs) are a promising class of heterogeneous materials that maximize atomic efficiency while providing well-defined, tunable active sites.1 By stabilizing isolated metal atoms on supports such as carbon, metal oxides, or MOFs, SACs bridge homogeneous and heterogeneous catalysis through coordination-environment engineering.2 Their tunable d-band structures impart unique electronic properties that enhance reactant adsorption and catalytic performance, leading to broad applications in energy conversion, environmental remediation, and sustainable organic synthesis.3 Motivated by these advantages, we developed several 3d-metal SACs and investigated their catalytic activity in organic transformations. Cobalt-based SACs were prepared via impregnation of cobalt precursors onto nitrogen-doped graphitic carbon, followed by pyrolysis and acid washing. The resulting Co-SACs efficiently activated diazo compounds for carbon-carbon bond formation via metal-carbene intermediates, affording inter- and intramolecular cyclopropanes from diverse styrenes and diazo substrates. The porous structure and electron-deficient cobalt centers were crucial for high reactivity. The catalyst was recyclable for up to nine cycles without significant loss of activity (Scheme 1).



***Scheme 1**: Co-SAC-catalysed electrophilic olefin cyclopropanation.*

Keywords: Single-atom catalysts, catalyst engineering, carbene transfer, cyclopropanation

References

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FP–02

M^{3+} or M^{4+}? Identifying the active sites for anodic oxidation reactions

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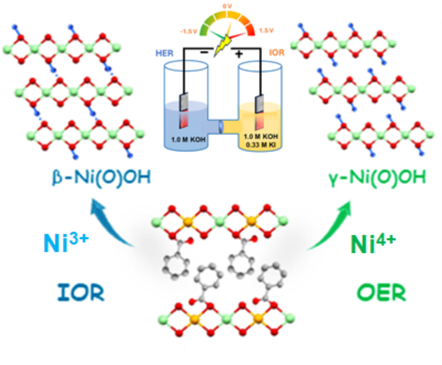
Iodide oxidation reaction (IOR) has emerged as an energy-efficient alternative to the oxygen evolution reaction (OER), yet the identification of true active intermediate responsible for the observed catalytic reaction remains unexplored. To elucidate the active sites in IOR and OER, we provide insights from a PBA-derived Co(O)OH active catalyst and a hydroxide-derived Ni(O)OH catalyst.[1,2] Electrochemical analysis combined with *in situ* Raman studies showed that Ni^{4+} governs OER, whereas Ni^{3+} acts as the active site for IOR.[3] In contrast, Co^{4+} species served as the active centre for both IOR and OER.[4] In this talk, I will provide mechanistic insights into the active sites governing IOR and OER in Ni and Co-based systems for the rational design of next-generation electrocatalysts.



***Scheme 1**: Active sites for IOR and OER*

Keywords: Active site identification, Iodide oxidation reaction, Oxygen evolution reaction

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FP–03

Enhanced Photocatalysis via Perovskite-Molecular Synergy and Surface Engineering

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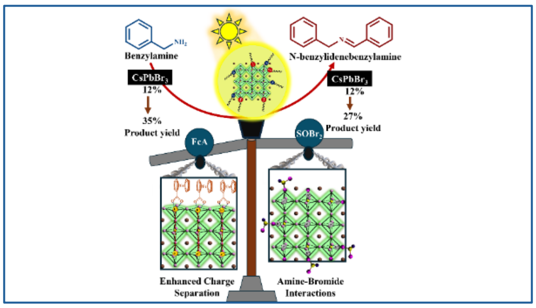
Cesium lead bromide ($CsPbBr_3$) nanocrystals exhibit strong light absorption and tunable optoelectronic properties, yet rapid charge recombination and inefficient exciton dissociation hinder their photocatalytic performance.[1] To address this, we engineered a composite system combining $CsPbBr_3$ with ferrocene carboxylic acid (FcA), a molecular hole acceptor. This integration facilitates charge separation through energy level alignment and suppresses recombination,[1] leading to a threefold increase in benzylamine oxidation yield (35 ± 5%) compared to pristine $CsPbBr_3$ (12 ± 2%).[2] Additionally, thionyl bromide ($SOBr_2$) treatment removes surface ligands and introduces bromide ions,[3] improving charge transport and substrate accessibility, with a 27 ± 5% yield in 3 hours. While $SOBr_2$ improves initial performance, its acidity may cause side reactions over time. These results highlight how molecular integration and surface engineering enhance perovskite photocatalysis by optimizing interfacial charge transfer dynamics, paving the way toward sustainable chemical transformations.



***Scheme1**: Comparative product yield in different perovskite-based photocatalytic systems.*

Keywords: Photocatalysis, $CsPbBr_3$ nanocrystals, ferrocene carboxylic acid, charge separation, active-site accessibility

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FP–04

Benzyl thioether: A Dynamic Covalent Motif for Covalent Adaptable Networks

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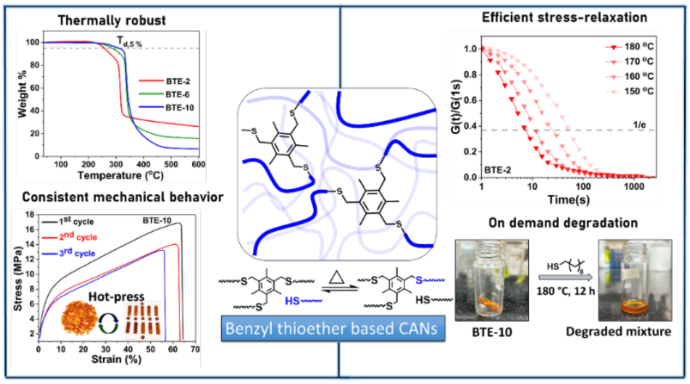
In recent decades, covalent adaptable networks (CANs) have emerged as promising materials to overcome the issues associated with irreversible crosslinks in thermosets. These polymers exhibit the unique combination of high strength and recyclability owing to the presence of dynamic linkages.[1] However, despite advancements in CAN literature, designing chemistry that imparts both robustness and consistent dynamic behavior remains a significant challenge. To this end, we have introduced benzyl thioether-based transthioetherification as a dynamic chemistry platform for designing recyclable crosslinked polymers.[2] To the best of our knowledge, this is the first report that introduces benzyl thioethers linkages to design robust and dynamic CANs. The exchangeability of the thioether bonds was demonstrated using small molecular model studies, implementing which linear as well as crosslinked polymers were prepared. Additionally, based on the spacer chain lengths between the dynamic bonds, a detailed structure-property relationship was explored, spanning our study towards a wider range of material properties. The CANs exhibited recyclability, thermal robustness, and chemical resistance owing to robust and dynamic thioether bonds. The viscoelastic behavior was studied using stress-relaxation measurements and were regulated by both the chain lengths as well as the catalyst concentration in the polymer matrix. The effect of stoichiometric variations on the dynamic behavior of the networks was also explored. Finally, as a proof of concept, the degradation of the crosslinked network with a thiol via transthioetherification reaction was demonstrated, making them on-demand degradable thermosets.



Keywords: Thermosets, Covalent adaptable networks, Viscoelastic, Transthioetherification, Degradation.

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FP–05

CO_2 Electroreduction to CO over Silver Nanoclusters: The Impact of Nuclearity on Synergistic Activity Modulation

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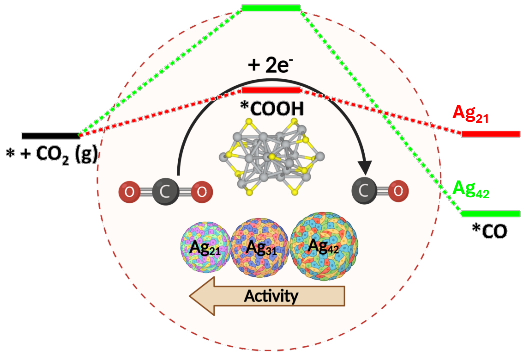
Electrochemical reduction of CO (eCO_2R) powered by renewable energy enables sustainable chemical production and decarbonization of hard-to-abate sectors. We investigate the structure-activity relationship of atomically precise silver nanoclusters (Ag NCs) Ag_{21}, Ag_{31}, and Ag_{42} for CO production, focusing on metal core nuclearity and ligand electronics. The CO Faradaic efficiency (FE_{CO}) increases and the potential for FE_{COmax} shifts positively with decreasing nuclearity, showing a near-quantitative trend (~70 mV and ~80 mV shifts in FE_{max} and $j_{CO(max)}$ per ~10 Ag atoms). Ag_{21} achieves 99.6% FE_{CO} at −0.59 V vs. RHE and 148 mA cm^{-2} at -0.7 V. Calculations attribute this enhancement to reduced activation barriers via modulation of surface charge distribution and electronic density of states at active Ag sites.



Keywords: Electrochemical CO_2 reduction, Silver nanocluster, Carborane-thiol, CO, Faradaic efficiency

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FP–

Customizable Microfluidic Platforms for Analyte and Pathogen Detection

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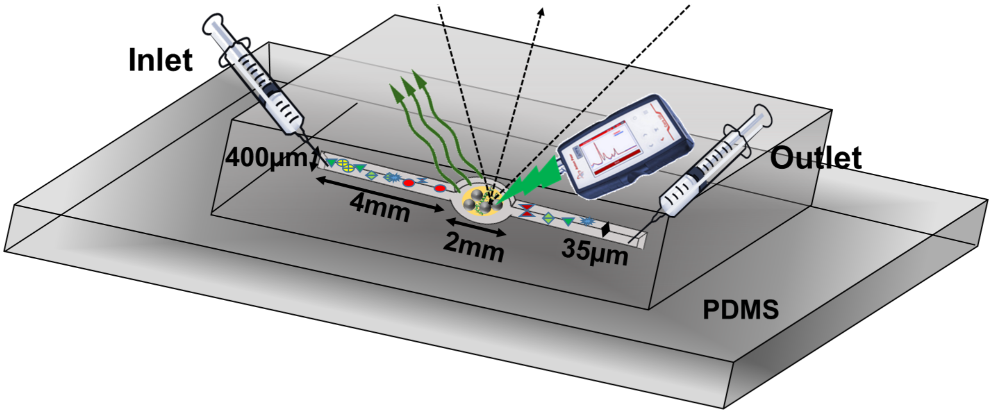
Microfluidic biosensing platforms enable controlled analyte transport and engineered surface interactions for sensitive detection in complex biological environments. We have previously developed and reported an indigenously fabricated microfluidic sensing device integrating a closed detection chamber with nanostructured interfaces for ultrasensitive analyte detection, validated for central nervous system (CNS) biomarker screening.[1,2] Building on this established platform, its design is intended to extend toward pathogen detection through modular customization of the sensing interface while retaining the microfluidic architecture. The detection region is engineered with antibiotic-embedded nanofiber surfaces selected for their defined binding affinities toward bacterial cell envelope components. Under laminar flow conditions, these interfaces are designed to promote selective bacterial interaction and localized release of bacteria-associated molecular markers, which are expected to be amenable to detection using the existing SERS based sensing framework. This highlights a materials-driven strategy for adapting a validated analyte-detection platform toward pathogen sensing.



***Scheme 1**: Prototype design of a sealed microfluidic device for analyte detection, Langmuir 2024, Indian Patent*

Keywords: Microfluidics, SERS, Detection Platform

References

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[2] Indian Patent no. 547959, Granted on August 16, 2024.

FP–

Mixed Viologens enabling Multichromic Phenomena: A Sum is Better than the Individuals

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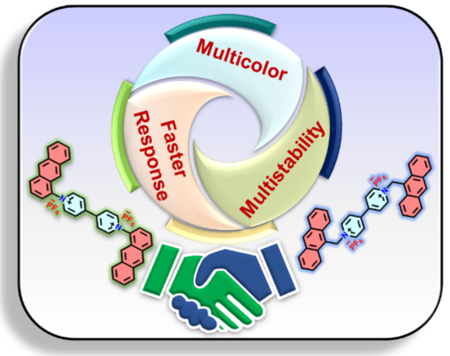
Electrochromic materials capable of reversible and tunable multicolour modulation are critical for next-generation smart windows, adaptive optical devices, and low-power displays.[1,2] Conventional viologens undergo two sequential one-electron reductions, resulting in limited color states defined by their intrinsic electronic structures.[3] Here, we demonstrate that rational mixing of structurally distinct viologen derivatives enables emergent multichromic behavior beyond the response of individual components. Integrating electronically differentiated alkyl- and aryl-substituted viologens establishes complementary redox potentials that collectively generate an effective four-electron reduction window within a single electrochemical system. Spectroelectrochemical analysis reveals stepwise formation of radical cation and neutral species with distinct absorption bands across the visible region, tunable intermediate hues, broader spectral coverage, improved electroactivity, producing enhanced color contrast, and greater cyclic stability than single-component analogues.



Scheme 1*: Mixed viologens enable fast, stable multicolor electrochromism*

Keywords: Electrochromism, Viologen, Multicolor, Cyclic Stability, Spectroelectrochemistry

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FP–

Next-Gen Energetic 3D MOFs for High Energy Density Materials and Iodine Encapsulation

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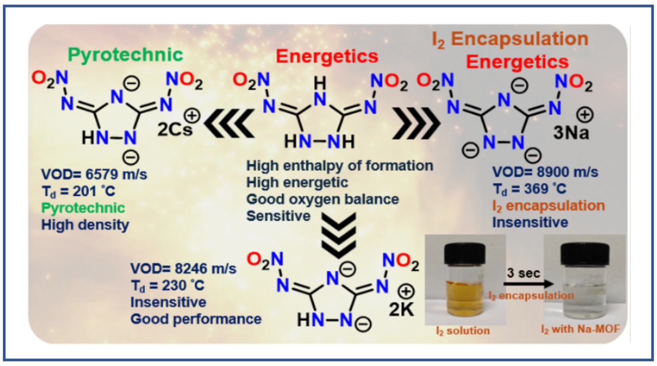
Energetic materials are essential for aerospace, defense, and civilian applications, and current research focuses on achieving high performance together with thermal stability and low sensitivity. Nitrogen-rich energetic metal–organic frameworks (E-MOFs) provide an effective platform to meet these requirements. Herein, three nitrogen-rich E-MOFs, Na-MOF (**1**), K-MOF (**2**), and Cs-MOF (**3**) were synthesized via hydrothermal self-assembly using dinitrimino triazole (DNT) as the energetic ligand and non-toxic alkali metals. Among them, Na-MOF exhibits outstanding detonation performance (VOD = 8900 m s^{-1}, DP = 26.21 GPa), exceptional thermal stability up to 369 °C, and remarkable insensitivity to impact (40 J) and friction (360 N), positioning it as a promising replacement for benchmark explosives such as RDX, HNS, and PYX. Although potassium-based dinitrimino energetic MOFs have traditionally served as primary explosives, the newly synthesized K-MOF behaves as a secondary energetic material, delivering high detonation performance (VOD = 8286 m s^{-1}, DP = 30.52 GPa) with low mechanical sensitivity. In addition, Cs-MOF shows potential for pyrotechnic applications through bright red flame emission, while Na-MOF also demonstrates excellent iodine adsorption capability.



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FP–09

Fabrication of high-loading SPAN cathodes for alkali metal-sulfur batteries via electrospinning

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Alternatives to the current state-of-the-art Lithium-ion Batteries (LIBs) are being sought as these are expensive, rely on non-abundant materials, and offer a limited energy density of approximately 250 Wh/kg. Lithium-sulfur (Li-S) and Sodium-sulfur batteries present a promising alternative with a much higher theoretical capacity and energy density of 1675 mAh g−1 and 2500 Wh/kg respectively. However, sulfur cathodes face challenges such as low cycle life, poor rate capability, polysulfide shuttling, and incompatibility with carbonate electrolytes. Sulfurized polyacrylonitrile (SPAN) is a composite sulfur cathode, which consists of sulfur chains covalently bound to carbonized polyacrylonitrile (PAN) backbone. It mitigates the main issue of polysulfide shuttling by binding the sulfur to the PAN chains, thereby demonstrating compatibility of the sulfur composite cathode with carbonate electrolytes. However, fabrication of cathodes with high active material loading, crucial for competing with state-of-the-art battery technologies, is a major challenge in this system. Electrospinning is a versatile technique to fabricate non-woven mats of polymer nanofibers, which have excellent porosity and mechanical strength. Although electrospun cathodes of SPAN have been reported in literature, the fabrication process involves electrospinning of PAN followed by its sulfurization. Such an approach results in a cathode with poor performance due to its low electronic conductivity. This work explores the synthesis of SPAN composite cathodes by directly electrospinning the slurry containing the sulfurized polymer, conductive additive, and the binder, instead of employing a traditional doctor blade coating method. The possibility of having improved porosity, while simultaneously allowing ultra-high loadings, will unlock high-performance yet scalable sulfur cathodes.

Keywords: SPAN cathodes, Lithium-Sulfur battery, Sodium-Sulfur battery, Electrospinning

FP–10

Enhancing efficiency of semi-transparent perovskite solar cells *via* additive engineering

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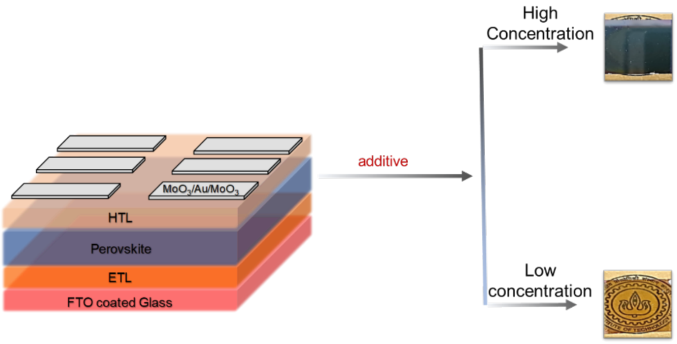
Semi-transparent perovskite solar cells (ST-PSCs) are gaining worldwide attention for their use in building-integrated photovoltaics, tandem solar cells, and other applications. ST-PSCs combine the excellent properties of metal halide perovskite materials, such as bandgap tunability, high absorption coefficient, long carrier diffusion length, and easy solution processing, with varying degrees of transparency to enable them for different applications. However, the main issue associated with ST-PSCs is the trade-off between power conversion efficiency (PCE) and average visible transmittance (AVT). Several strategies have been reported to simultaneously increase PCE and AVT values to obtain high-performance ST-PSCs. In this work, we employed an additive engineering strategy to fabricate semi-transparent formamidinium-based perovskite solar cells incorporating a $MoO_3/Au/MoO_3$ dielectric–metal–dielectric (DMD) top transparent electrode. The initial transparency of the perovskite was controlled by varying the molarity of the perovskite precursor, and optimization of the concentration of a novel zwitterion-based additive enhanced both PCE and AVT. A maximum PCE of around 16% with an AVT of 20% was obtained using this approach.



***Scheme 1**: Device architecture of ST-PSC*

Keywords: Solar cells, Perovskites, Semitransparent, Power conversion efficiency

Reference

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FP–11

Helper lipids accelerate the mass transfer of cationic lipid nanoparticles, resulting in an efficient gene delivery

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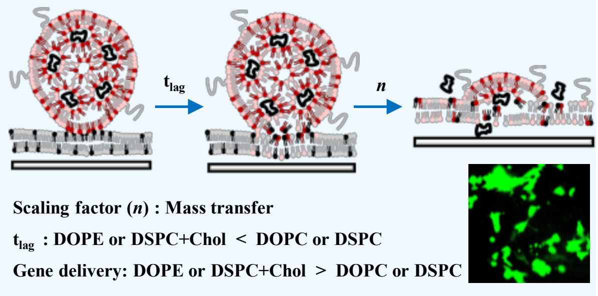
Lipid nanoparticles (LNPs) have attracted significant attention following the clinical success of the Onpattro drug and mRNA vaccines.[1-2] Two major challenges remain: (i) designing LNPs for gene therapy targeting non-liver tissues[3] and (ii) overcoming inefficient endosomal escape of conventional LNPs.[4] Cationic LNPs have been reported to shift the organ tropism[c], but their endosomal escape is yet to be evaluated. Here, we investigated the fusion dynamics of cationic LNPs with model membranes at the single-particle level. We found that membrane fusion occurs through a unique mass-transfer pathway, involving a one-step transition that forms a metastable intermediate that fully coalesces with the target membrane. A moderately high concentration (31 mol%) of the cationic lipid (DOTAP), combined with either DOPE or DSPC + cholesterol helper lipids, accelerates the fusion kinetics by reducing the lag time. The enhanced fusogenicity of these compositions aligns with the bulk-phase lipid mixing results. Endosomal localization and eGFP expression upon gene delivery in a range of mammalian cell lines confirm effective endosomal escape of DOPE- or DSPC + cholesterol-rich cationic LNPs. Overall, these findings represent a step toward designing optimal cationic LNP candidates for efficient gene delivery to organs beyond the liver.



***Scheme 1**: Composition-dependent fusion dynamics of cationic lipid nanoparticles (LNPs).*

Keywords: Lipid nanoparticles (LNPs), Gene delivery, Endosome, Vaccines, Fusion dynamics

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FP–12

Molecule Based 2D-Materials for Electronic Applications

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Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are emerging as promising π-conjugated materials for thin-film electronics. Their extended in-plane conjugation theoretically enables charge-carrier mobilities approaching ~1000 $cm^2\ V^{-1}\ s^{-1}$, making them attractive for electronic device applications. However, achieving uniform, highly crystalline films with long-range order remains a major challenge. Here, we demonstrate band-like charge transport in two highly crystalline semiconducting 2D imine-COF thin films synthesized via quasi-equilibrium Schiff base condensation. By rational precursor design, we precisely control the nitrogen content within the unit cell producing frameworks with six and ten nitrogen atoms (6N- and 10N-imine-COFs). Two-electrode measurements over 1 mm channel lengths reveal reproducible linear I–V characteristics, confirming uniformity and band-like transport across large-area films. Notably, the 10N-imine-COF exhibits ~36-fold higher conductivity than the 6N analogue. This scalable synthetic strategy provides a pathway to tailor nitrogen content and engineer electronic properties in 2D imine-COFs, advancing their integration into next-generation thin-film electronic devices.

Keywords: Covalent organic framework, Thin film, Charge transport, Optoelectronic materials.

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Poster No.	Name of Presenter	Title of Poster
P01	Anupama K	Highly Promising Primary Explosive: A Metal-Free, Fluoro-Substituted Azo-Triazole with Unmatched Safety and Performance
P02	Balakumaran K	Hydrothermally Engineered Ni-Deposited Cu Foam as a Tandem Electrocatalyst for Selective Nitrate-to-Ammonia Conversion
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P11	Sagar Eknath Nehe	Fused Azo-Bridged Triazolo-Pyridazine-Derived Energetic Materials
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P14	Palak	Development and optimization of flexible solid-state electrolytes for high-performance Li-ion batteries
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P25	Anamika Yadav	Coordination Site Engineering Induced Lattice Distortion in 2D Precatalyst for Efficient Anodic Oxidation Reaction
P26	Monika Yadav	Free-Standing Blatter Radical Polymer Thin Films with Controlled Nanometer Thickness and their Redox-Optical Behaviour
P27	Sandeep Yadav	Ni–Fe MOFs and Hydroxides for Oxygen Evolution: Mechanistic Insights via Chemical Probes and pH Studies

PP–01

Highly Promising Primary Explosive: A Metal-Free, Fluoro-Substituted Azo-Triazole with Unmatched Safety and Performance

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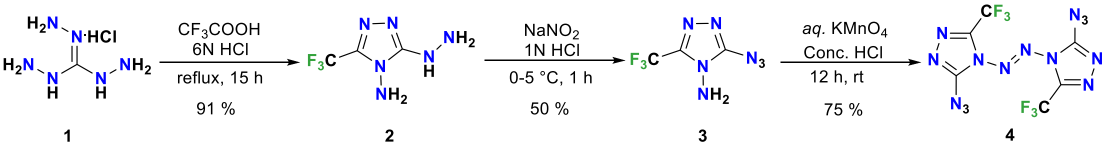
Primary explosives are a special class of energetic materials that can detonate with very little external stimulus, such as heat, shock, friction, or a spark. Because of their sensitivity and fast response, they play a crucial role in initiating the less sensitive secondary explosives. Lead azide (LA) has long been the go-to primary explosive due to its consistent and powerful initiation capability. However, the presence of toxic heavy metals like lead, and its environmental persistence, has raised serious health and ecological concerns, making the development of cleaner, safer alternatives a high priority. Primary explosives are small in quantity but immense in strategic importance. Their performance, reliability, and safety directly influence a country's military effectiveness, technological edge, and readiness for conflict or deterrence. Advancing new, safer alternatives is not just a scientific challenge but a strategic national security imperative. In this context, we have developed a novel organic primary explosive, (*E*)-1,2-bis(3-azido-5-(trifluoromethyl)-4*H*-1,2,4-triazol-4-yl) diazene **(4)** **(Scheme 1)**. This compound is synthesized through a simple, scalable reaction using commercially available starting materials. Structurally, **4** features an *N,N'*-azo-1,2,4-triazole framework modified with two trifluoromethyl and azido groups. These functional groups not only enhance the detonation performance but also contribute to its thermal stability and reduced sensitivity to non-explosive stimuli. Compound **4** meets key criteria for modern green primary explosives: it is completely free from metals and perchlorates, exhibits high density and excellent priming capability, and maintains strong resistance to environmental degradation. Notably, **4** can be initiated by a laser and demonstrates high thermal stability, traits that are highly desirable in advanced ignition systems. In performance tests, **4** successfully initiated the detonation of 500 mg of PETN using only 40 mg of material, matching the efficiency of lead azide. It also outperforms other reported green primary explosives like ICM-103 (MPC: 60 mg) and DDNP (MPC: 70 mg), highlighting its superior initiation ability. Given its excellent detonation power, environmental safety, simple and cost-effective synthesis, and potential for large-scale production, compound **4** stands out as a strong candidate to replace traditional primary explosives such as lead azide and DDNP in future energetic applications.



Scheme 1*: Synthesis of (E)-1,2-Bis(3-azido-5-(trifluoromethyl)-4H-1,2,4-triazol-4-yl) Diazene (4)*

Keywords: Primary Explosive, Detonation Test, Laser Ignition, Azo bridged.

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PP–02

Hydrothermally Engineered Ni-Deposited Cu Foam as a Tandem Electrocatalyst for Selective Nitrate-to-Ammonia Conversion

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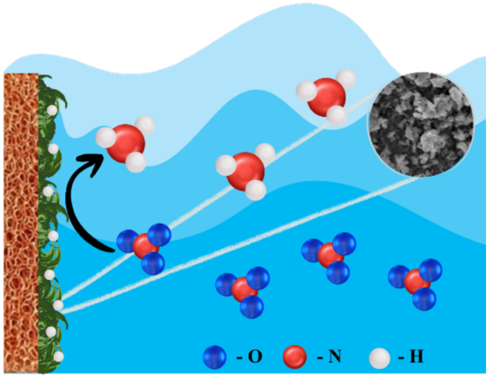
Electrocatalytic nitrate reduction reaction (NO_3RR) offers a sustainable route for ammonia synthesis under ambient conditions, serving as a decentralized alternative to the energy-intensive Haber-Bosch process while simultaneously addressing nitrate-contaminated wastewater remediation. However, achieving high ammonia selectivity over the competing hydrogen evolution reaction (HER) remains challenging due to complex multi-electron transfer pathways and intermediate stabilization requirements. Herein, we report a hydrothermally engineered Ni-deposited Cu foam ($CuNi_{170}$) as a binder-free, three-dimensional electrocatalyst for selective NO_3RR. Systematic variation of hydrothermal temperature and reaction time enabled precise control over surface morphology, Ni loading, and Ni-Cu electronic interactions, thereby optimizing catalytic performance. Electrochemical activity was evaluated using ECSA, Electrochemical Impedance Spectroscopy, and Chronoamperometry. Ammonia, nitrite, and residual nitrate were quantified via UV-vis spectroscopy using indophenol and Griess methods, while ammonia was also validated by NMR analysis. Faradaic efficiency and ammonia yield rate were calculated based on charge passed and quantified products, demonstrating the effectiveness of hydrothermal parameter optimization. This study underscores the critical role of hydrothermal parameter optimization in designing high-performance tandem catalyst for selective green ammonia synthesis.



Scheme 1: *$CuNi_{170}$ electrocatalyst for efficient conversion of nitrate (NO_3^-) to ammonia(NH_3).*

Keywords: Green Ammonia Synthesis; Hydrothermal Engineering; Copper based catalyst.

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PP–03

Heterometallic Molecular Ni-Salen Catalysts for Efficient Electrocatalytic Oxygen Evolution Reaction

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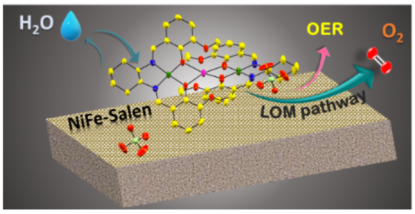
Electrocatalytic oxygen evolution reaction (OER) plays a pivotal role in overall water splitting but remains kinetically sluggish due to the involvement of a multistep four-electron/proton transfer process, necessitating the development of efficient, stable, and earth-abundant catalysts.[1] Herein, we report a series of salen-based heterometallic nickel complexes as molecular electrocatalysts for OER under alkaline conditions. Among them, complex **Ni-Fe(Salen)** exhibits outstanding catalytic performance, delivering a current density of 50 mA cm^{-2} at a low overpotential of 350 mV and maintaining excellent operational stability for 24 h. Mechanistic investigations indicate that the OER proceeds via a lattice oxygen mechanism (LOM), highlighting the non-innocent participation of ligand-derived oxygen species during catalysis.[2,3] Detailed electrochemical analyses reveal the in-situ formation of a heterointerface between complex **Ni-Fe(Salen)** and Ni(O)OH, which serves as the catalytically active phase and significantly enhances OER activity.[4,5] The synergistic interaction at this molecular-inorganic interface facilitates efficient charge transfer and stabilizes high-valent nickel intermediates during turnover. This work underscores the potential of rationally designed heterometallic molecular complexes to construct active heterointerfaces and provides new insights into leveraging lattice oxygen participation for high-performance OER catalysis.



***Scheme 1**: Ni–Fe Salen Complex Promotes Water Oxidation through a Lattice Oxygen Pathway*

Keywords: Electrocatalysis, Oxygen evolving reaction, lattice oxygen mechanism, salen

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PP–04

Unleashing the true Potential of Halide-rich Perovskites in Superior Charge Transport Dynamics through Strategic Ligand Engineering

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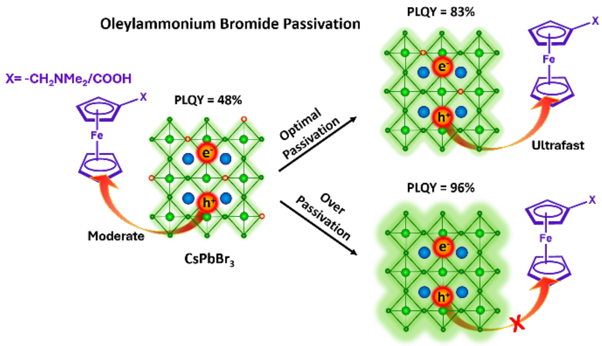
Perovskite nanocrystals (NCs) offer significant potential for photovoltaics, but optimizing surface passivation while ensuring efficient charge transport remains a challenge. This study employs oleylammonium bromide (OAmBr) to modulate ligand density in $CsPbBr_3$ (CPB) NCs, enhancing charge extraction while mitigating surface traps. By systematically varying OAmBr concentrations, we investigate the impact of bromide-rich surface sites and ligand density on charge extraction efficiency, revealing distinct charge transfer mechanisms for FcA and FcAm. Lower ligand densities improve FcA transport by enhancing surface accessibility, whereas FcAm transfer is governed by both ligand density and bromide-rich surface sites. Notably, CPB12 exhibits superior FcAm charge transfer due to its accessible bromide-rich surface. While surface passivation boosts charge transport to hole acceptors, excessive ligand densities (CPB150) hinder extraction. These findings provide a strategic framework for optimizing ligand engineering to enhance perovskite-based photovoltaics.



Keywords: Perovskite nanocrystals, halide-rich perovskite nanocrystals, surface chemistry, trap state passivation, charge separation, hole transfer

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PP–05

Exploring Low-Frequency Infrared Spectra of LiTFSI in Tetrahydropyran using Polarizable Models

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Tetrahydropyran (THP) exhibits high chemical stability, favourable ionic conductivity, and compatibility with various electrode materials. Its low volatility and strong solvating ability enhance battery performance and safety. These properties suggest tetrahydropyran is a promising candidate for advanced electrolyte design in energy storage systems.[1,2] The low-frequency vibrational regime of cyclic ether-based systems, particularly THP, remains largely unexplored, leaving an important gap in the fundamental understanding of collective ion-solvent dynamics that govern ion transport. The low-frequency IR region is primarily sensitive to intermolecular and collective motions,[3] including solvent librations, Li^+ cage motion, contact ion pair formation, and ion aggregation processes.[4] These modes are directly linked to solvation strength and ionic mobility. In this work, we use polarizable models for simulating LiTFSI in THP and calculating the low-frequency IR spectra of electrolyte solutions at varied LiTFSI:THP ratios. We dissect the spectra into intra- and inter-species components and analyse vibrational features associated with Li^+-THP coordination. This way, one can resolve collective modes that are difficult to isolate experimentally and relate the low-frequency spectral features to microscopic solvation structures and dynamics.

Keywords: Energy storage, Li-ion battery, cyclic-ether, polarizable model, linear spectroscopy

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PP–06

Structural Tuning of 1,3,4-Oxadiazoles via Bridging for Controlled Energetic Output

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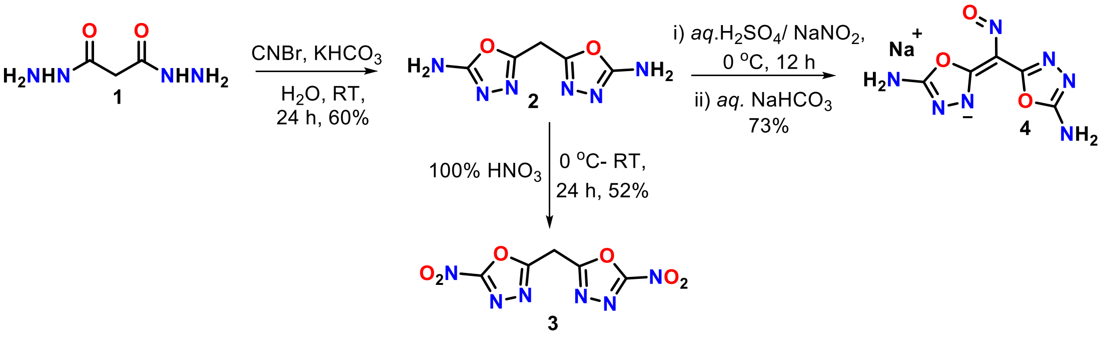
Energetic materials store substantial chemical energy and release it rapidly upon stimulation, enabling applications in defense systems, aerospace propulsion, mining, and other civilian technologies. Nitrogen-rich compounds are particularly attractive due to their high energy density and favorable physicochemical properties. Nitrogen-containing heterocycles act as compact energy reservoirs, where abundant N-N and N-O bonds promote rapid heat and gas generation during detonation. Unlike purely nitrogen-based rings such as triazoles and tetrazoles, oxadiazoles incorporate oxygen atoms within the heterocyclic framework, improving oxygen balance, crystal density, and structural stability. Among them, the 1,3,4-oxadiazole motif has emerged as a promising platform for next-generation energetic materials. Herein, methylene- and nitroso-bridged architectures (**2-4**) based on the 1,3,4-oxadiazole core were synthesized through efficient and scalable methodologies. Notably, methylene bridging significantly enhanced insensitivity without compromising detonation performance or thermal stability, demonstrating their potential as advanced high-energy-density materials.



***Scheme 1**: Synthesis of compounds 1-4 for multiple applications.*

Keywords: Energetic materials, methylene bridged, oxadiazole, nitro

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PP–07

Single-Source Synthesis of Bifunctional Pyrazole-Triazole Energetic Materials with Modulated Stability and Sensitivity

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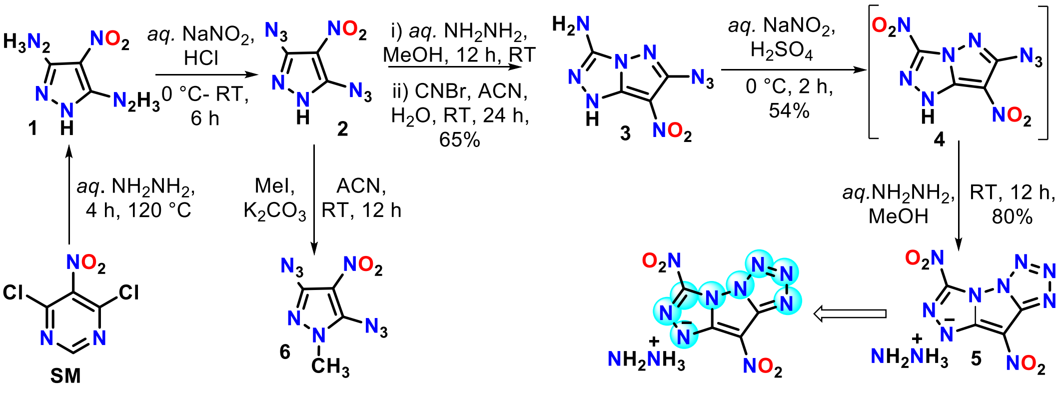
Energetic materials play a crucial role across a wide range of applications, including defense technologies, space exploration, and civilian uses. In recent years, nitrogen-rich compounds have attracted significant attention owing to their propensity to decompose into environmentally benign gaseous products. These materials further offer desirable characteristics such as low volatility and high thermal stability, enabling their incorporation into diverse formulations, including energetic ionic liquids and hydrocarbon-based systems. Energetic materials are typically tailored for specific functions; for instance, explosives are engineered to release energy rapidly and commonly incorporate explosophoric groups such as nitro (-NO_2) and azide (-N_3) moieties to enhance their performance. Current state-of-the-art research is focused on the development of high-energy-density materials that combine superior detonation performance with reduced sensitivity to mechanical stimuli. In this context, five-membered heterocyclic frameworks, such as tetrazole, triazole, furazan, and pyrazole, along with their functionalization using energetic groups, provide versatile platforms for advancing next-generation energetic materials.



***Scheme 1**: Synthesis of compounds 1-6 for multiple applications.*

Keywords: Energetic materials, fused rings, catenation, tetrazole, triazole, azide

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PP–08

Repurposing Cu scrap into a multi-functional catalytic anode for energy conversion reactions

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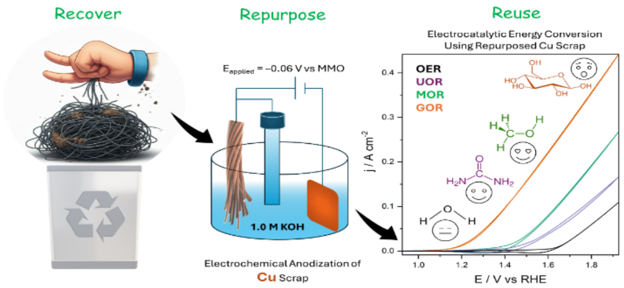
As global emphasis on sustainable development is growing every year, the efficient recovery, repurposing and reusing of metals from waste has become an urgent priority. A novel approach has been developed to recover copper (Cu) scrap wires from e-waste, utilizing a simple pre-cleaning process followed by potential-controlled anodization. This method forms a dense layer of $Cu(OH)_2/CuO$ nanoneedles on the surface of the Cu wires, which are then employed as electrocatalytic interfaces for the oxidation of various small molecules. Our results indicate that $Cu(OH)_2/CuO$ nanoneedle arrays exhibit high efficiency for the oxidation of urea (UOR), methanol (MOR), and glucose (GOR) in 1.0 M KOH, with potentials required to achieve a current density of 10 mA cm^{-2} of 1.499 V, 1.438 V, and 1.192 V respectively. Notably, these electrodes exhibit significant OER-masking capability, requiring 157 mV less for UOR, 218 mV less for MOR, and 464 mV less for GOR compared to the OER. By integrating Cu wire recycling into electrocatalysis, this approach not only adds value to electronic waste but also reduces the environmental impact of wastewater while addressing the global challenge of the approximately 9 million metric tons of copper scrap generated annually.



***Scheme 1**: Repurposing Cu scrap for different electrooxidation reactions*

Keywords: Potential-Controlled Anodization, Nanoneedles, Electrocatalytic Interfaces, OER Masking, Electrocatalysis

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PP–09

A New Direction in Catalyst Synthesis toward High-Performance OER via an Eccentric Corrosion Method

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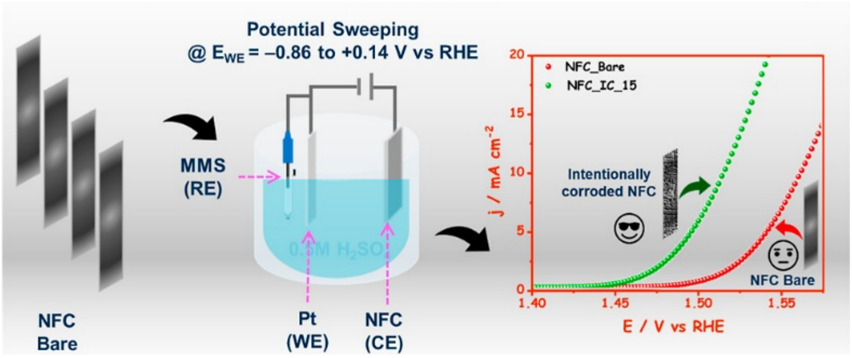
For scalable and sustainable hydrogen production, it is essential to utilize non-noble metals and adopt synthesis methods that are easy to implement. Therefore, an easy method of enhancing the oxygen evolution reaction (OER) performance of an economically viable Fe-rich NiFeCo (NFC) alloy has been developed. This approach employs HER on the Working Electrode (WE), which indirectly induces anodic potential at the Counter Electrode (CE). NFC was intentionally corroded indirectly by using it as a CE during potential sweeping HER with a Pt WE.

The indirectly corroded NFC (NFC_IC), featuring mostly γ-NiFeOOH and γ-NiCoOOH entities on the surface, began OER at an onset overpotential of 250 mV and reached 10 mA cm^{-2} at 290 mV, which is 60 and 55 mV lower than bare NFC and RuO_2, respectively, with faster kinetics as evidenced by a smaller Tafel slope of 30 mV dec^{-1}. Overall, this work offers insights into designing trimetallic alloy-based OER electrocatalysts and opens a new avenue for developing improved self-supported OER electrodes for more efficient H_2 production via water electrolysis.



***Scheme 1**: Intentionally Corroded Fe-rich NiFeCo Alloy with Enhanced OER Activity*

Keywords: Electrocatalysis, Oxygen Evolution Reaction, Hydrogen Production

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PP–10

Novel Co(III) NHC Catalysts for Highly Efficient Dehydrogenation and Recycling of Formic Acid: Approach Towards Carbon-Neutral System and Green Energy

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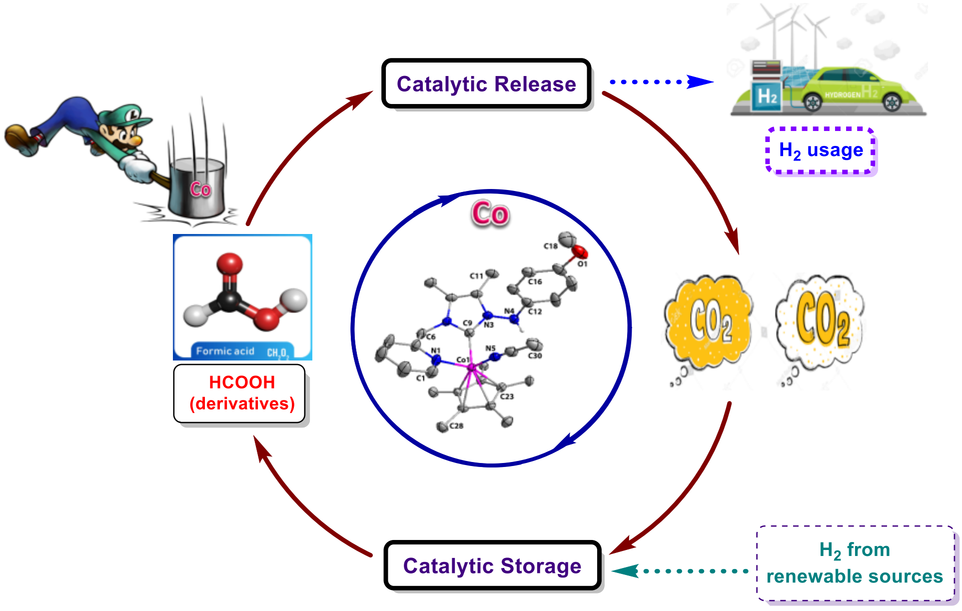
Implementation of 'hydrogen economy' facilitating sustainable energy as a lucrative alternative to fossil fuels is critically dependent upon methods to safely store & controllably release hydrogen. The released CO_2 from dehydrogenation of FA, one of the potential LOHCs possessing high hydrogen content (4.4 %), high energy density (1.77 kWh L^{-1}) and non-toxicity[1], (i.e. FADH) can be recaptured to regenerate FA creating a closed-loop[2]. The meticulously designed Co(III) complex is found to achieve additive and/or temperature-dependent TOFs ranging from 3,800 (60 $^{\circ}$C) to 295,000 h^{-1} (95 $^{\circ}$C) and upto 2.7 million TONs for FADH thus giving a tough competition to state-of-the-art systems. The elevated efficiency coupled with exceptionally low cost & facile synthesis of the catalyst (< \$30/g) are attractive characteristics for industrial applications.



♣ Inexpensive 3d metal catalyst ♣ Air & moisture stable and dormant catalyst
♣ Exceptionally high TON values ♣ Handsome TOF values under base-free conditions

***Scheme 1**. Catalytic cycle for FA hydrogen storage*

Keywords: Organometallic Catalyst, Hydrogen Economy, Sustainability

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PP–11

Fused Azo-Bridged Triazolo-Pyridazine-Derived Energetic Materials

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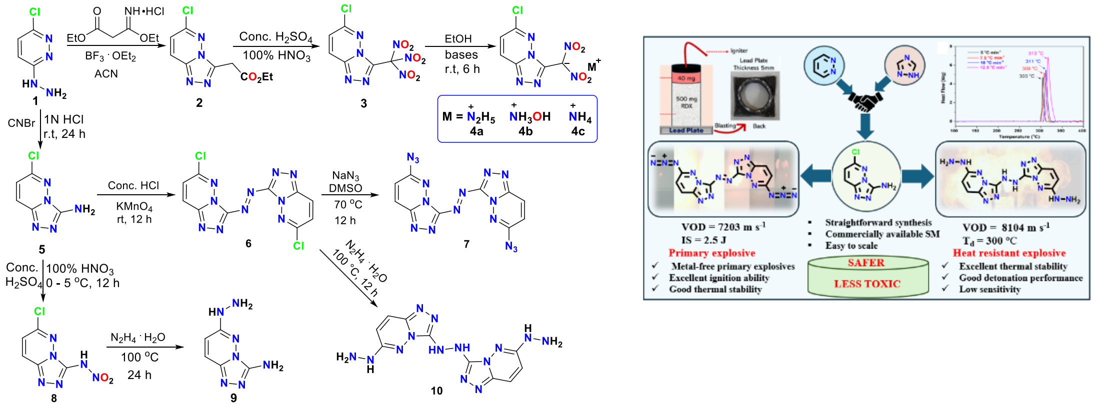
Energetic materials are essential in military, aerospace, and civilian applications. Nitrogen-rich compounds are particularly attractive due to their high energy content and environmentally benign decomposition to N_2. In this study, nitrogen-rich fused heterocyclic systems incorporating nitramine, azide, hydrazine, and azo functionalities were designed and synthesized as potential high-performance, metal-free explosives.

The new compounds exhibited favorable densities (1.60–1.76 g cm^{-3}), high detonation velocities (6642-8104 m s^{-1}), moderate to controlled sensitivities (IS: 2.5-40 J; FS: 120–360 N), and thermal stability ranging from 128-300 °C. Notably, compound **10** showed outstanding thermal stability (300 °C) as a heat-resistant explosive, while compound **7** demonstrated strong potential as a lead-free primary explosive with an ultralow primer charge of 40 mg.



Scheme 1: *Synthesis of fused-ring energetic compounds 3 to 10.*

Keywords: High-energy density materials; Metal-free primary explosives; Heat-resistant explosives

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PP–12

Design of Imidazolium Based cationic COF Polymer composite Electrolyte for high performance advanced solid-state Electrolytes for Lithium-Ion Batteries

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Developing powerful, safe, and durable energy storage systems is essential for modern devices, from portable gadgets to electric vehicles. While lithium-ion batteries (LIBs) are common, their flammable liquid electrolytes pose safety risks, especially at high energy levels. Solid polymer electrolytes enhance safety and compatibility with battery components but often have low ion conductivity. In this study, we developed a new Imidazolium covalent organic framework (Im-COF) loaded with acid and combined it with polyethene oxide (PEO) to create a solid composite electrolyte. This PEO-COF composite exhibits improved ion conductivity at room temperature 1.1×10^{-5} Scm^{-1} and a higher lithium-ion transfer (0.56) than typical PEO systems. The cationic Im-COFs is a porous structure which facilitates anion trapping in the matrix and allows only Li to migrate through the channels. Stripping plating shows stability with lithium metal for over 1000 hours at low current of 0.1 $mA.cm^{-2}$ and sustained stability at higher current till 0.3 $mA.cm^{-2}$. In a solid-state lithium-ion battery with a $LiFePO_4$ cathode, Li metal as anode and this composite electrolyte, delivers a high discharge capacity of 110 mA. hg^{-1} at C/3 rate and retains 75% capacity after 1200 charge cycles at 60 °C. These results demonstrate that Im-COF-based polymer composites are a promising solid-state electrolyte offering safety, ease of production, and strong battery performance for future lithium-ion batteries.

Keywords: Solid-state electrolyte (SSE), Lithium-ion Battery (Li-ion Battery), Imidazolium Covalent Organic Framework (Im-COF)

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PP–13

Evolution of self-assembled chessboard-like structures by recurrent phase separation and coalescence of domains to obtain multifunctional heterostructures

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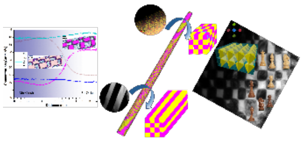
Well-organized, multi-phase microstructures enable superior multifunctional properties that are difficult to achieve in bulk materials of the same composition. This Solid-state self-assembly is a viable approach for creating such ordered microstructures. The CB-like nanostructures evolve through a complex sequence of twinning, subdomain formation via recurrent pseudo-spinodal decomposition, and domain coalescence along specific crystallographic axes. The process begins with cross-penetration of compound deformation twins accompanied by subtle chemical segregation between domains, ultimately leading to a polymorphic transformation into cubic and tetragonal phases. This work describes the evolution mechanism of a chessboard-like, multi-phase self-assembled nanostructure composed of Mn-rich ($CoMn_2O_4$) and Mn-lean ($CoFe_2O_4$) phases in $CoFe_xMn_{2-x}O_4$. In this system, magnetic coercivity increases by severalfold following the formation of the CB-like nanostructure, making these materials promising candidates for high-density memory and energy storage applications. Differences in lattice parameters between the cubic ($CoFe_2O_4$) and tetragonal ($CoMn_2O_4$) phases produce rotationally oriented product domains. Correlative TEM and APT analyses further reveal that recurrent pseudo-spinodal decomposition within the CB-like domains gives rise to finer CB-like nanodomains.



Scheme 1: self-assembled chessboard-like structures by recurrent phase separation and coalescence of nano domains in CoFeMnO system

Keywords: Chessboard-like microstructure, Correlative microscopy, Nanoarchitectonics, Pseudo-spinodal decomposition, solid-state Self-assembly.

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PP–14

Development and optimization of flexible solid-state electrolytes for high-performance Li-ion batteries

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The present work displays the development and optimization of the lithium phosphorous sulphur chloride (Li6PS5Cl) solid electrolyte for high-performance lithium-ion batteries. This study presents a systematic optimisation of polyethylene oxide (PEO) binder concentration and its impact on the properties of the sulphide-type solid electrolyte. Different concentrations of PEO (i.e. 0, 5, 10, and 15 weight percent) are added to LPSCl using a dry mixing approach, and the properties of the synthesized solid electrolyte composites are studied. Ionic conductivity, interfacial resistance, and relative density are measured using electrochemical impedance spectroscopy, and pellet physical characterization. Morphological and structural properties of the synthesized solid electrolyte composites are investigated through scanning electron microscopy (SEM) and X-ray diffraction technique (XRD), respectively. It is observed that solid electrolyte composites containing 10 wt% PEO performed better than all other compositions. Although ionic conductivity (IC) decreased as anticipated, a consistent reduction in interfacial resistance (IR) is also observed.

Keywords: Sulphide electrolyte, Flexible Battery, Ionic conductivity, LiPSCl, PEO

PP–15

Catenated Nitrogen-Rich Triazine-Tetrazole Molecules for Advanced Explosives and Gas-Generator Applications

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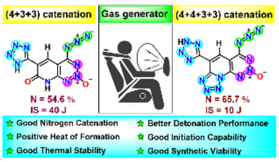
Catenated nitrogen-rich energetic materials are important building blocks for explosives, propellants, pyrotechnics and gas generators. They play a key role in military, aerospace, and civilian applications.[1] But the trade-off between performance and safety further limits their modern applications. As we know, Sodium azide, as a traditional catenated nitrogen-rich gas generator, is widely used in automobile airbags. Over time, its use has reduced due to the production of sodium-based residues upon combustion, toxicity, and instability during long-term storage.[2] These problems have encouraged the search for safer, cleaner, and more stable nitrogen-rich alternatives. Recently, researchers have considered tetrazole and 1,2,3-triazine compounds as greener options, as they mostly release nitrogen gas upon decomposition. Therefore, in view of this, we undertook the synthesis of a tricyclic compound with a bicyclic core, 4-azido-7-oxo-6-(1*H*-tetrazol-5-yl)-7,8-dihydropyrido[2,3-*d*][1,2,3]triazine 2-oxide, which features 4+3+3 nitrogen catenation and tetracyclic compound with a tricyclic fused core, 6-azido-4-(2*H*-tetrazol-5-yl)tetrazolo[1',5':1,6]pyrido[2,3-*d*][1,2,3]triazine 8-oxide, which exhibits 4+4+3+3 catenation through a facile synthetic route. All the compounds are fully characterized and exhibit high densities, good thermal stabilities, detonation velocities, detonation pressures, and high insensitivity. Overall, Synthesized compounds demonstrate strong potential as next-generation EMs and viable candidates to replace traditional gas generators.



Keywords: High-energy density materials (HEM), Gas generator, Catenation, Detonation velocity, Detonation pressures, and Sensitivity.

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PP–16

Lubricant Infused Surface: Role of Lubricant Viscosity on Fog Collection

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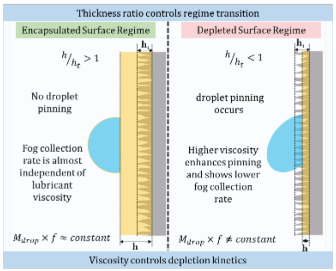
Nepenthes-inspired lubricant-infused surfaces offer high efficiency for fog harvesting but are often limited by lubricant depletion. Although lubricant depletion is often correlated to lubricant viscosity, the role of lubricant viscosity on fog harvesting was not explicated.[1] To address this, LIS of various lubricant viscosities were fabricated via a two-step immersion procedure. Fog collection experiments, conducted for short-term (30 min) and multicyclic trials exhibit distinct behaviour. To explain this, we established a mechanistic framework based on the thickness ratio (h/h_t), defining two distinct interfacial states: the encapsulated regime ($h/h_t > 1$) and the depleted regime ($h/h_t < 1$). Data analysis confirmed that while viscosity dictates depletion kinetics, the thickness ratio governs the regime transition and the onset of droplet pinning. In the encapsulated regime, collection rates remain high and viscosity-independent. Conversely, in the depleted regime, higher viscosity exacerbates pinning, leading to a sharper performance decline. Based on the proposed framework, maintaining a prolonged encapsulated state is critical for long-term efficiency. This work establishes a thickness-ratio-governed framework for designing durable, high-performance fog harvesters.



Keywords: Nepenthes, slippery surface, fog harvesting

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PP–17

N-centered persistent organic radicals: potential organic materials for next-gen optoelectronics

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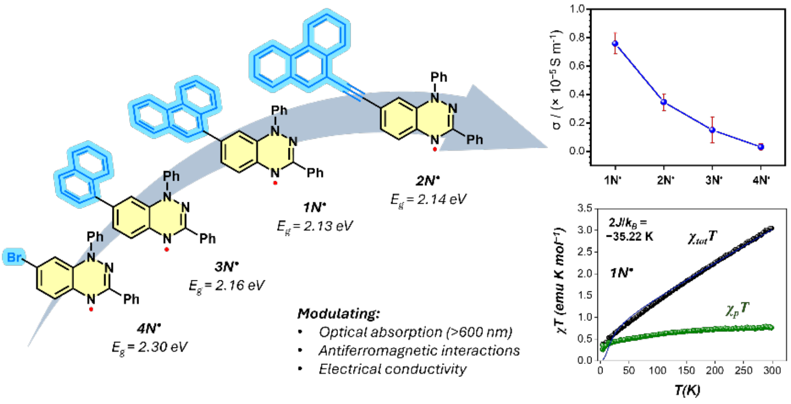
Open-shell organic molecules that possess active spin in their singly occupied molecular orbital (SOMO) and exhibit unique physical properties such as reversible multicycle redox behavior, low band gaps, and magnetic properties. Among them, Blatter radicals received significant interest recently due to their additional high air, chemical, and thermal stability, particularly for applications in organic electronics, optoelectronics, spintronics, high-energy storage, molecule-based magnets, etc. Herein, I discuss how optoelectronic properties are modulated in Blatter radicals (**1N$^\bullet$** – 4N$^\bullet$) through systematic structure modulation and demonstrate this in molecular junctions. As a highlight, the optical properties were modulated to the NIR range, while the antiferromagnetic interactions were tuned with exchange interactions (*$2J/k_B$)* in the range of −35.22 K, and the solid-state thin film conductivity was tuned to ca.7.2 × 10^{-6} Sm^{-1} compared to non-conjugated Blatter radical, **4N$^\bullet$** (2.85 × 10^{-7} Sm^{-1}).



Scheme 1: Schematic illustration of modified Blatter radical derivatives for electrical conductivity

Keywords: Open shell molecules, NIR absorption, antiferromagnetic interactions, thin films, electrical conductivity.

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PP–18

Ionic Liquid assisted Interfacial Engineering for Quasi–Solid-State Lithium Metal Batteries

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In this presentation, we use LATP, a NASICON-type solid-state electrolyte that conducts lithium ions. A key challenge in solid-state batteries is the poor electrode–electrolyte contact, which leads to high interfacial impedance, along with additional resistance arising from grains and grain boundaries. To address these issues, we incorporate a solvated ionic liquid (SIL), which promotes intimate and stable interfacial contact at both electrodes. This approach also helps mitigate filament (dendrite) formation, improving overall stability. Unlike conventional liquid electrolytes, the SIL is non-flammable and can lower the population of free, highly mobile ions, which can be beneficial for interfacial control. We evaluate the system using electrochemical techniques including EIS, LSV, CV, lithium stripping/plating, and galvanostatic charge–discharge testing. Structural and chemical characterization is carried out using XRD, FESEM, and FTIR. Additional characterization and extended electrochemical results will be presented in the poster.

Keywords: LATP, metal-electrolyte interface, solid-state lithium batteries, solvated ionic liquid

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PP–19

Polymer Derived and Ni-Single Atom Doped Carbon Nanofibers for CO_2 Capture and Electroreduction to CO

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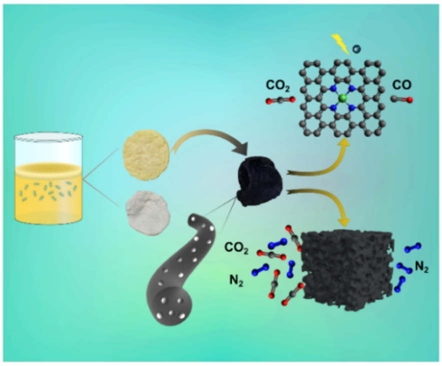
Unique properties of carbon nanofibers (CNFs), such as high surface area, tunable porosity and heteroatom doping capability, make them archetypes for CO_2 capture and conversion applications. Single-atom catalysts (SACs) with metal-nitrogen-carbon motifs have been transformative in electrocatalytic CO_2 reduction (eCO_2R), due to their high atomic utilization, under-coordinated active sites, and unique electronic structures. Herein, porous CNFs from three polymers, viz. Bacterial cellulose, Aramid, and Zylon are optimally synthesized. The textural and porous architectures of the CNFs are exploited for ambient and high-pressure CO_2 capture, with Aramid-CNFs exhibiting the highest CO_2 adsorption capacity of 4 mmol g^{-1} at 1 Bar, 273K. Subsequently, the N-doped CNFs of carbonized bacterial cellulose (N-CBC) are explored for hosting Ni single atoms to yield Ni-N-CNF SACs. Extended x-ray absorption fine structure (EXAFS) analysis, microscopic studies and corroborative density functional theory (DFT) calculations confirmed the atomic dispersion of Ni sites on N-CBC matrix having $Ni\text{-}N_4$ coordination. Ni-N-CBC at a mere 0.1 wt% Ni loading exhibited competitive and durable eCO_2R-to-CO performance with Faradaic efficiency (FE_{CO}) of 94±3% at 0.53 V versus reversible hydrogen electrode (RHE) and a high turnover frequency (TOF) of 35.26 s^{-1}. This work underscores the properties and potential of CNFs for sustainable CO_2 capture and conversion.



Keywords: Aramid, Bacterial Cellulose, Zylon, Carbon nanofibers (CNFs), Electrocatalytic CO_2 reduction (eCO_2R), Ni single atom catalyst (Ni-SAC)

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PP–20

Exploring Prussian Blue Analogue-derived W-doped FeNi-LDH for Electrocatalytic Anodic Oxidation Reactions

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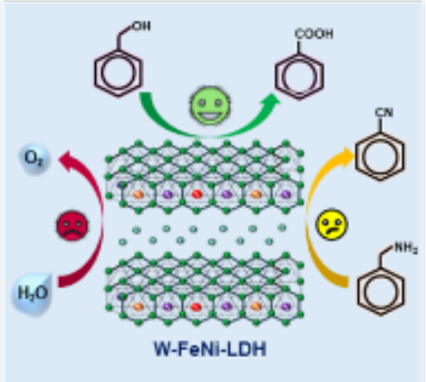
Electrocatalytic water splitting is a highly promising method for H_2 production. However, the oxygen evolution reaction (OER) poses a considerable challenge of sluggish kinetics and high energy demand. Anodic oxidation reactions (AORs) provide an efficient alternative, enabling hydrogen generation while producing valuable chemicals.[1-2] This study evaluates the benzylamine oxidation reaction (BAmOR) and benzyl alcohol oxidation reaction (BAOR) using a single W^{6+}-incorporated FeNi-layered double hydroxide (W-FeNi-LDH) catalyst. The high-valent W^{6+} enhances charge transfer, increases the number of active sites, and improves electrochemical performance.[2-3] The W-FeNi-LDH reaches 100 mA cm^{-2} at 1.48 V (1.59 V) vs. RHE for BAOR and BAmOR, with nearly 100% selectivity for benzonitrile (FE = 95.8%) and benzoic acid (FE = 97.6%), respectively.[1] This work highlights that benzyl alcohol is a suitable substrate for AORs, with potential improvements in H_2 production, energy efficiency, and faradaic efficiency compared to water and benzylamine.



Scheme 1: A Prussian blue analogue derived W-FeNi-LDH catalyst has been explored to evaluate the suitable substrate for anodic oxidation reaction.

Keywords: Electrocatalysis, Anodic Oxidation Reactions, H_2 Production

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PP–21

Galvanic Displacement Strategy for Fabricating Pt-Decorated Cu Electrodes Towards Efficient HER

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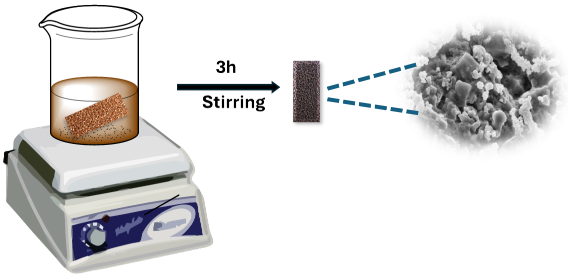
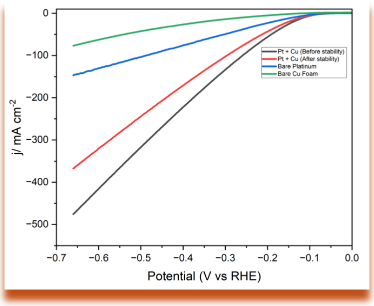
Hydrogen is a promising alternative to non-renewable fossil fuels, and enhancing the hydrogen evolution reaction (HER) is essential for environmentally friendly hydrogen generation via electrochemical water splitting.[1] Pt-based electrocatalysts are widely used because of their high activity and stability; however, their scarcity and high-cost limit large-scale applications. To address this challenge, we report the synthesis of Pt nanostructures on Cu foam with enriched CuO/Pt interfaces through a galvanic replacement reaction, reducing Pt usage to only 5.68% (1/4th of commercial Pt content in commercial Pt/C 20 wt.%). Our investigations confirmed the successful formation of Pt nanoparticles with an average grain size of 3.25 nm, as revealed by transmission electron microscopy (TEM). XRD and Raman analyses indicated the coexistence of CuO phases and Pt nanoparticles, evidencing partial oxidation of the copper support. Electrochemical evaluations demonstrated substantial improvements in catalytic activity after Pt deposition. The electrocatalyst demonstrated an outstanding performance with only 98 mV overpotential to achieve the 100 mA cm^{-2} current density and demonstrated stability for 12 h. This study underscores galvanic displacement as a simple and efficient approach to design Pt-decorated Cu foam electrodes with enhanced surface properties, offering a cost-effective pathway for advanced electrocatalytic applications.[2]





Keywords: HER, Electrocatalyst, H_2 Production

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PP–22

Terephthalate-Induced Lattice Defects in NiCo-Hydroxide for Corrosion-Tolerant Seawater Oxidation

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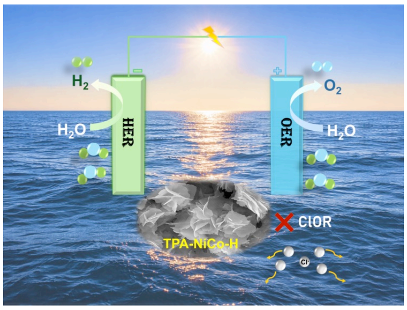
Unlike freshwater, seawater oxidation faces significant challenges due to the competing chloride oxidation reactions (ClOR) and chloride-induced corrosion. Herein, a molecular intercalation strategy has been developed to design NiCo-hydroxide by incorporating terephthalate (TPA) anions derived from waste plastic bottles. The incorporated TPA modulated the electronic structure of metal centres, expanded the interlayer spacing, and induced lattice disorder through edge dislocations. Consequently, TPA-NiCo-H exhibited enhanced seawater oxidation performance, requiring only 310 mV overpotential to achieve a current density of 10 mA cm^{-2}, outperforming pristine NiCo-H and RuO_2. Interlayer-anchored TPA suppressed chloride-induced corrosion and structural degradation in seawater, maintaining continuous operation for over 5 days. *In-situ* Raman studies confirmed the formation of Ni^{4+} as an active species, while electrochemical impedance spectroscopy (EIS) suggested accelerated charge-transfer kinetics in TPA-NiCo-H. This work highlighted the organic linker intercalation as an effective strategy to enhance activity, stability, and corrosion resistance for seawater oxidation.



***Scheme 1**: Terephthalate-coordinated NiCo-hydroxide for chloride-resistant seawater oxidation*

Keywords: Organic linker intercalation, lattice distortion, seawater oxidation, corrosion resistant, long-term stability

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PP–23

Upconversion-Assisted Solar Hydrogen Evolution on β-SiC with Surface and Thermoelectric Modulation

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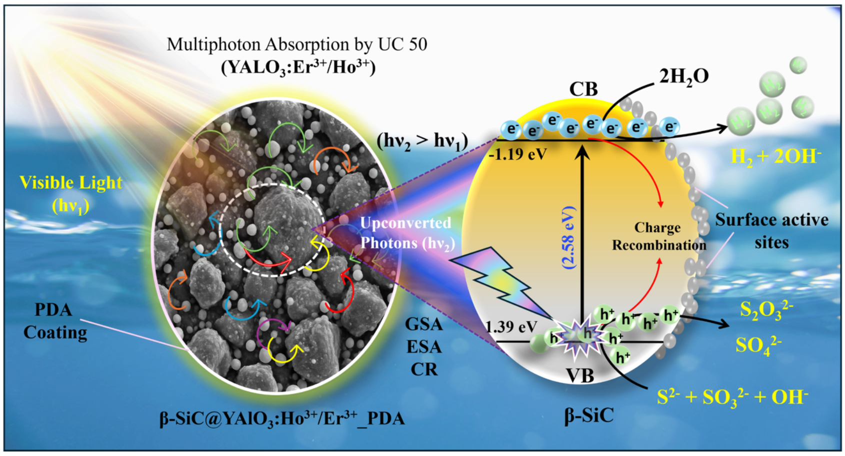
The limited absorption of sub-bandgap photons by conventional photocatalysts such as CdS, TiO_2, and β-SiC restricts solar-to-hydrogen conversion efficiency. Herein, we developed a broadband activation strategy by integrating Ho^{3+}/Er^{3+}-doped $YAlO_3$ upconversion phosphor (UC-50) with β-SiC, followed by conductive polydopamine (PDA) surface engineering. The resulting β-SiC@UC-50_PDA nanosystem coupled with photon upconversion and interfacial charge modulation. Under visible-light irradiation in 0.1 M Na_2S/Na_2SO_3, β-SiC@UC-50 achieves a 3.9-fold enhancement in H_2 evolution over pristine β-SiC, while PDA functionalization increases activity to 4.6-fold with excellent dispersibility. An apparent quantum efficiency of 11.53% at 650 nm confirms effective sub-bandgap photon utilization, and a ~2.9-fold higher photocurrent at 1.5 V vs RHE indicates improved charge separation. In situ electrochemical analysis verifies elemental sulfur formation from S^{2-} oxidation. Integration with a thermoelectric generator (TEG) further improves overall energy utilization by converting photothermal losses into electrical bias.



Scheme 1: Schematic Overall Mechanism for UC-assisted Solar Hydrogen generation.

Keywords: Green Hydrogen, Sustainable Energy, Photocatalysis, Upconversion, Solar Fuels

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PP–24

Interlayer Engineering in Layered Double Hydroxides for Efficient Electro-Oxidation of 1,4-Butanediol

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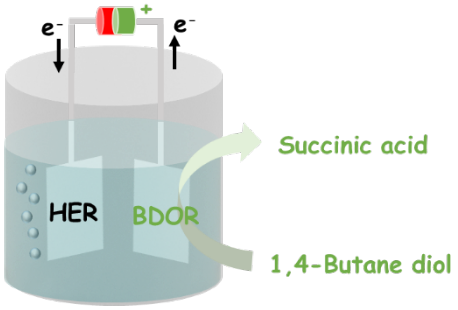
Growing emphasis on green and sustainable development has increased demand for succinic acid (SA), attracting considerable attention due to its role as a key monomer in the production of polybutylene succinate (PBS). Conventional industrial production of SA depends on hydrogenation of maleic anhydride under high temperature and pressure with external H_2, raising economic and environmental concerns. As a cleaner alternative, the electrocatalytic oxidation of 1,4-butanediol (BD) to SA offers a simpler and greener pathway. Building on this approach, NiFe-layered double hydroxide catalyst was modified using disodium terephthalate (NiFe-TPA) intercalation derived from waste polyethylene terephthalate. Consequently, NiFe-TPA exhibited enhanced 1,4-butanediol oxidation reaction (BDOR), requiring only 1.48 V to achieve 100 mA cm^{-2} current density, outperforming pristine NiFe-LDH. The incorporation of TPA expands the interlayer spacing, stabilize the structure, and tunes the electronic and redox properties of NiFe active sites. Electrochemical impedance spectroscopy confirmed enhanced charge transfer and faster reaction kinetics upon TPA incorporation, while in-situ Raman analysis highlighted the active participation of electro-generated Ni^{3+} species during BDOR.



***Scheme 1**. Schematic representation of electrocatalytic BDOR*

Keywords: Layered double hydroxide, terephthalate anion, 1,4-butane diol oxidation, succinic acid

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PP–25

Coordination Site Engineering Induced Lattice Distortion in 2D Precatalyst for Efficient Anodic Oxidation Reaction

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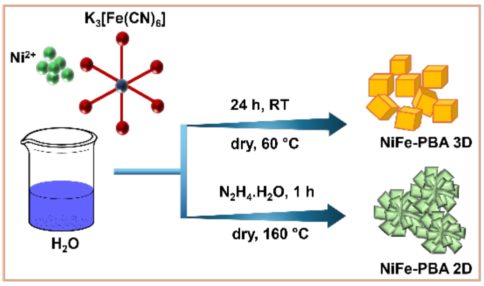
Electrocatalytic urea oxidation reaction (UOR) is an efficient approach for the waste-water treatment and replace sluggish oxygen evolution reaction (OER) for the improved hydrogen production.[1] In this work, we have developed a 2D Prussian blue analogue (PBA) precatalyst for electrocatalytic urea oxidation. Using a site-selective reduction method, we successfully induce the formation of 2D-NiFe-PBA nanosheets containing unsaturated coordination sites. The 2D-NiFe-PBA precatalysts exhibited altered structural and electronic features.[2] As a result, it required only 1.56 V to reach 100 mA cm^{-2} for OER and 1.42 V for UOR. Mechanistic analysis reveals that Ni^{4+} centers generated during applied anodic potential drive OER through a lattice oxygen mechanism, while Ni^{3+}/Fe^{3+} species catalyse UOR. Overall, this study highlights 2D catalyst engineering as a promising strategy for efficient UOR.



***Scheme**: Synthesis scheme for PBA tuning morphology*

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PP–26

Free-Standing Blatter Radical Polymer Thin Films with Controlled Nanometer Thickness and their Redox-Optical Behaviour

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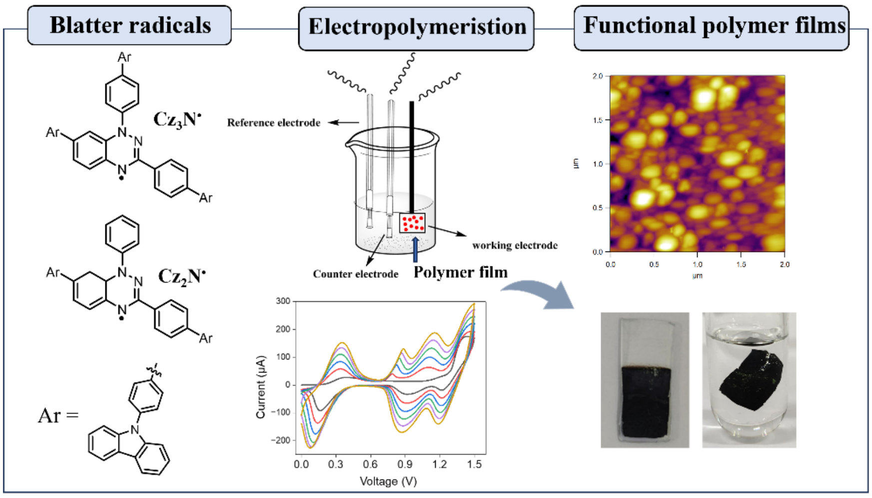
Polymerization of air-stable Blatter radicals into processable/free-standing thin films while retaining their redox properties is crucial for applications in electrochemical devices such as redox flow batteries, metal-ion batteries or for electrocatalysis. Herein, we elucidate the electropolymerization-assisted generation of carbazolyl Blatter radical polymer thin films with nanometer-precision thickness control, as well as into free-standing thin films with the retained redox characteristics of Blatter radicals integrated within polymeric thin films, and demonstrate their structure-property relationship, particularly the modulation of optical, electronic, and magnetic properties. The π-conjugated Blatter radicals exhibited NIR absorption properties compared to pristine Blatter radical due to extended π-conjugation and exhibit solid-state antiferromagnetic interactions due to spin-spin coupling interactions via intermolecular π-π interactions.



__Scheme 1__: Schematic illustration of modified Blatter radical derivatives into free standing polymer thin films.

Keywords: Organic radicals, Electropolymerisation, Free-standing thin films, Antiferromagnetic interactions.

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PP–27

Ni–Fe MOFs and Hydroxides for Oxygen Evolution: Mechanistic Insights via Chemical Probes and pH Studies

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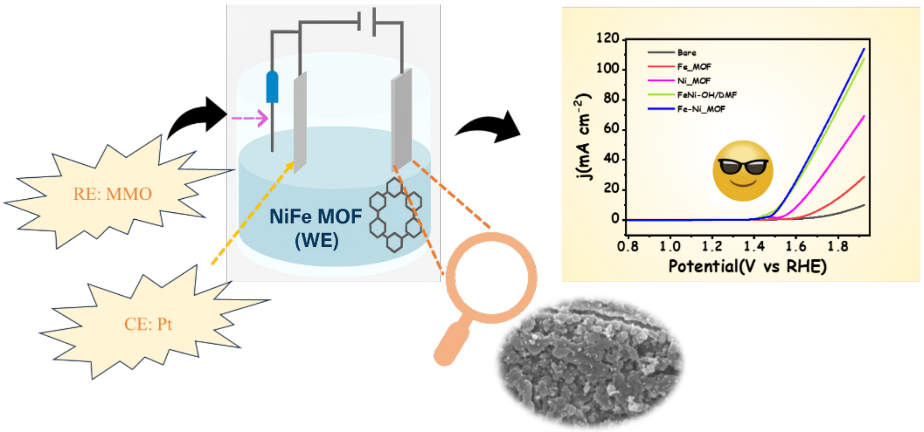
Nickel–iron (NiFe) materials are promising earth-abundant electrocatalysts for the oxygen evolution reaction (OER). In this work, Ni-MOF, Fe-MOF, and NiFe-MOF were synthesized by solvothermal methods using terephthalic acid (H2BDC) as the linker. On the other hand, NiFe hydroxide (NiFe–OH) was obtained via KOH-triggered biphasic precipitation in DMF. Electrochemical tests (CV, LSV, EIS) showed that NiFe-MOF exhibited the highest OER activity, with NiFe–OH showing comparable performance. Mechanistic studies with pH variation and chemical probes (methanol, TMAH) confirmed a pH-independent adsorbate evolution mechanism (AEM). These findings highlight design strategies for efficient NiFe-based OER catalysts.



Scheme 1: *Electrochemical water splitting in a three-electrode Configuration, and corresponding polarization curve*

Keywords: NiFe-MOF; NiFe–OH; OER; Electrocatalysis

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