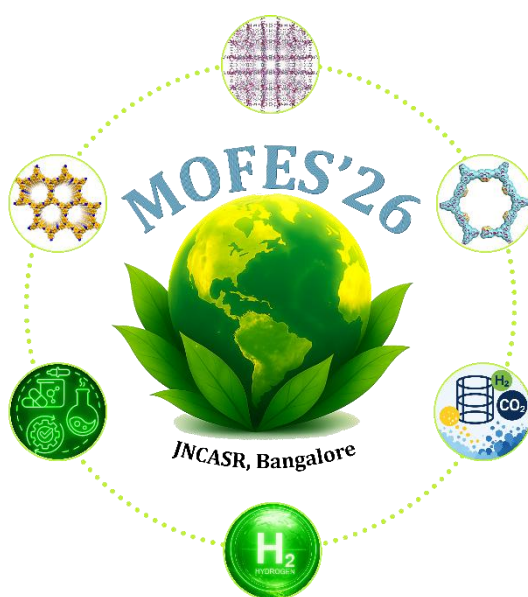




# International Conference on Metal-Organic Frameworks and Porous Organic Polymers for Energy and Sustainability, 2026 (MOFES'26)



**Jawaharlal Nehru Centre for Advanced Scientific  
Research (JNCASR)  
Bangalore**

**12 – 15 January, 2026**



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## Message from the Convener

*It is my great pleasure to welcome you to MOFES'26: the International Conference on Metal-Organic Frameworks (MOFs) and Porous Organic Polymers (POPs) for Energy and Sustainability, being held during January 12-15, 2026 at the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India.*

*MOFES'26 is organized at a truly historic moment for the global chemistry and materials science community. The year 2025 marked a watershed in the field with the Nobel Prize in Chemistry recognizing the pioneering contributions to Metal-Organic Frameworks, crystalline porous materials that have transformed the way chemists design, understand, and apply as functional materials. This recognition not only celebrates decades of fundamental innovation in reticular chemistry, coordination chemistry, and solid-state science, but also underscores the profound societal relevance of MOFs in addressing grand challenges related to energy, environment, and sustainability.*

*Over the past two decades, MOFs and related porous organic materials, including COFs and POPs have evolved from elegant laboratory curiosities into powerful platforms for gas capture and separation, catalysis, CO<sub>2</sub> conversion, hydrogen generation and storage, water harvesting, sensing, and energy storage. Their unparalleled structural tunability, modularity, and multifunctionality continue to inspire new concepts at the interface of chemistry, physics, materials science, and engineering. MOFES'26 aims to reflect this rich scientific landscape while also charting future directions for the field.*

*This conference is particularly significant as it represents one of the first large-scale international conferences in India dedicated exclusively to MOFs and porous organic materials, bringing together a vibrant and diverse community. MOFES'26 hosts 300+ participants, including nearly 200 students and young researchers, and features approximately 80 lectures consisting of plenary, keynote, and invited talks delivered by leading international and national experts, alongside strong participation from industry leaders and major scientific journal publishing houses. The program has been carefully curated to encourage deep scientific discussions, cross-disciplinary exchange, and meaningful interactions between academia, industry, and early-career researchers.*

*The Abstract Book you hold reflects the breadth and depth of contemporary research in MOFs, COFs, and POPs, spanning fundamental design principles to translational and industrial perspectives. We hope it will serve not only as a record of MOFES'26, but also as a valuable reference and source of inspiration for future research.*

*I would like to express my sincere gratitude to all the speakers, contributors, session chairs, sponsors, student volunteers, and members of the organizing and advisory committees for their enthusiastic support and commitment. I am also grateful to JNCASR for providing an outstanding academic environment to host this important event.*

*I warmly welcome all delegates to MOFES'26 and hope that the conference fosters stimulating discussions, lasting collaborations, and new ideas that will shape the next chapter of porous materials research in the post-Nobel era.*

With best wishes,



**(Prof. Tapas K. Maji)**

Convener, MOFES'26

Chemistry and Physics of Materials Unit (CPMU)

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)

Bangalore, India



## Message from the President

*We are absolutely delighted to see the International Conference on Metal-Organic Frameworks and Porous Organic Polymers for Energy and Sustainability (MOFES) being hosted at JNCASR.*

*Metal Organic Frameworks are remarkable crystalline solids that exhibit high porosity, surface area, flexibility and a wide range of functional properties, as endorsed by their recognition with a Nobel Prize in Chemistry in 2025. They can be discovered, chemically developed and their properties can be engineered with definite design principles, making them intrinsically diverse and classifiable, suitable for numerous applications. Consorted efforts among researchers based on free exchange of ideas and organic collaborations are key to development of MOFs based technologies that will address societal grand challenges and strive towards sustainability.*



*It is great that MOFES conference during Jan 12-15, 2026 will initiate a series of conferences that will provide an interactive platform to facilitate advancement of research in MOFs and Porous Organic Polymers, and has chosen to focus on the problems of energy conversion and storage, and environment with relevance to sustainability. Its scientific programme highlights the rich scientific ideas that cut across disciplines and will make the conference an exciting event in this important area in materials science. The diversity in representation from academia, industry and national labs in MOFES'26 will surely facilitate by exchange of ideas, cooperation and collaboration that would promote pathbreaking research in various geographical regions.*

*JNCASR is a research institution deemed to be university is well-suited to host this conference as it is particularly known for the interdisciplinary research in materials science that covers hard and soft materials, with strengths in theory and experiment. With critical in-house research activity in soft matter, porous materials and their interactions with molecules, liquids and external fields, JNCASR is in a strong position to host MOFES'26. As the time may permit during the event, we encourage its participants to explore beautiful campus and other activities of JNCASR.*

*Congratulating the organizers for their leadership, efforts and having formulated this potentially impactful conference, and we wish you all a vibrant event that will help in achieving your scientific objectives.*

**Prof. Umesh V. Waghmare**

President

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)

Bangalore, India

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## Conference Schedule

### Day 1: 12<sup>th</sup> January, 2026 (Monday)

Time	Event				
07:45 AM-09:00 AM	<b>Registration at JNCASR Auditorium</b> Breakfast Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR				
09:00 AM-09:20 AM	Welcome Address and Inaugural Session				
<b>Session I</b> Event Venue: JNCASR Auditorium <b>Chair of the Session:</b> Prof. Umesh V Waghmare (JNCASR)					
Time		Speakers			
09:20 AM-10:00 AM	PL	<b>Prof. Roland A. Fischer</b> <i>Photoactive Metal-Organic Frameworks</i>			
10:00 AM-10:30 AM	KL	<b>Prof. Amanda J. Morris</b> <i>Catch and Release: Controlling MOF Photo-Dynamics</i>			
10:30 AM-11:00 AM	KL	<b>Prof. Jarugu Narasimha Moorthy</b> <i>Multi-functional MOFs and POPs by a Bottom-Up Rational Design: Synthesis and Applications</i>			
11:00 AM-11:30 AM	Group Photo at JNCASR Auditorium Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR				
<b>Session II</b> Event Venue: JNCASR Auditorium <b>Chair of the Session:</b> Prof. Chandrabhas Narayana (JNCASR)					
Time		Speakers			
11:30 AM-12:00 PM	KL	<b>Prof. Dominik Eder</b> <i>Designing Active Sites in MOF-based Photo/Electrocatalysis</i>			
12:00 PM -12:30 PM	KL	<b>Prof. Masaki Kawano</b> <i>MOF Crystallography for Natural Products</i>			
12:30 PM-01:00 PM	KL	<b>Prof. Stefan Wuttke</b> <i>Combining Reticular Pore Design with Green Promises to Sustainable Practices</i>			
<b>Session III</b>					
Event Venue: JNCASR Auditorium <b>Chair of the Session:</b> Prof. Ranjani Viswanatha (JNCASR)			Event Venue: AMRL Conference Hall, JNCASR <b>Chair of the Session:</b> Prof. Thimmaiah Govindaraju (JNCASR)		
Time		Speakers			Speakers
02:00 PM-02:25 PM	IL	<b>Prof. Idan Hod</b> <i>Metal-Organic Frameworks as a Heterogeneous Platform for (Photo)-Electrocatalytic Solar Fuel Production</i>		IL	<b>Prof. Kuntal Manna</b> <i>Engineering Earth-Abundant Metal Catalysts using Metal-Organic Frameworks for Selective Methane Functionalization</i>
02:25 PM-02:50 PM	IL	<b>Dr. Suman Kalyan Samanta</b> <i>Bandgap Engineered Conjugated Porous Organic Polymers in</i>		IL	<b>Prof. Madhab C. Das</b> <i>Chemically Programmed Molecular Diffusion in Metal-Organic Frameworks</i>

		<i>Photocatalysis and Pollutant Removal</i>		
02:50 PM-03:15 PM	IL	<b>Dr. Monika Singh</b> <i>Metal–Organic Frameworks (MOFs) for Sustainable Energy and Environmental Solutions</i>	IL	<b>Dr. Nivedita Sikdar</b> <i>Amine-Rich Metal–Organic Framework/Polymer Hybrid Interfaces for Non-Faradaic Capacitive Halide Sensing</i>
03:15 PM-03:30 PM	EIL	<b>Dr. Arshad Aijaz</b> <i>MOF-Derived Single-Atom-Catalysts for Energy Applications</i>	EIL	<b>Dr. Seemita Banerjee</b> <i>Application of MOF and Related Materials towards Energy Storage &amp; Conversion</i>
03:30 PM-04:00 PM	Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel, Football Ground, and AMRL Foyer, JNCASR			
<b>Session IV</b> Event Venue: JNCASR Auditorium <b>Chair of the Session:</b> Prof. M. Eswaramoorthy (JNCASR)				
<b>Time</b>		<b>Speakers</b>		
04:00 PM-04:30 PM	KL	<b>Prof. Shuhei Furukawa</b> <i>Van der Waals Porous Solids</i>		
04:30 PM-05:00 PM	KL	<b>Prof. Sujit K. Ghosh</b> <i>Nuclear-Wastes Sequestration by MOFs+ for Safe Drinking Water</i>		
05:00 PM-07:00 PM	<b>Session V</b> <b>Refreshment &amp; Poster Session</b> Event Venue: SSL Foyer and SAMat Building, JNCASR <b>Chair:</b> Prof. Rajeswara Rao M (IIT Dharwad) & Dr. Papri Sutar (NIT Silchar)			
Cultural Programme (07:00 PM-08:00 PM) Venue: JNCASR Auditorium				
Dinner (08:00 PM onwards) Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR				

## Day 2: 13<sup>th</sup> January, 2026 (Tuesday)

Time	Event			
08:00 AM-09:00 AM	Breakfast Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR			
Session VI Event Venue: JNCASR Auditorium Chair of the Session: Prof. Giridhar U. Kulkarni (JNCASR)				
Time		Speakers		
09:00 AM-09:40 AM	PL	<b>Prof. Stefan Kaskel</b> <i>Flexible Metal-Organic Framework</i>		
09:40 AM-10:10 AM	KL	<b>Prof. Jing Li</b> <i>Molecular Sieving Based Separation of Liquid Hydrocarbons by Flexible MOFs</i>		
10:10 AM-10:40 AM	KL	<b>Prof. Christof Wöll</b> <i>Electrode-Integrated Functional Molecular Solids via Programmed Assembly: The SURMOF Approach – or: Digitalization of Materials Research</i>		
10:45AM-11:15 AM	Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR			
Session VII Event Venue: JNCASR Auditorium Chair of the Session: Prof. K. N. Ganesh (JNCASR)				
Time		Speakers		
11:15 AM-11:45 AM	KL	<b>Prof. Jorge A. R. Navarro</b> <i>Reactive Zeolitic Imidazolate Framework Crystal Facets</i>		
11:45 AM-12:15 PM	KL	<b>Prof. Jin-Chong Tan</b> <i>Resilient Triboelectric Nanogenerators and Sensing Devices Engineered from MOF-Based Composites</i>		
12:15 PM-12:45 PM	KL	<b>Prof. Samar Kumar Das</b> <i>MOF-based Composite Materials for Sustainable Development</i>		
12:45 PM-01:00 PM	ET	<b>Dr. Sally Howells-Wyllie</b> RSC publishing in India-supporting you to publish your best research		
Session VIII				
Event Venue : JNCASR Auditorium Chair of the Session: Prof. Kanishka Biswas (JNCASR)		Event Venue: AMRL Conference Hall, JNCASR Chair of the Session: Dr. Thanasekaran Pounraj (Pondicherry University)		
Time		Speakers		Speakers
02:00 PM-02:25 PM	IL	<b>Prof. Arvind Rajendran</b> <i>How Can Process Engineering Enable the Discovery/Screening of MOFs for CO<sub>2</sub> Capture</i>	IL	<b>Dr. Soumya Mukherjee</b> <i>Crystal Engineering of Transiently Porous and Ultramicroporous Networks as Adsorbents</i>
02:25 PM-02:50 PM	IL	<b>Prof. Sanjit Konar</b> <i>Stimuli Responsive Magnetic Switching in Hofmann type of MOFs</i>	IL	<b>Prof. Kamalakannan Kailasam</b> <i>Metal-free Heptazine based Photoredox Catalysts (HMPs) for Sustainable Fuels and Chemicals</i>
02:50 PM-03:15 PM	IL	<b>Prof. Debajit Sarma</b> <i>Coordination-Driven Framework Materials for</i>	IL	<b>Dr. Subhadip Neogi</b> <i>Task-Specific Functionalization in Framework Materials for</i>

		<i>Catalytic and Sensing Applications</i>		<i>Environmental Remediation and Sustainable Catalysis</i>
03:15 PM-03:40 PM	IL	<b>Prof. Himanshu Aggarwal</b> <i>Using Molecular Building Block Approach Towards MOF Design for Sensing, Separation, and Catalysis Applications</i>	IL	<b>Prof. Jayaramulu Kolleboyina</b> <i>Surface Functionalization of Hybrid Porous Materials for Next-Gen Applications (SFP Nex-Gen)</i>
03:40 PM-03:55 PM	EIL	<b>Dr. Venkata Suresh Mothika</b> <i>Systematic Acceleration of Photocatalytic H<sub>2</sub>O<sub>2</sub> Generation using Conjugated Microporous Polymers</i>	EIL	<b>Dr. Sanjog S. Nagarkar</b> <i>Sustainable Chemistry with Glassy &amp; Liquid Metal-Organic Frameworks</i>
03:55 PM-04:10 PM	EIL	<b>Dr. Samrat Ghosh</b> <i>Solar Rechargeable Porous Organic Semiconductors</i>	EIL	<b>Dr. Suresh Babu Kalidindi</b> <i>Exploring MOF/COFs as Next-Generation Materials for Room-Temperature Hydrogen Sensing</i>
04:10 PM-04:45 PM	Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel, Football Ground, and AMRL Foyer, JNCASR			
Session IX Event Venue: JNCASR Auditorium Chair of the Session: Prof. Subi J. George (JNCASR)				
Time		Speakers		
04:45 PM-05:15 PM	KL	<b>Prof. Paolo Falcaro</b> <i>3D Oriented Polycrystalline MOF Films and Patterns</i>		
05:15 PM-05:45 PM	KL	<b>Prof. Satoshi Horike</b> <i>Disordered Systems and Microstructures of Coordination Polymers and MOFs</i>		
05:45 PM-06:15 PM	KL	<b>Prof. Ramaswamy Murugavel</b> Organophosphate Based SBUs for MOF-like Porous Solids and C3-Symmetric Triarylborane COF Building Blocks		
Conference Dinner (07:00 PM onwards)				

## Day 3: 14<sup>th</sup> January, 2026 (Wednesday)

Time		Event		
08:00 AM-09:00 AM		Breakfast Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR		
Session X Event Venue: JNCASR Auditorium Chair of the Session: Prof. K. Ganapathy Ayappa (IISc)				
Time			Speakers	
09:00 AM-09:40 AM		PL	<b>Prof. Christian Seree</b> <i>Biocompatible Metal-Organic Frameworks : From Green Synthesis to the Treatment of Severe Diseases</i>	
09:40 AM-10:10 AM		PL	<b>Prof. Randall Q. Snurr</b> <i>Hydrogen Storage in Metal-Organic Frameworks: Effect of Topology and Efforts toward Room-Temperature Storage</i>	
10:10 AM-10:40 AM		PL	<b>Prof. Guillaume Maurin</b> <i>Advancing MOF Simulations with Machine-Learned Potentials</i>	
10:45AM-11:15 AM		Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR		
Session XI Event Venue: JNCASR Auditorium Chair of the Session: Prof. Srinivasan Natarajan (IISc)				
Time			Speakers	
11:15 AM-11:45 AM		KL	<b>Prof. Arne Thomas</b> <i>Design of Sustainable Catalysts using Covalent Organic Frameworks</i>	
11:45 AM-12:15 PM		KL	<b>Prof. Rahul Banerjee</b> <i>Reticular Chemistry: Covalent Organic Frameworks to Porous Crystalline Nitrogen Doped Graphite</i>	
12:15 PM-12:45 PM		KL	<b>Prof. Asim Bhaumik</b> <i>Sustainable Catalysis over MOFs and POPs</i>	
12:45 PM-01:00 PM		IT	TRANE Technologies	
Session XII				
Event Venue: JNCASR Auditorium Chair of the Session: Prof. Partha Sarathi Mukherjee (IISc)			Event Venue: AMRL Conference Hall, JNCASR Chair of the Session: Prof. Sebastian C. Peter (JNCASR)	
Time		Speakers		Speakers
02:00 PM-02:25 PM	IL	<b>Prof. Ravichandar Babarao</b> <i>Accelerating the Discovery of Metal Organic Frameworks for Capture, Separation and Activation of Small Molecules</i>	IL	<b>Dr. Jan Kazimierz Zaręba</b> <i>Using Nonlinear Optical Processes for Post-Synthetic Modification of Metal-Organic Frameworks and Coordination Polymers</i>
02:25 PM-02:50 PM	IL	<b>Prof. Abhijit Patra</b> <i>Porous Organic Materials for Energy and Environmental Sustainability</i>	IL	<b>Prof. Bishnu P. Biswal</b> <i>Covalent Organic Framework Membranes for Molecular Separations and Beyond</i>
02:50 PM-03:15 PM	IL	<b>Dr. Renjith S. Pillai</b> <i>Metal-Organic Frameworks and Porous Organic</i>	IL	<b>Prof. Debashis Adhikari</b> <i>Covalent Organic Frameworks for Efficient Organic Transformations</i>

		<i>Polymers: A New Frontier in Space Materials</i>		
03:15 PM-03:30 PM	IT	Thermo Fisher Scientific	IT	Micromeritics
03:30 PM-04:00 PM	Meet the Editors (RSC); Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel, Football Ground, and AMRL Foyer, JNCASR			
Event Venue: JNCASR Auditorium <b>Chair of the Session:</b> Prof. Pratap Vishnoi (JNCASR)			Event Venue: AMRL Conference Hall, JNCASR <b>Chair of the Session:</b> Dr. Ujjwal Pal (CSIR-IICT)	
04: 00 PM-04: 25 PM	IL	<b>Prof. Debajyoti Ghoshal</b> <i>Excited-state Intramolecular Proton Transfer (ESIPT) in Metal Organic Frameworks</i>	IL	<b>Prof. Biplab Maji</b> <i>A <math>\pi</math>-Conjugated COF as an Integrated Photoredox Catalyst for Energy/Electron Transfer–Driven Cross-Coupling Reaction</i>
04: 25 PM-04: 50 PM	IL	<b>Prof. Pradip Pachfule</b> <i>Harnessing the Sunlight for Photocatalytic Hydrogen Peroxide Generation</i>	IL	<b>Prof. Nagaraja C. M.</b> <i>Strategic Design of Framework Materials for Chemical Fixation of Carbon Dioxide to Value-Added Chemicals</i>
05: 00 PM-07:00 PM	Session XIII <b>Refreshment &amp; Poster Session</b> Event Venue: SSL Foyer and SAMat Building, JNCASR <b>Chair:</b> Dr. Ashish Singh (Guru Ghasidas Central University) & Dr. Arijit Mallick (Jawaharlal Nehru University)			
Dinner (07:00 PM onwards) Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR				

## Day 4: 15<sup>th</sup> January, 2026 (Thursday)

Time		Event			
08:00 AM-09:00 AM		Breakfast Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR			
Time			Speakers		
Session XIV Event Venue: JNCASR Auditorium Chair of the Session: Prof. Swapan K. Pati (JNCASR)					
09:00 AM-09:40 AM	PL	Prof. Hiroshi Kitagawa <i>Electrical conduction and proton rectifying property in MOFs</i>			
09:40 AM-10:10 AM	KL	Prof. Takashi Uemura <i>MOFs for Advanced Polymers</i>			
10:10 AM-10:35 AM	IL	Prof. Pravas Deria <i>Artificial Photosystem Metal–Organic Frameworks</i>			
10:35 AM-11:00 AM	IL	Prof. Jürgen Senker <i>Understanding Guest-Host Materials for Photocatalytic Carbon Dioxide Reduction Using NMR Crystallography</i>			
11:00 AM-11:30 AM	Tea/Coffee Break Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR				
Session XV					
Event Venue: JNCASR Auditorium Chair of the Session: Prof. Prabal K. Maiti (IISc)			Event Venue: AMRL Conference Hall, JNCASR Chair of the Session: Prof. Sarit S Agasti (JNCASR)		
Time		Speakers			Speakers
11:30 AM-11:55 AM	IL	Prof. Nirmalya Ballav <i>Facing the Interface: Hetero-Structured Thin Films of Coordination Polymers</i>		IL	Prof. Rajeev Gupta <i>Sustainable Catalysis Using Visible Light, Air and Water</i>
11:55 AM-12:20 PM	IL	Prof. Kumar Varoon Agrawal <i>Molecular and Ionic Sieving Metal-Organic Framework Membranes with a Thickness of Just One Unit Cell</i>		IL	Prof. Shaikh M. Mobin <i>Design and Development of Metal-Organic Frameworks Based Triboelectric Nanogenerator for Sustainable Power Generation</i>
12:20 PM-12:45 PM	IL	Prof. Shyam P. Biswas <i>Development of Water-Stable Metal-Organic Frameworks for Fluorescence Sensing, Oil-Water Separation and Heterogeneous Catalysis</i>		IL	Dr. Ritesh Haldar <i>Chemically Programmed Molecular Diffusion in Metal-Organic Frameworks</i>
12:45 PM-01:00 PM	IT	Bruker		EIL	Dr. Sattwick Haldar <i>Dual-Functional Organopolysulfide Frameworks Cathodes: Bridging Organic and Chalcogen Battery Chemistry</i>
Session XVI					
Event Venue: JNCASR Auditorium			Event Venue: AMRL Conference Hall,		



Chair of the Session: Prof. K. S. Narayan (JNCASR)			JNCASR Chair of the Session: Dr. Chanchal Samanta (BPCL)	
Time		Speakers		Speakers
02:00 PM- 02:25 PM	IL	<b>Dr. Saona Seth</b> <i>Advancing Porous Solids for Selective Carbon Capture and Utilization</i>	IL	<b>Prof. Prem Felix Siril</b> <i>Structure–Function Correlations in COFs: Toward Optimized Nanocarriers for Lung Cancer Therapy</i>
02:25 PM- 02:50 PM	IL	<b>Dr. Vincent Guillerm</b> <i>Harnessing Hierarchical Porosity in MOFs through the Templated Assembly of Face-decorated Platonic Cages</i>	IL	<b>Prof. Tamas Panda</b> <i>Mechanochemistry as a Tool for Disorder Engineering in Macromolecular Frameworks</i>
02:50 PM- 03:15 PM	IL	<b>Prof. Prakash Kanoo</b> <i>Nanochannel-Assisted Organic Transformations in Metal–Organic Framework</i>	IT	Verder Scientific (02:50 PM-03:05 PM)
			IT	Rigaku (03:05 PM-03:20 PM)
03:45 PM- 04:15 PM	<b>Presentation of Poster Prizes and Vote of Thanks</b> Event Venue: JNCASR Auditorium			
04:15 PM onwards	<b>High Tea and Departure</b> Venue: 5 <sup>th</sup> Block SR Hostel and Football Ground, JNCASR			

PL: Plenary Lecture; KL: Keynote Lecture; IL: Invited Lecture;

EIL: Emerging Investigator Lecture; IT: Industry Talk; ET: Editorial Talk



# Photoactive Metal-Organic Frameworks

Prof. Roland A. Fischer

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## Abstract

Metal-Organic Frameworks, MOFs, offer unique opportunities to integrate physico-chemical properties and functionalities by the choice and the design of the building blocks, such as metal nodes, organic linkers, hosted guests by the tailoring of their spatial arrangement, i.e. via reticular synthesis. The lecture will focus on photoactive MOFs which are characterized by using chromophores as linkers. Four case-studies will be presented and discussed (Figure): (1) Photocatalytic CO<sub>2</sub>-to-syngas evolution with dual molecular catalyst loaded NU-1000, that features a pyrene-chromophore.<sup>1</sup> It delivers energy efficiently to the active sites, conceptually yielding a nanozyme function with benchmark turnover numbers and record incident photon conversions up to 36%. (2) Decoupled solar energy storage and dark photocatalysis in 3D MOFs.<sup>2</sup> The embedding of Mn and Re redox centers in the confined space of the photoactive framework unlocks a unique electron accumulating property under visible-light irradiation. About 15 C g<sub>MOF</sub><sup>-1</sup> of electric charges can be concentrated and stored for over weeks. (3) Photochromic MOFs, functionalized with spiropyranes, feature stimulus-adaptable performance and demonstrate the ability to shift between multiple relaxation pathways as a function of the excitation wavelength. It resulted in photoswitch-directed tailoring of model phosphinylation reaction outcomes.<sup>3</sup> Finally, (4) the tailoring and optimization of the multiphoton-absorption efficiency by MOF crystal engineering involves subtle interaction phenomena induced by pyrene, carbazole and perylene diimide chromophore packing, conformational strain and rigidification.<sup>4</sup> The examples will be put into the wider perspective of the development of multifunctional photoactive porous network materials.

## References

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Roland A. Fischer studied Chemistry from 1981-1986 and obtained Dr. rer. nat. in 1989 and Dr. rer. nat. habil. in 1995 at Technical University of Munich (TUM), where he has been Chair of Inorganic and Metal-Organic Chemistry since 2016. He is also Managing Director of the TUM Catalysis Research Centre. Previously he was Professor of Inorganic Chemistry at Ruhr-University Bochum (1997-2015) and at Heidelberg University (1996-1997). He served as a vice President of the German Research Foundation (2016-2021). He is a member of the award selection committee of the Alexander von Humboldt Foundation and member of the scientific advisory board of the German Chemical Industry Fund. His research interest focusses on functional molecular materials for advancing applications in energy conversion, catalysis, gas storage and separation, chemical sensing, and photonics. His research is documented in about 700 journal publications and was, for example, more recently recognised in 2022 by the International Award of the Japanese Society of Coordination Chemistry and in 2025 by the Wilhelm-Klemm-Prize of the German Chemical Society.

# Biocompatible Metal-Organic Frameworks: from green synthesis to the treatment of severe diseases

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## Abstract

Nanoparticles of biocompatible metal organic frameworks (nanoMOFs) are particularly appealing due to their low toxicity and biodegradable character. [1] Their large ordered porosity is often associated with the presence of open metal sites and/or functional groups. This results in the loading of record quantities of challenging drugs or biological gases together with a controlled release in body fluids while the release of bioactive metals (Fe...) can be associated with the formation of ROS. This enables to develop multi-therapies of interest in the field of cancer treatment, inflammation and more recently antibacterial or wound healing. I will propose a review of the different classes of biocompatible Fe, Ti or Zr MOFs and related composites, their synthesis under green ambient pressure conditions,[2] the engineering of their surface coating, and disclose representative examples of their in vitro and in vivo biomedical properties such as cancer treatment using MOF-inorganic nanoparticles composites to wound healing using new MOF based gasotransmitters.[3-5]

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Christian Serre obtained his PhD in materials' chemistry in 1999 at the university of Versailles in France. After a post-doc in USA at Rhodia Inc (Princeton), he became a CNRS researcher in 2001 at the Lavoisier Institute in Versailles (France) where he discovered most of the MIL class of MOF materials. Christian was the first to propose the use of MOF nanoparticles as drug carriers with exceptional loading capacity. He was promoted as a CNRS research director in 2008 and headed Institut Lavoisier in 2015. He moved in 2016 to Ecole Normale Supérieure and ESPCI in Paris to create a new Institute fully dedicated to porous solids and related composites for health, the environment and energy. To date, he has published more than 460 articles and holds 45 patent families. He is one of the co-founders of SquairTech, a start-up dedicated to indoor air quality. He has received many awards and is a member of the French Academy of Sciences since 2024 and since 2025 of the European Academy of Sciences.

# Flexible Metal-Organic Frameworks

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## Abstract

In the field of porous materials adaptive materials are rare. The ability to adaptively transform pore size and shape initiated by a molecular stimulus is a unique feature of some selected MOFs. Developing *in situ*-methodologies for monitoring local and global structural features along an adsorption isotherm has been instrumental to unravel the mechanisms and understanding of flexibility phenomena in MOFs. The presentation will illustrate tailorable switchability by means of building block adjustment exemplified by prototypical model systems such as pillared layer MOFs. A counterintuitive phenomenon is also negative gas adsorption. We will analyze important factors governing flexibility such as crystal size, shape, defects and surface deformation. Despite nowadays a wide variety of MOFs are known to show flexibility, several open questions in field remain open fostering the development of innovative customized instrumentation. Flexible MOFs offer ultrahigh selectivity in gas separation applications, sensing, but are also discussed as shock absorbers, actuators and gas storage systems. Fundamental research and functional exploration are crucial to develop the platform of flexible MOFs for real world applications in future.

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Stefan Kaskel studied chemistry at Eberhard Karls University, Tübingen (Germany), and received his Ph.D. degree in 1997. As a Feodor-Lynen Fellow of the Alexander von Humboldt foundation he worked with J. Corbett at Ames Laboratory, USA (1998-2000) on intermetallic compounds. He was a group leader at the Max-Planck-Institut für Kohlenforschung in Mülheim a.d. Ruhr (2000-2004) in the group of F. Schüth and after his habilitation at Ruhr University (Bochum) in 2004 in the area of heterogeneous catalysis, he became full professor for Inorganic Chemistry at Dresden University of Technology. Since 2008 he is also business field leader at Fraunhofer IWS, Dresden (part time).

His research interests are focused on porous and nanostructured materials (synthesis, structure, function) for applications in energy storage, catalysis, batteries and separation technologies. His major activity at Fraunhofer IWS is the development of next generation battery technologies. He received the nanotechnology award of the German Ministry of Science and Education in 2002, the JSPS award from Japan in 2016, and the Joseph von Fraunhofer Award in 2025. He is an elected member of the European Academy of Sciences and a corresponding member of the Göttingen Academy of Sciences and Humanities in Lower Saxony. Stefan Kaskel has authored more than 700 publications (h-index 137) and has contributed as inventor to more than 60 patent applications. He was recognized multiple times as a Highly Cited Researcher of world's most influential scientific minds by Clarivate Analytics.

# Electrical conduction and proton rectifying property in MOFs

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## Abstract

For more than 30 years, we have developed a metal-dimer-assembled MMX chain system as a model of pure 1-D electrons system, because this system has a wide variety of possible electronic phases. There are four dominant interactions in this system, transfer integral  $t$ , on-site Coulombic repulsion  $U$ , nearest neighbor Coulombic repulsion  $V$ , and electron-lattice interaction  $S$ , those are competing to each other in energy. It exhibits metallic conduction, representing the first example of a metallic coordination-network complex. Recently, we have also developed conductive MOF nanotube and other electrically conductive MOFs, including proton and ionic conduction. More recently, we have also developed a rational control of unidirectional proton transport using free-standing membranes of a proton-conducting two-dimensional porous coordination polymer and a hydroxide ion-conducting layered double hydroxide. The current–voltage measurements revealed that the heterogeneous membrane exhibits a significant unidirectional proton transport with a proton rectification ratio exceeding 200 under 90% relative humidity in the initial voltage scan. This value is the highest among the reported all-solid-state proton rectifiers. Our recent work on electron and proton conductions, and proton rectification in MOFs is presented [1-8].

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HK received his Ph.D. from Kyoto University in 1992 and, after working as an assistant professor at the Institute for Molecular Science and the Japan Advanced Institute of Science and Technology, was appointed associate professor at the University of Tsukuba in 2000. He became a professor at Kyushu University in 2003 and returned to Kyoto University in 2009. He was employed at the Japan Science and Technology Agency (JST) as Director of "Science and Creation of Innovative Catalysts" and is now employed at JST as Director of "Exploring Innovative Materials in Unknown Search Space" and as Program Officer of the Materials Science Panel, Fusion Oriented Research for Disruptive Science and Technology. He was also Chief Program Officer in Chemistry Group, Japan Society for the Promotion of Science (JSPS) from 2020 to 2024. He is a previous President of the Japan Society of Coordination Chemistry from 2020 to 2024. He is also Vice Provost of Kyoto University for Planning and Coordination. He has published more than 560 original research papers on solid-state chemistry, coordination chemistry, nanoscience, low-dimensional electron systems and molecule-based conductors.

# Electrode-Integrated Functional Molecular Solids via Programmed Assembly: The SURMOF Approach – or: Digitalization of Materials Research

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The deliberate assembly of 'Designer Solids' from extensive libraries of prefabricated units is a compelling goal that has garnered significant interest, particularly within the domain of metal–organic frameworks (MOFs). This lecture will spotlight recent breakthroughs in MOF-based device development, encompassing electrochemical, photoelectrochemical, photovoltaic, and sensing technologies based on MOFs incorporating different types of organic linkers, such as porphyrins, phthalocyanines, naphthalene diimides, and triphenylene. Additionally, we will delve into the potential of internal interfaces in MOF heterostructures for photon upconversion and diode manufacturing. Since the fabrication of reliable and reproducible electrical contacts to MOF-materials represent a major challenge, we have developed a layer-by-layer (lbl) deposition method to produce well-defined, highly oriented and monolithic MOF thin films on appropriately functionalized conducting substrates. The resulting films are referred to as SURMOFs [1,2] and have very appealing properties in particular with regard to optical applications.[3] The fabrication of hetero-multilayers is rather straightforward with this lbl method. In this talk, we will describe the principles of SURMOF fabrication as well as the results of systematic investigations of electrical and photophysical properties exhibited by empty MOFs. Band structure effects occurring in crystalline porphyrin arrays assembled using the SURMOF approach will also be discussed.[5] We close by presenting the first metallic MOF thin film [6], which shows clear evidence of Dirac-cone band transport from temperature-dependent measurements.

This progress—metallic conductivity being a holy grail for MOFs—was enabled by unattended experimentation, for which SURMOFs are especially suited. Robot systems guided by machine learning efficiently optimize film properties such as orientation, crystallinity, and conductivity. We will highlight this in the context of SURMOF-based sensors and metallic MOF thin films.

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Christof Wöll is Director of the Institute of Functional Interfaces (IFG) at the Karlsruhe Institute of Technology (since 2009). He studied Physics at the University of Göttingen and received his PhD in 1987 at the Max-Planck-Institute of Dynamics and Self-Organization. After several years of postdoctoral activity at the IBM Research laboratories in San Jose, USA and at Heidelberg University, in 1996 he took over the chair for Physical Chemistry at the University of Bochum (until 2009) and founded the collaborative research center SFB 558. He has received several awards including the Max-Planck Medal for his PhD thesis (Max-Planck Society) and the van't Hoff Prize of the German Bunsen Association. He is a member of the German National Academy of Sciences, Leopoldina and was the Spokesperson of the German Physical Society (DPG) Surface Physics Division (2016–2018). His research activities focus on fundamental processes in Surface Physics and Surface Chemistry, in particular development and advancement of techniques for the characterization of molecular adsorbates, oxide surfaces, and surface-mounted metal-organic frameworks (SURMOFs).



# Hydrogen Storage in Metal-Organic Frameworks: Effect of Topology and Efforts toward Room-Temperature Storage

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## Abstract

Hydrogen is a clean alternative to fossil fuels and can be produced by using renewable energy sources. However, due to its low volumetric energy density, H<sub>2</sub> storage requires low temperatures and/or high pressures for practical applications. H<sub>2</sub> storage using metal–organic frameworks (MOFs) has been investigated for over 20 years due to the large surface areas and highly tunable nature of MOFs, but suitable materials for room-temperature storage remain elusive. We performed ab initio calculations to study H<sub>2</sub> storage at room temperature in two anionic MOFs and examined the effects of different exchanged metal cations on hydrogen adsorption [1]. Our results show that the H<sub>2</sub> adsorption enthalpy on Mg<sup>2+</sup> cations is the highest among the cations studied, with average adsorption enthalpies around –20 kJ/mol at three H<sub>2</sub> molecules per Mg<sup>2+</sup>, which is in the desired range for room temperature storage. We further estimated the volumetric H<sub>2</sub> uptake for 2,058 anionic MOFs using assumptions based on our modeling and found that 459 MOFs could potentially exhibit a volumetric uptake of more than 15.0 g/L. Further DFT calculations show that water molecules can bind strongly to the Mg<sup>2+</sup> cations, which may make it difficult to remove water and access these adsorption enthalpies experimentally. For application under cryogenic conditions, past work has run into a ceiling on performance due to a trade-off in the volumetric deliverable capacity (VDC) versus the gravimetric deliverable capacity (GDC). We computationally constructed and screened 105, 230 MOF structures based on 529 nets to explore the effect of underlying topology on the hydrogen storage performance of the resulting materials [2]. A machine learning model was developed based on simulated hydrogen uptake to facilitate screening of the entire dataset. We identified a promising structure based on the **tsx** topology that exhibits both VDC and GDC higher than the current benchmark material, MOF-5. Our data-driven analysis indicates that nets with higher net density yield MOFs with enhanced volumetric and gravimetric surface areas, thereby improving maximum VDC while shifting the capacity trade-off toward higher GDC.

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# Molecular Sieving Based Separation of Liquid Hydrocarbons by Flexible MOFs

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## Abstract

Flexible metal-organic frameworks (FMOFs) represent a distinct sub-class of MOFs that often exhibit adsorption properties markedly different from those of their rigid counterparts (RMOFs). This difference arises from the inherent flexibility of FMOFs, which leads to structural responses that are absent in rigid systems. In this presentation, I will highlight our recent progress in the development and study of robust FMOFs, with particular emphasis on their intriguing temperature- and adsorbate-dependent adsorption behaviors.<sup>1-11</sup> Special attention will be given to their potential applications in highly selective, molecular sieving-based separations of important liquid hydrocarbons accompanied by both high adsorption capacity and fast kinetics.

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# Advancing MOF Simulations with Machine-Learned Potentials

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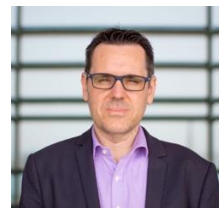
## Abstract

Machine-learned potentials (MLPs) are transforming materials science by enabling accurate and efficient modeling of complex materials, such as metal-organic frameworks (MOFs). These data-driven approaches overcome the limitations of traditional methods like density functional theory (DFT), which are computationally prohibitive for large-scale simulations. MLPs offer a hybrid alternative by learning the potential energy surfaces from quantum mechanical data, thereby providing rapid and precise predictions of material properties across extended length and time scales. One area where MLPs prove especially valuable is in the modeling of flexible MOFs, which can exhibit phase transitions and mechanical deformations in response to external conditions (thermal, mechanical pressure). Using MLPs, we explore the MOF CALF-20's phase space with unprecedented efficiency, revealing distinct two-step elastic deformation and high fracture strain, which are critical for potential applications in flexible electronics and sensors. Furthermore, MLPs extend their utility to adsorption simulations, particularly for MOFs with open metal sites (OMS), where strong host-guest interactions are challenging for classical force fields to describe accurately. We demonstrate this by developing an MLP for H<sub>2</sub> adsorption in Al-soc-MOF-1d, an OMS-containing framework. The MLP accurately models H<sub>2</sub> binding and diffusion, offering insights into adsorption performance that can guide the design of MOFs for hydrogen storage applications. MLP is also a key feature to describe the guest-assisted local dynamics of narrow pore MOFs like MIL-120(Al). These examples illustrate the potential of ML-based approaches to advance the computational modeling of MOFs.

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Guillaume Maurin is a Full Professor at the University of Montpellier and a distinguished Senior Chair at the Institut Universitaire de France. His research focuses on developing and applying advanced modelling/numerical simulation tools to aid the design of MOF nanoporous MOFs and related membranes for energy and environmental applications. So far he has published 400+ publications with H-factor 100+ and 50k+ citations.



# Reticular Chemistry: Covalent Organic Frameworks to Porous Crystalline Nitrogen Doped Graphite

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## Abstract

Covalent Organic Frameworks (COFs) represent a novel class of highly porous, crystalline polymers with uniformly ordered pore channels. Despite their extensive use for storing various molecular species such as gases, nanoparticles, enzymes, and drugs, the potential of their ordered pore channels for molecular separation still needs to be utilized. A significant obstacle is fabricating COF particles into self-standing, stable membranes. Beyond processability, other significant barriers to the real-world application of COFs include (i) chemical stability, (ii) complex synthesis procedures, and (iii) scalability. In this context, we have successfully addressed the chemical stability issue by synthesizing  $\beta$ -ketamine-based frameworks. Furthermore, recent advances in Reticular Chemistry have led to the development of Covalent Organic Nanotubes (CONTs), which extend the principles of COF design into one-dimensional architectures. These CONTs, formed by linking molecular building blocks in a reticular fashion, offer unique properties such as tunable pore sizes and enhanced stability, making them promising candidates for molecular separation, catalysis, and nanofiltration applications. Integrating reticular chemistry in one dimension opens new avenues for designing functional materials with precise control over their structural and chemical features. Our findings highlight that COMs and CONTs have significant potential to address some of the world's most challenging separation problems, including wastewater treatment and drug recovery in the pharmaceutical industry.

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# Multi-functional MOFs and POPs by a Bottom-Up Rational Design: Synthesis and Applications

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## Abstract

The development of porous organic–inorganic hybrid (MOFs, metal-organic frameworks) and purely organic (POPs, porous organic polymers) materials remains an exciting area of research due to their wide range of applications in gas adsorption and storage, separations, catalysis, and sensing, among others. Numerous MOFs have been constructed from organic linkers and metal ions, and their applications demonstrated in a number of areas. In recent years, POPs have gained prominence because of their exceptional physicochemical stability.

Our research relies on the premise that properties of bulk organic materials depend on two key factors: the structures of the constituent molecular building blocks and their organization. By dealing with the structures of molecular building blocks and controlling their organization based on structural attributes, organic materials with pre-determined properties can be developed in a bottom-up fashion. I will exemplify our de novo approaches to the development of MOFs<sup>1</sup> and POPs<sup>2</sup> for a variety of applications by a rational design of organic building blocks.

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# Organophosphate Based SBUs for MOF-like Porous Solids and C<sub>3</sub>-Symmetric Triarylborane COF Building Blocks

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Our laboratory has been employing an organic soluble organophosphate (ArO)P(O)(OH) (Ar = 2,6-diisopropylphenyl) as the primary building unit (PBU) to assemble a large number of polyhedral molecules that resemble one or more zeolite secondary building units (SBUs). The reaction of this phosphate with a divalent metal ion (e.g. Zn<sup>2+</sup>) in a donor solvent predominantly leads to the isolation of stable tetranuclear metal phosphates [(ArO)PO<sub>3</sub>Zn(L)]<sub>4</sub> which possess a Zn<sub>4</sub>O<sub>12</sub>P<sub>4</sub> D4R SBU inorganic core. In recent times, however, we have unraveled that it is possible to also isolate other SBUs from the same set of reactants by making small variations in the reaction conditions. It is now possible to isolate hitherto unknown discrete D6R and D8R SBUs (which possess Zn<sub>6</sub>O<sub>18</sub>P<sub>6</sub> and Zn<sub>8</sub>O<sub>24</sub>P<sub>8</sub> cores, respectively) by switching the solvent from methanol to acetonitrile and the co-ligand from DMSO to either 4-formylpyridine or 4-cyanopyridine. From a series of experimental observations, it has become apparent that, irrespective of the conditions employed, S4R SBUs are formed as the initial products. A rationalization of these building principles and application of these building newer type of Metal Organic Frameworks (MOFs) and their use as catalysts, and magnetic materials will be presented in this lecture. A portion of the lecture will also deal with our efforts in building main-group based Covalent Organic Frameworks (COFs) and other porous polymers.

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# Sustainable catalysis over MOFs and POPs

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## Abstract

Metal–organic frameworks (MOFs) and porous organic polymers (POPs) are attracting increasing interest over the years in the liquid phase heterogeneous catalysis by virtue of their exceptionally high specific surface area, in-built pores of nanoscale dimensions and the ease of tuning reactive surface functional groups.<sup>1,2</sup> Sustainability in the catalytic processes is highly demanding from the industrial perspective considering the economy and renewable resource management. Poly(hydroxy)urethane, a bulk polymer used in foam can be synthesized through a very ecofriendly way (iso-cyanate free green approach) from the bis-epoxide utilizing CO<sub>2</sub> as C1 source followed by the reaction with diamines over a MOF-based catalyst.<sup>3</sup> Selective electrochemical oxidation of alcohols using water as the oxygen source over a MOF-based electrocatalyst is another sustainable catalytic route as the overall process is coupled with high yield green H<sub>2</sub> production.<sup>4</sup> Conversion of biomass derived abundant glycerol into solketal (fuel additive) by using a MOF based catalyst<sup>5</sup> is also very promising. Catalytic conversion of raw biomass into 5-hydroxymethylfurfural (HMF) is another very demanding chemical reaction, where POP based solid acid catalysts have huge opportunities.<sup>6</sup> HMF can be selectively reduced to biofuel 2,5-dimethylfuran (DMF) by using these porous materials as supports. On the other hand, N-rich POPs with high surface area and strong surface basicity can be explored in the catalytic CO<sub>2</sub> fixation into fuels and fine chemicals.<sup>7,8</sup>

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# MOFs for Advanced Polymers

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## Abstract

Metal-Organic Frameworks (MOFs) composed of metal ions and organic ligands have been extensively studied. The characteristic features of MOFs are highly regular channel structures with controllable pore sizes approximating molecular dimensions and designable surface functionality. We have successfully utilized the regular and tunable channels of MOFs for a field of polymerization, which can allow multi-level controls of polymers, nanoparticles, and nanographenes.<sup>[1]</sup> In addition, construction of nanocomposites between MOFs and polymers provides unprecedented material platforms to accomplish many nanoscale function.<sup>[2]</sup> We have also developed direct insertion of polymers into nanochannels of MOFs, which enables powerful macromolecular recognition and separation technologies with exceptionally high selectivity.<sup>[3]</sup> Designing nano-sized pores of MOFs with a regular arrangement of reactive/interactive/responsive entities offers the possibility of universal polymer production and purification that cannot be accomplished by conventional methods.

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# Disordered Systems and Microstructures of Coordination Polymers and MOFs

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## Abstract

Coordination polymers and metal-organic frameworks, MOFs, are composed of metal ions and bridging ligands connected by coordination bonds, and many applications are currently being explored. We are interested in the phase transitions of coordination polymers and MOFs, which include glass, supercooled liquid, and liquid states (Figure).<sup>1</sup> The reversible phase transitions and disordered states facilitate various materials designs for ion conductivity and electro/photocatalysis.<sup>2,3</sup>

For instance, the glassy state of the 3-D Prussian blue analogue exhibits distinct semiconductive behavior compared to its crystalline state and functions as a CO<sub>2</sub> photocatalyst for selective CO production.<sup>4</sup> Two meltable 1-D coordination polymers with Cu<sup>+</sup> and imidazolate derivatives can form a polymer-melt blend, and the resulting quenched glass film demonstrates flexibility and bendability even at cryogenic temperatures.<sup>5</sup> Recent exploration of disordered systems and microstructures of coordination polymers and MOFs for energy will be discussed.

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# Van der Waals Porous Solids

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## Abstract

Strong, directional interactions between building blocks have been prerequisites for the assembly of permanently porous frameworks. For instance, permanent porosity is realized in metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and hydrogen-bonded organic frameworks (HOFs) by the rigid, directional natures of coordination, covalent, and hydrogen bonds, respectively. Conversely, van der Waals (vdW) interactions, or dispersion interactions, a ubiquitous attraction among molecules, have been rarely used in the construction of permanently porous frameworks due to their weak interaction energy and lack of directionality. In this study, we demonstrate that vdW interactions drive the assembly of three-dimensional open frameworks from supramolecular building blocks, so-called metal-organic polyhedra (MOPs), a group of cage-shaped metal complexes with high structural modularity like MOFs.[1] Particularly, we designed octahedral MOPs and assembled them into diamond networks. The resulting porous solids assembled via vdW showed high chemical stability, high thermal stability over 300 °C and high surface area (one is over 2,000 m<sup>2</sup>/g). By altering the surface functionality of MOPs, we also created one and two-dimensional MOP assemblies that showed structural flexibility.[2] We will discuss how vdW interactions can be tuned to generate dynamics in materials.

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# Nuclear-Wastes Sequestration by MOFs+ for Safe Drinking Water

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## Abstract

With rising global energy demand and environmental concerns associated with fossil fuels, sustainable energy supply to the global community remains a great challenge. A clean, low-carbon, sustainable energy source that is becoming more and more vital to the advancement of human society is nuclear energy. Uranium is a key element in the nuclear industry. However, its limited availability on land is the major concern, but in contrast, the oceans contain more than 4.5 billion tons of uranium, sufficient to provide energy to the world for next 1000 years. For that reason, recently Uranium extraction from seawater (UES) is considered one of the seven chemical separations, which have the potential to change the world. However, Uranium recovery from seawater is extremely challenging due to its ultra-low concentration (~3.3 ppb). On the other hand, safe handling and effective disposal of radioactive waste produced during spent fuel processing and reprocessing are essential to the long-term viability of nuclear power. Radioactive pollutants such as  $^{131}\text{I}$ ,  $^{140}\text{Ba}$ ,  $^{137}\text{Cs}$  and  $^{90}\text{Sr}$ ,  $^{99}\text{Tc}$ ,  $^{126}\text{Sn}$ ,  $^{79}\text{Se}$ ,  $^{93}\text{Zr}$ ,  $^{135}\text{Cs}$ ,  $^{107}\text{Pd}$ ,  $^{129}\text{I}$  get transferred into environment and are known to be toxic in nature. Natural and man-made Uranium (U) contamination of groundwater is another major concern due to its toxic nature. In this lecture I will discuss regarding various advanced porous materials developed in our group for efficient extraction of Uranium from seawater and also sequestration of toxic nuclear-wastes pollutants from water for environmental remediation particularly for safe drinking water (Scheme 1).<sup>1-5</sup>

**Scheme 1:** Advanced porous materials as efficient scavenger of radionuclides.

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# MOF-based composite materials for sustainable development

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## Abstract

ZIF-8 is a versatile metal organic framework containing compound. There will be a discussion on electrochemical water oxidation by ZIF-8 MOF-based host-guest type composites (as heterogeneous catalysts). The central element Co(II) of a Keggin-type polyoxometalate (POM) anion  $[\text{Co}^{\text{II}}\text{W}_{12}\text{O}_{40}]^{6-}$  is, as such, not catalytically active. This becomes an efficient electrocatalyst for water oxidation,<sup>1</sup> when the relevant POM anion is encapsulated inside the well-defined confined space of the MOF, ZIF-8. A Bi(III)-aqua-functionalized POM compound  $\text{K}_5[\text{Bi}(\text{H}_2\text{O})_2\text{SiW}_{11}\text{O}_{39}] \cdot 13\text{H}_2\text{O}$  per se decomposes in the neutral pH aqueous medium — but when it is confined in the ZIF-8's cavities, its  $-\text{Bi}(\text{OH}_2)$  functionality acts as an active site for oxygen evolution reaction (OER) in a wide pH range (from pH 4.0 to pH 7.0 through pH 13.0).<sup>2</sup> When a versatile coordination complex  $[\text{Fe}^{\text{III}}(\text{salen})\text{Cl}]$ , that undergoes decomposition at a moderate anodic potential, is encapsulated in a confined space of ZIF-8 MOF, it turns into stable active site for electrocatalytic water oxidation.<sup>3</sup> Likewise, a Co(II)-porphyrin complex, [5,10,15,20-tetrakis(4-methoxyphenyl)porphyrinato]cobalt(II), CoTMPP usually acts as an ORR (oxygen reduction reaction) catalyst, not as a OER catalyst. However, when it is encapsulated inside ZIF-8, the resulting host-guest material becomes an efficient electrocatalyst for water oxidation.<sup>4</sup> During all these electrocatalyses, the ZIF-8 MOF does not get decomposed, retaining its overall architecture. However, there are some well-known MOFs that are collapsed in the electrochemical cell in an alkaline pH and form nano-scale metal hydroxide that exhibits efficient electrochemical OER. We could synthesize CoMOF-74 in two different conditions, yielding materials with two different morphologies: (i) nanoscale particles (CoMOF-74/RT) via room temperature wet-synthesis and (ii) conventional spindle-shaped bulk crystals (Co-MOF-74/ST) through solvothermal synthesis. CoMOF-74/RT exhibits superior oxygen evolution reaction (OER) activity in alkaline 1M KOH solution, delivering a current density of  $100 \text{ mA cm}^{-2}$  (with an excellent operational stability over a period of 7 days) at an overpotential of 433 mV, along with a Tafel slope of  $83 \text{ mV dec}^{-1}$ , outperforming its crystalline counterpart (Co-MOF-74/ST).<sup>5</sup> But post-electrolysis characterization reveals the transformation of the CoMOF-74/RT into  $\beta\text{-Co}(\text{OH})_2$  nanosheets, that acts as actual catalyst for this OER. Finally, MOF (MIL-101)–GO (graphene oxide) composites exhibiting enhanced proton conductivity will be discussed.<sup>6</sup>

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# 3D Oriented polycrystalline MOF films and patterns

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## Abstract

Metal-Organic Framework (MOF) materials are promising materials for a variety of applications including sensing, microelectronics, and optics. Despite the exceptional functional properties, protocols for the microfabrication of MOF-based components are still underdeveloped. However, this is a key-enabling process: controlling the geometrical position, shape, and crystal orientation in micropatterns will enable the implementation of MOF materials in technologically relevant devices.<sup>(1)</sup> In this presentation, we will discuss the recent developments in the field of oriented MOF films and patterns.<sup>(2,3,4)</sup> Protocols for the deposition of 3D-oriented polycrystalline Cu-based MOFs via hetero-epitaxial growth from Cu-based ceramics will be presented.<sup>(2,3)</sup> The recent strategy that enables the extension to photolithography for the microfabrication of oriented porous patterns will be illustrated.<sup>(4,5)</sup>

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Paolo Falcaro is an Italian materials scientist known for his pioneering work in porous materials, particularly metal-organic frameworks (MOFs). After a Master's degree in Materials Science (Padova University, Italy) he earned his PhD in Materials Engineering from the University of Bologna in 2006. His early career involved applied research at CIVEN and NanoFab in Italy, where he developed nanostructured materials for industrial applications. In 2009, he joined Australia's Commonwealth Scientific and Industrial Research Organisation (CSIRO), leading a team focused on engineering porous crystals and bio-composites. In 2016, Falcaro was appointed Full Professor of Bio-based Materials Technology at the Institute of Physical and Theoretical Chemistry at Graz University of Technology (TU Graz) in Austria. He has been appointed as an adjunct professor at the University of Adelaide in Australia and guest professor at Osaka and Kyoto University. His research focuses on the synthesis and application of MOFs, mesoporous materials, and functional nanoparticles, with applications spanning sensing, biotechnology, and environmental remediation. His methodologies include sol-gel processes, self-assembly, and film deposition techniques. A significant milestone in his career was receiving the European Research Council (ERC) Consolidator Grant in 2017 for the POPCRYSTAL project, which aims to develop crystalline materials with precisely aligned pores for use in optics and sensing technologies. Additionally, he co-leads the "Porous Materials @ Work for Sustainability" initiative at TU Graz, focusing on the development of sustainable porous materials.

# Reactive Zeolitic Imidazolate Framework Crystal Facets

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## Abstract

A general assumption of reticulated porous materials is that the primary interaction site is the pore surface/void space. In this regard, while bulk and pore nanospace properties of these materials have been extensively studied, the chemistry of the external crystal surface remains underexplored.

In this report, we have selected a series of both porous and non-porous zinc imidazolate frameworks (ZIFs) with different topologies, crystal sizes and shapes in which we propose their reactivity is mainly dictated by the crystal surface (Scheme 1).

Some of the essayed ZIF systems exhibits a high reactivity towards hydrolytic degradation of extremely toxic G-type nerve agents, Soman (GD) and simulant diisopropylfluorophosphate (DIFP). The reactivity of the crystal surface of ZIF towards P-F bond breakdown, gives rise to cascade of events including: i) crystal surface degradation releasing its structural components and ii) released nucleophilic imidazole moieties reactivate organophosphate inhibited Acetylcholinesterase within 10 min.<sup>[1,2]</sup> This detoxification process can be taken as a proof of concept for reversing organophosphorous poisoning. More generally, this approach underscores the importance of crystal surface nature and composition to control the reactivity of reticular materials.

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Jorge A. R. Navarro is Professor of Inorganic Chemistry at the University of Granada since 2010. His main research interest are the synthesis and biomedical and environmental applications of metal-organic framework materials. He has authored ca 160 publications which have received > 10,700 citations (H-index = 52). >2.0 million € in research funding (EU, National, Regional) managed as Project coordinator and PI in the last 5 years. > 500,000 € from contracts with Industry and Institutions. Regular invitations as plenary, keynote, invited lectures and invited seminars at major scientific conferences and research institutions (Materials Research Society, MOF, EuroMOF, Spanish Royal Society, MOFSchool, EliteCat, etc.). Organization of Major Scientific Events: Chair of 5<sup>th</sup> EuroMOF-2023 (750 participants) and XXXV Spanish Royal Society of Chemistry-2022 (> 1,600 participants). Transfer of knowledge: Founding member of Spin-Off Company: Porous Materials in Action S.L. Stablished in 2021.

## Designing active sites in MOF-based photo/electrocatalysis

## Abstract

Metal-Organic frameworks (MOFs) have recently gained interest as an innovative class of photocatalytic and electrocatalytic materials owing to catalytically active oxo-metal clusters connected to photoactive organic linkers through a well-ordered micropore network that yields exceptionally high surface areas. In dynamic processes and especially in liquid phase catalysis, the accessibility of active sites becomes a critical parameter as the reactant diffusion is often limited by the inherently small micropores of MOFs.

In this talk, I will present a promising strategy to overcome this challenge. It involves the synthesis of mixed-ligand MOFs, followed by selective ligand removal (SELIRE) upon thermal stimulus to design microporous-mesoporous MOFs [1]. As an example, we synthesized photoactive MOFs of the MIL-125-Ti family with two distinct hierarchical pore architectures resembling either large cavities or branching fractures, both of which significantly improved the photocatalytic hydrogen evolution (HER) rates of the MOFs by up to 500%. In another example, we show that these pores also greatly enhanced the potential of these MOFs to adsorb large molecules, such as glyphosate, from waste water [2]. The enhancements induced by the SELIRE process originate from 1) the formation of new under-coordinated adsorption sites and 2) better access to catalytic sites by facilitating reactant diffusion through the pores.

We will further demonstrate how this mixed-ligand approach can greatly enhance the structural integrity and durability of zeolitic imidazolate frameworks (ZIFs) in water-based environments und applied irradiation and electric fields as well as their conductivity and activity towards (photo)electrocatalytic HER and OER reactions [3,4]. Moreover, we will discuss how the creation of open-metal sites through the SELIRE process affects the rate limiting steps for these reactions [5]. In the last part, we will briefly explore the benefits of photoactive MOFs with 2D-arranged Ti-SBUs (i.e. COK-47 as an example) on facilitating charge separation, transport and extraction to adsorbed reactants [6].

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Prof. Dominik Eder, FRSC, received his Ph.D. in Physical Chemistry from the University of Innsbruck in 2003. In 2005, he joined the University of Cambridge as an Erwin Schrödinger Fellow and established his own research group in 2006 through the APART Fellowship of the Austrian Academy of Sciences. In 2011, he became Junior Professor at the University of Münster, and in 2015, he was appointed Full Professor of Materials Chemistry and Head of the Molecular Materials Chemistry Division at TU Wien. His research focuses on functional materials for energy and environmental applications, including nanocarbons, 1D/2D inorganic materials, MOFs, COFs, and mesoporous transition metal oxides. His group combines fundamental mechanistic studies for photocatalysis, electrocatalysis, and photovoltaics using in-situ and operando spectroscopy with the development of scalable systems, including large-scale reactors. Prof. Eder has published over 160 peer-reviewed articles, holds two patents, and has edited two academic books. He was elected Fellow of the Royal Society of Chemistry in 2018 and received the Chang Jiang Scholar Award in 2023.

# Catch and Release: Controlling MOF Photo-Dynamics

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## Abstract

Metal-organic frameworks (MOFs) offer precise chemical control and unique photophysical behavior, but understanding their dynamic excited states remains a challenge. This talk highlights how subtle linker modifications can dramatically tune the lifetime of a photoinduced “deligation” event—where a carboxylate ligand transiently detaches from an iron-based MIL-101 node. Using time-resolved infrared and visible transient absorption spectroscopy, we show that introducing electron-donating ( $-\text{NH}_2$ ) or electron-withdrawing ( $-\text{NO}_2$ ) groups alters intramolecular interactions, extending or shortening excited-state lifetimes by nearly three orders of magnitude. Supported by computational modeling, these findings reveal how Coulombic attractions or repulsions between functional groups and carboxylates govern back-electron-transfer energetics. The result is a molecular design strategy for precisely controlling photochemical reactivity in carboxylate-based MOFs, with implications for photocatalysis, light harvesting, and dynamic materials

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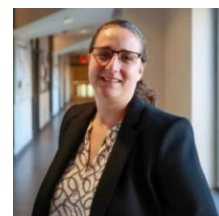
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Amanda Morris is a Professor of Inorganic and Energy Chemistry and Chair of Chemistry at Virginia Tech. Her research education, conducted at Penn State University (B.S.), Johns Hopkins University (Ph.D.), and Princeton University (Postdoctoral), was focused on addressing critical environmental issues with fundamental science, including water remediation, solar energy harvesting and storage, and carbon dioxide conversion. As her publication record shows, Morris is a classically trained photo-electrochemist with demonstrated success utilizing various techniques (cyclic voltammetry, spectroelectrochemistry, and pulsed-laser spectroscopy) to explore new frontiers in renewable energy. Her research group's current focus is on light-matter interactions and catalysis. She has received numerous awards for her research pursuits. She serves as an Associate Editor of Chemical Physics Reviews and sits on the Editorial Advisory Boards for the Journal of the American Chemical Society, ChemSocRev, ACS Applied Energy Materials, and EnergyChem.



# MOF crystallography for natural products

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## Abstract

We have developed metal–organic frameworks (MOFs) incorporating interactive ligands to trap metastable structures and construct responsive pore environments. An interactive ligand is defined as a bridging ligand bearing functional groups capable of engaging in supramolecular interactions. These ligands enable a range of fascinating functions, including kinetic trapping [1], selective guest recognition [2], ion conductivity [3], non-volatile memory storage [4], and more.

Notably, we have designed adaptable pores capable of visualizing natural products at atomic-level resolution [5]. While the crystalline sponge method has proven effective for analyzing small molecules [6], it still faces several challenges, such as limitations in molecular size, chemical and physical stability, and issues arising from pseudo-symmetry.

To address these challenges, we are developing new MOF systems tailored for enhanced structural elucidation of natural products. In this presentation, we will share our recent progress, with a particular emphasis on the structural analysis of nucleophilic natural products and medium-sized molecules [7].

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Since 2024, he has been the founder and CSO of TEKMOF.

His research interests include Coordination chemistry, Supramolecular chemistry, MOF, In situ chemical crystallography, Crystalline-state photochemistry, ab initio powder X-ray crystallography.

# Resilient Triboelectric Nanogenerators and Sensing Devices Engineered from MOF-Based Composites

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## Abstract

Triboelectric nanogenerators (TENG) are simple devices constructed from a pair of tribo-positive and tribo-negative material, which convert waste mechanical energy into useful electrical power. Because of their compact architecture and lightweight design, TENG devices are attractive as low-cost energy harvesters for scavenging energy from mechanical vibrations, human motions, and renewable sources. Likewise, TENG can be tailored to function as self-powered sensors to enable chemical detection and sensing of physical stimuli. Compared with contemporary triboelectric materials, such as perovskites, metal oxides, and MXenes, which typically exhibit a limited power output, MOF-based TEGs offer notable key advantages [1-2]. The rich topology of MOFs and variability of MOF-based composites, constructed from tunable organic and inorganic building blocks, confer a huge combination of structural versatility and multifunctionality not found in conventional materials. In this talk, recent exemplars of resilient MOF-based TENG devices will be presented. Attention will be given to the tailoring of dielectric properties, interfacial response, and time-dependent mechanical behavior including surface adhesion in the context of TENG output [3]. Chemical stability and humidity effects on electrical output and long-term performance and device resilience will be discussed. The underlying mechanisms [3-4] were interrogated through multimodal techniques, encompassing nanoscale-resolved mechanical and chemical studies *via* near-field infrared spectroscopy (nanoFTIR with a ~20 nm spatial resolution) [5] and tip-force microscopy (TFM) nanoanalytics, in conjunction with density functional theory (DFT) calculations of electrostatic potentials. Potential practical applications demonstrated include energy harvesters both in the contact- and non-contact modes, shear-type tactile sensors, and a self-powered Morse code generator of high sensitivity.

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# Design of Sustainable Catalysts using Covalent Organic Frameworks

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## Abstract

Catalysis is a crucial technology with significant implications for both economic and ecological sustainability. It plays a central role in developing resource-efficient, sustainable processes for energy and material conversion. Porous functional materials, characterized by large accessible surface areas and well-defined surface functionalities, are vital as catalysts in a wide range of viable chemical reactions.

Among these materials, are covalent organic frameworks (COFs). They combine the advantages of organic polymers with those of conventional inorganic or hybrid porous materials, such as zeolites, activated carbon, or metal-organic frameworks.<sup>[1]</sup> COFs feature ordered pore structures and tunable pore sizes, along with exceptionally high porosity and surface area. Moreover, their exclusively organic composition allows for precise control over both the chemical properties of their surfaces and the physical characteristics of the overall framework.

These unique features make COFs highly attractive for emerging applications, including freshwater generation, energy storage, and also opens up innovative prospects in electro- and photocatalysis. In this presentation, it will be shown how the surface of COFs can be precisely tailored to meet the requirements of specific catalytic applications<sup>[2]</sup> and how COFs can be used to modify the surfaces of inorganic catalysts<sup>[3]</sup> and to stabilize biological catalysts.<sup>[4]</sup>

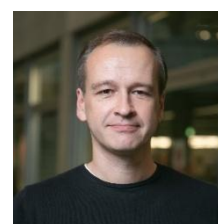
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Arne Thomas heads the Functional Materials group at the Institute of Chemistry at TU Berlin. He studied Chemistry in Gießen, Marburg and Edinburgh and completed his doctoral thesis at the MPI of Colloids and Interfaces, Potsdam/Golm, under Markus Antonietti. After a postdoctoral stay at the University of California, Santa Barbara, USA, in the group of Galen Stucky, he returned to the MPI-KGF as a group leader. In 2009, he was appointed to a professorship for Functional Materials at the TU Berlin. His group is interested in nanostructured and porous inorganic and organic materials and their diverse applications in gas separation, energy storage or catalysis. He serves as Advisory Editor for *Angewandte Chemie* and *Advanced Energy Materials*. Furthermore, he is the mentor and scientific advisor of two start-up companies. He is a highly cited researcher (Clarivate Analytics), with so far 290 Publications cited > 70.000 times.



# Combining Reticular Pore Design with Green Promises to Sustainable Practices

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## Abstract

Metal-organic frameworks (MOFs) reticular pore chemistry addresses the precise control over the position and spatial arrangement of the installed functionalities guided by the framework scaffold. Its chemistry operates in an infinite space of composition, structure, property, application and hence has given us an infinite freedom to build an enormous variety of new porous materials – but also placed upon us a profound responsibility to use it wisely. The responsibility – especially after winning the Nobel Prize in Chemistry – lies in identifying:

1. What are the key scientific questions that still need to be answered?
2. What are the societal challenges that reticular science can address?
3. How can reticular chemistry can provide real and sustainable solutions?

In this talk, we will explore these questions and reflect on our role in shaping the future of high-performance MOF materials enabling sustainable technologies. Our group has used reticular pore chemistry to develop a general platform to systematically build noncovalent interactions by using a MOF as a molecular scaffold to position selective chemical groups in defined geometry, combined with rigorous measurements of the electric fields associated with these interactions.<sup>[1]</sup> Electric fields provide a universal and physics-based metric for these interactions. Using this platform, we discovered and study a series of noncovalent interactions with a wide range of electric fields. Further we would like to introduce MOF-based aerogels designed for highly efficient atmospheric water harvesting or removal of per- and polyfluoroalkyl substances (PFASs) from drinking water.<sup>[2,3]</sup> In this context, we wish to discuss the critical need to align the development of MOF materials with sustainability principles. The core aspect revolves around the "sustainability paradox": materials designed for sustainable technologies often rely on resource-intensive and environmentally detrimental synthesis methods. We wish to emphasize that qualitative "green" claims are insufficient; true sustainability demands quantitative validation with Life-Cycle Assessment (LCA), which provides a standardized framework to quantify environmental impacts from raw material extraction to disposal.<sup>[4,5]</sup> Further, we would like to introduce the Performance-Sustainability Indicator (PSI) that balance impact against value, linking a MOF's functional benefits to its environmental footprint.<sup>[5]</sup> By integrating sustainable principles into reticular chemistry practice, MOF materials can evolve beyond scientific curiosities to become important contributors to a sustainable future that embodying environmental responsibility.

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Stefan Wuttke created the research group "WuttkeGroup for Science", initially hosted at the Institute of Physical Chemistry at the University of Munich (LMU, Germany). Currently, he is an institute professor and director of the Department of Functional Materials and Nanomagnetism at Academic Centre for Materials and Nanotechnology of the AGH University of Krakow (Poland), and also a visiting Professor of Functional Materials at Lincoln University (UK). His principal focus is the design, synthesis, and functionalization of MOFs and their nanometric counterparts to target diverse applications. At the same time, he aims to establish a basic understanding of the chemical and physical elementary processes involved in the synthesis, functionalization, and application of these hybrid materials.

# Metal-Organic Frameworks as a Heterogeneous Platform for (Photo)-Electrocatalytic Solar Fuel Production

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## Abstract

In a world that is running out of natural resources, there is a growing need to design and develop sustainable and green energy resources. In that respect, photo-electrocatalytically driven reactions for the production of alternative fuels (such as water splitting or CO<sub>2</sub> reduction) hold the potential to provide a route for future carbon neutral energy economy. Nevertheless, the slow kinetics of those catalytic reactions demands the development of efficient catalysts in order to drive it at lower overpotentials. Indeed, a variety of molecular catalysts based on metal complexes are capable of electrochemically reducing CO<sub>2</sub> and/or protons. Yet, despite the significant progress in this field, practical realization of molecular catalysts will have to involve a simple and robust way to assemble high concentration of these catalysts in an ordered, reactant-accessible fashion onto a conductive electrode.

Our group utilizes Metal-Organic Frameworks (MOFs) based materials as a platform for heterogenizing molecular electrocatalysts. Their unique properties (porosity and flexible chemical functionality), enables us to use MOFs for integrating all the different functional elements needed for efficient catalysts: 1) immobilization of molecular catalysts, 2) electron transport elements, 3) mass transport channels, and 4) modulation of catalyst secondary environment. Thus, in essence, MOFs could possess all of the functional ingredients of a catalytic enzyme. In this talk, I will present our recent study on (photo)-electrocatalytically active MOFs incorporating molecular catalysts for solar fuel reactions.

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Idan received all his degrees from Bar-Ilan University, including a B.Sc. in chemistry and computer science, an M.Sc. in molecular crystal engineering under the supervision of Prof. Yitzhak Mastai, and a Ph.D. in the photo-electrochemistry of quantum dot-sensitized solar cells with Prof. Arie Zaban. His interest in materials science and electrochemistry led him to a three-year postdoctoral stint as a Fulbright scholar with Prof. Joseph T. Hupp at Northwestern University's Department of Chemistry, where he studied the electrochemical properties of porous coordination polymers. In 2016, Idan accepted a faculty position as an assistant professor in the Chemistry Department at Ben-Gurion University of the Negev. His primary research interests center on developing novel concepts for the molecular-level manipulation of heterogeneous catalysts using functional, porous materials, and their application in electrocatalytic small-molecule activation reactions, such as CO<sub>2</sub> reduction, O<sub>2</sub> reduction, H<sub>2</sub> evolution, and ammonia electrosynthesis.

# Design and Development of Metal-Organic Frameworks Based Triboelectric Nanogenerator for Sustainable Power Generation

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## Abstract

TENGs have gained significant attention due to their ability to convert mechanical energy into electricity. Advancements in materials like metal-organic frameworks (MOFs) and device architecture have led the improvements in performance. Recently, the metal-organic frameworks (MOFs) based TENGs has attracted attention due to their triboelectrification properties and charge trapping ability. In this regard, we present series of MOFs-TENGs devices which generated a maximum output power density: (i) the Cd-MOF-TENG device was attached to the fingers of a glove and used to control the mouse movement in a computer *via* finger movements as “Air Mouse”, (ii) another case the V-shaped Zn-MOF-TENG is utilized for low-powered electronics and smart sports sensor in detection and monitoring and (iii) Mn-MOF-TENG device as Parking Sensor.

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# Harnessing the Sunlight for Photocatalytic Hydrogen Peroxide Generation

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## Abstract

Covalent organic frameworks (COFs) are crystalline, porous, two- and three-dimensional materials that are well known for their customizable topologies and tunable functionalities.<sup>[1, 2]</sup> Due to their tunable pore sizes, large surface areas, high chemical stability, and visible-light absorption, COFs have attracted considerable attention in photocatalysis. Consequently, COFs have been investigated for their applications in photocatalytic water splitting, organic transformations, CO<sub>2</sub> reduction, and dye degradation.<sup>[3]</sup> Among these applications, the generation of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) using photocatalysis has received particular attention due to the dual role of H<sub>2</sub>O<sub>2</sub> as a green oxidant and a sustainable energy carrier.<sup>[4]</sup> It also has the potential to replace the conventional anthraquinone process with a cleaner, sunlight-driven alternative. In our efforts to design efficient, recyclable COFs for photocatalytic H<sub>2</sub>O<sub>2</sub> production from pure water, we have demonstrated that tuning the density of hydrazone linkages, introducing metal clusters, enabling proton-coupled electron transfer and incorporating donor-acceptor functionalities into the COF backbone can significantly enhance activity and stability, highlighting the remarkable versatility of COFs in photochemistry.<sup>[5-7]</sup>

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Dr. Pachfule is an Associate Professor at the S. N. Bose National Centre for Basic Sciences, Kolkata, India. He obtained his Ph.D. from the National Chemical Laboratory (NCL), Pune, and conducted postdoctoral research at the Advanced Institute of Industrial Science & Technology, Osaka (Japan), and subsequently at Technische Universität Berlin (Germany). His group's research lies at the intersection of chemistry and materials science. The group is focusing on designing and synthesizing covalent organic frameworks (COFs) for use in energy and environmental applications. These include photocatalytic water splitting for hydrogen generation, the production of hydrogen peroxide, and organic transformation. Dr. Pachfule has made significant contributions in the fields of photocatalysis, electrocatalysis, and energy storage, with special emphasis on sustainable hydrogen and hydrogen peroxide generation, CO<sub>2</sub> reduction, and organic transformations. His work has been published in leading journals such as *Nature Chemistry*, *JACS*, *Angewandte Chemie*, *Advanced Materials*, *Small*, etc., and he has authored over 85 peer-reviewed publications. He is a recipient of prestigious fellowships, including the Alexander von Humboldt Fellowship and the JSPS Fellowship, and currently leads several nationally funded research projects.

# Artificial Photosystem Metal–Organic Frameworks

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## Abstract

Developing entirely artificial photosystem has been challenging by the system design where molecular assembly hosts all the crucial photophysics, including efficient light harvesting, control over the operating spin manifold, and proton-coupled electron transfer. Each of these defines an independent subject area and consists of subordinate areas and their own challenges. Material design must consider scalability for ease of deployment. MOFs define heterogeneous photocatalytic platforms with highly chemical accessibility of the interior surface – where the pigment (strut) assemblies around the well-defined pores characterize the evolution of unique yet intuitively predictable excitonic properties possible through structural, environmental, and dielectric modulation. The presentation will highlight MOFs as an artificial photosystem-I, featuring antenna behavior to generate high-potential redox equivalents through symmetry-breaking charge transfer process with complete control over the triplet formation and populations (i.e. 0-150% of the initial singlet), proton-couples electron transfer to generate natural PS-I like chemical reducing agent.

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Deria started his research as a JNCASR summer fellow (2020) at IISc Bangalore working on developing enantioselective epoxidation. He then worked on developing heterogeneous catalysts for phosphate ester toxin decompositions at IIT Kanpur and came back to IISc for a second summer (JNCASR summer fellow) working on MOLY-driven sugar functionalization. His doctorate research at Penn involved ionic conjugated polymer-wrapped SWNTs and their hierarchical assemblies for unique optoelectronic properties. His postdoctoral tenure at Northwestern involved developing a widely used MOF-functionalization method called Solvent-Assisted Ligand Incorporation (SALI). His group at SIU is focused on developing porous solids for photo-, electro-, and photoelectrocatalytic transformations and energy conversion. Research on developing efficient artificial light-harvesting antenna systems has been supported by *NSF CAREER* award whereas heterogeneous photocatalytic work is currently on NIH support. This research fundamentally addresses how to manipulate molecular excitons (like displacing them to far sites and splitting them into redox equivalents) in the solid porous assembly for energy conversion much like the way it occurs in biological systems.



# Crystal Engineering of Transiently Porous and Ultramicroporous Networks as Adsorbents

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## Abstract

This seminar will focus on our recent results (including published and ongoing studies) on the crystal engineering of several classes of transiently porous and ultramicroporous reticular sorbents,<sup>1</sup> key to advancing the state-of-the-art in physisorbent design. At the heart of this field is the use of bottom-up nanomaterial design principles, applying crystal engineering approaches to develop advanced adsorbents.<sup>2</sup> Key takeaways include new scientific understandings of sorption performances that address commodity chemical separations, including light hydrocarbon and freshwater purifications. The overarching goal is set at meeting the United Nations Sustainable Development Goals 3 (Good Health and Well-being), 6 (Clean Water and Sanitation), 7 (Affordable and Clean Energy), and 13 (Climate action).<sup>3</sup> Despite these advances, challenges remain to be addressed for commercial adoption.

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Dr Soumya Mukherjee, an Associate Professor in Materials Chemistry at the Department of Chemical Sciences, University of Limerick, is an early-career academic with an outstanding research record. Prof Mukherjee (SM) has won the University of Limerick President's Research Excellence and Impact Award 2022, the Mid-Career Researcher Award 2024 from the Bernal Institute, the Thieme Chemistry Journals Award 2025, and has secured several competitive research grants from Research Ireland, the Alexander von Humboldt Foundation, the EU Commission, and the Royal Society of Chemistry. With >110 peer-reviewed publications and >10,000 citations in materials chemistry, SM has featured in the Stanford University's list of globally highly cited (top 2%) researchers for five years in a row. SM's research team develops advanced porous materials, including organic and metal-organic polymers to address the global grand challenges in chemical purification, air, and water treatment. SM's most impactful contributions to date address benchmark materials for water purification, trace carbon capture, and hydrocarbon purification.



# Coordinated Solvents Driven Proton Conduction in Crystalline Solids

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## Abstract

The presentation includes the discussion on design strategy, synthesis and proton conduction properties of Coordination Polymers (CPs) and Metallo-Hydrogen Bonded Organic Frameworks (MHOFS) performed at 'Framework Laboratory' of IIT-KGP. Recent past witnessed considerable progress of such materials as solid-state proton conductors (SSPCs) due to their several structural superiority and architectural diversity. A variety of *intrinsic* and *extrinsic* protonic sources have been installed onto these frameworks so far, conversely, metal-coordinated solvent molecules (water, ammonia and dihydrogen-phosphates) acting as *solely intrinsic* proton sources by virtue of their enhanced acidity (due to polarization) are largely unknown in bringing conductivity onto such systems. Those key examples will be focused in this presentation.

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Madhab C. Das completed his BS in Chemistry from Midnapore College in 2002 followed by MS in Chemistry from Vidyasagar University in 2004. He did his Ph.D. in Supramolecular Chemistry at Indian Institute of Technology (IIT) Kanpur under the supervision of Professor P. K. Bharadwaj (2009). Then, he worked with Professor Banglin Chen at the University of Texas at San Antonio, Professor George K.H. Shimizu at University of Calgary, and Professor Hiroshi Kitagawa at Kyoto University as postdoctoral fellow (Dec, 2009–Nov, 2013). At Kyoto University he worked as a JSPS postdoctoral researcher. He joined at IIT Kharagpur as an Assistant Professor in Dec, 2013. Since Aug, 2019, he is an Associate Professor at IIT Kharagpur. He was a visiting AvH Experienced Fellow at University of Augsburg in the summers of 2023-2025. His work is focused on functional MOFs and HOFs mostly toward gas separations and proton conduction application domains.

# Strategic Design of Framework Materials for Chemical Fixation of Carbon Dioxide to Value-Added Chemicals

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## Abstract

The escalating carbon dioxide content in the atmosphere has led to pervasive consequences such as global warming, variations in climate, and erratic weather conditions. To address these detrimental environmental issues, it is imperative to attenuate atmospheric carbon dioxide concentration through selective capture and subsequent storage/utilization. Consequently, carbon capture and utilization (CCU) as a C1 feedstock to generate value-added chemicals and fuels offers dual advantages of mitigating the rising CO<sub>2</sub> concentration and sustainable generation of high-value compounds and fuels.<sup>1,2</sup> Especially, selective carbon capture and utilization from direct air has attracted tremendous attention due to its practical applications.<sup>3,4</sup> In this direction, our research group is working on the rational design of functional framework (MOF/COF) materials incorporated with a high density of CO<sub>2</sub>-philic and catalytic sites suitable for simultaneous capture and conversion of carbon dioxide into high-value chemicals at mild conditions.<sup>5-8</sup> The highlights of the ongoing research work on strategic design, synthesis, and catalytic investigation of the framework materials for chemical fixation of CO<sub>2</sub> into various value-added chemicals will be presented.

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Dr. Nagaraja is a professor of chemistry at the Indian Institute of Technology (IIT) Ropar. He earned his BS and MS degrees from Bangalore University. In 2007, he received his Ph.D. from the Indian Institute of Science, Bangalore. Thereafter, he carried out postdoctoral research work at Brandeis University, USA, and Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore. His research group is mainly working on the design of multifunctional framework (MOF/COF) materials for the utilization of carbon dioxide and generation of solar fuels. He has been awarded the Japan Society for the Promotion of Science (JSPS) invitational fellowship-2024 and the Chemical Research Society of India (CRSI) Bronze medal for the year 2026.

# Metal-free Heptazine based Photoredox Catalysts (HMPs) for Sustainable Fuels and Chemicals

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## Abstract

One of the oldest organic moiety reported in the 19<sup>th</sup> century, Heptazines (tri-*s*-triazines) are one of the forefront moiety in the form of polymeric graphitic carbon nitrides (especially known as g-C<sub>3</sub>N<sub>4</sub> or g-CN) today.<sup>1</sup> It attained profound importance after it's application as first organic semiconductor for water splitting to generate hydrogen in the visible light.<sup>2</sup> From that point there is no looking back, where it was applied in variety of energy and environment related applications. Our group utilised it extensively in synergistic photoredox catalysis to produce solar fuels and fine chemicals in more sustainable way.<sup>3</sup>

Even though, this *s*-heptazine moiety has not been explored much due to it's solubility issues in common organic solvents. After eventual breakthrough in 2002, the basic constituting unit of g-CN, heptazine, has driven scientists to develop various functional materials.<sup>4-6</sup> Especially our group is involved in various material-designs on synthesizing molecular compounds and heptazine based micro-/mesoporous organic polymers (HMPs) for photoredox catalysis. In particular, synergistic photocatalytic CO<sub>2</sub> reduction to selective CO and CH<sub>4</sub> and photocatalytic Baeyer- Villiger Oxidation will be presented in brief.<sup>7-9</sup>

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# MOLECULAR AND IONIC SIEVING METAL-ORGANIC FRAMEWORK MEMBRANES WITH A THICKNESS OF JUST ONE UNIT CELL

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## Abstract

Metal-organic frameworks (MOFs) have emerged as one of the most promising gas-selective nanoporous materials for application as a thin selective layer of membranes [1]. Pore size, adsorption affinity, lattice flexibility, grain-boundary defects, linker vacancies, and film thickness determine gas separation performance from a polycrystalline MOF membrane [2]. Restricting the lattice flexibility in a MOF film is crucial to achieve selectivity between similar-sized gas molecules. Lattice flexibility in bidentate MOFs, such as ZIF-8, arises from the flip-flop motion of the linker. The flexibility could be arrested by a simple yet effective post-synthetic treatment technique involving heating the membrane in the air for a few seconds, resulting in attractive CO<sub>2</sub>/N<sub>2</sub> selectivity from polycrystalline ZIF-8 membranes [3][4].

Unit-cell-thick MOF films can be considered the ultimate membrane for molecular separation. This is because ordered intrinsic porosity allows one to obtain high molecular selectivity, while the combination of unit-cell-thickness and large porosity (1 pore/nm<sup>2</sup>) allows high molecular flux. However, the state-of-the-art MOF films have thicknesses exceeding 50 nanometers. Unit-cell-thick, oriented, continuous, and pinhole-free MOF films could be prepared by suppressing the out-of-plane growth of MOF films [5]. This could be achieved using an ultradilute growth solution and atomic-smooth substrates that offer a crystallographic registry with the lattice of the MOF film. Three distinct two-dimensional (2D) MOF films could be prepared with this strategy, with film thickness down to a single unit cell. These are Zn(methylimidazole)<sub>2</sub> [5], Zn<sub>2</sub>(benzimidazole)<sub>4</sub> [6], and UiO-66 [7]. Thanks to the presence of size-sieving pores in these films and the elimination of lattice flexibility due to the two-dimensional confinement of the structure, large molecular and ionic selectivity could be achieved. In particular, record-high H<sub>2</sub>/N<sub>2</sub> and H<sub>2</sub>/CO<sub>2</sub> separation performance could be achieved. The method will accelerate the development of 2D crystalline and ultrathin MOF films for membranes.

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# Structure–Function Correlations in COFs: Toward Optimized Nanocarriers for Lung Cancer Therapy

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## Abstract

Over the past decade, covalent organic frameworks (COFs) have emerged as promising chemotherapeutic drug-delivery nanocarriers (DDNs) owing to their precise pore channels combined with tunable framework chemistry. Unlike non-porous analogues, this synergy has led to remarkable drug-loading capacities (up to 70-90 wt%), stimuli-responsive drug-release profiles and exceptionally high biocompatibility (up to 800 µg/mL). Although, a lot of progress has been achieved in the past decade, critical parameters regulating drug-loading capacity, release kinetics, *in vivo* chemotherapeutic performance of COF-based DDNs, such as immune response, sub-100 nm particle size control, long-term colloidal stability and blood circulation half-life along with precise clearance pathways remain underexplored.<sup>1</sup> We focused on exploring the role of pore-interface engineering in enhancing anticancer drug-loading in COF DDNs.<sup>2</sup> The results highlight the importance of pore-wall functionalization over surface area to achieve high drug-loading capacity and better drug-COF interaction. The in-vitro biological studies confirmed the biocompatibility of bare COFs and the efficacy of doxorubicin-loaded COF in killing cancer cells. Further, we have successfully synthesized isorecticular sub-100 nm COF DDNs with different functionalities while maintaining uniformity in their morphology and suspension stability. Apart from this, we have also investigated how different functionalities in these COF DDNs regulate their uptake and intracellular fate within the cancer cells. Findings of our studies highlight towards making COFs more suitable candidates for anticancer drug delivery by overcoming the existing challenges.

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Prem Felix Siril serves as a Professor at the School of Chemical Sciences, Indian Institute of Technology (IIT) Mandi. He became part of IIT Mandi in 2010, after pursuing postdoctoral research at the University of Paris-Sud in France and the University of Huddersfield in the UK. His research spans diverse areas including nanomaterials, porous frameworks, heterogeneous catalysis, and drug delivery systems. Additionally, he has a keen interest in synthesizing materials through flow chemistry techniques. He is a recipient of Marie-Curie international incoming fellowship, Royal Society network fellowship as well as BMBF visiting fellowship.



# Sustainable Catalysis Using Visible Light, Air and Water

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## Abstract

Functional materials featuring semiconductor-like behavior have attracted significant interest in photocatalysis due to their widespread applications. However, traditional materials, such as metal oxides, metal sulfides, metal phosphides, and perovskites, not only suffer from low surface area and limited stability but also from absorption in the UV region of the solar spectrum. In this context, metal-organic frameworks (MOFs) offer not only a large surface area but also robust and tailorable architectures. Our research group has pioneered the development of metalloligand-based MOFs to have better structural control of the resultant materials.<sup>1</sup> The step-wise design strategy successfully controls the structural dimensionality and the functional aspect of the resultant MOFs by varying the linker groups a metalloligand offers and selecting both primary and secondary metal ions. Notably, such metalloligands absorb light in the visible region of the solar spectrum, allowing them to function as the light-harvesting unit (i.e., photosensitizer) in the resultant MOFs.<sup>2</sup> As a result, such MOFs function as remarkable heterogeneous photocatalysts for various catalytic reactions, including selective oxidation of substrates, cross-coupling reactions, and oxidative coupling only using visible light, air, and water.<sup>2-4</sup> This talk will discuss a few selected molecular architectures that offer tunable band gaps for excellent light harvesting properties to achieve desirable photocatalytic reactions.

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Rajeev Gupta is a Senior Professor in the Department of Chemistry, University of Delhi. Prof. Gupta's research interests are in the area of Coordination and Supramolecular Chemistry with the focus on functional materials, sensing, catalysis, energy-transfer, and photocatalysis. Under his supervision, 21 students have obtained their PhDs, whereas 8 students are presently working in his research laboratory. He is an elected Fellow of the Indian Academy of Sciences (2025), a recipient of Prof. Priyadarajan Ray Memorial Award (2023) from the Indian Chemical Society; Bronze Medal (2016) from the Chemical Research Society of India; Science Flame Award (2015) from the World Science Congress; and Indo – US Research Fellowship (2009) from the Department of Science & Technology. Prof. Gupta has served as a member of the Programme Advisory Committee of SERB, the Expert Committee of the INSPIRE Fellowship Program of DST, the Special Assistance Program (SAP) of UGC, Expert Panels of the Central Pollution Control Board, and the Food Safety & Standards Authority of India, in addition to the Board of Studies of various universities and institutions across the country.



# Covalent Organic Framework Membranes for Molecular Separations and Beyond

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## Abstract

Membrane-based separation is vital in various industrial processes because of its low energy consumption, compact design, and ease of operation. The advancement of this technology hinges on the development of innovative membrane materials. While polymer-based membranes have been used for a long time, their efficiency is limited by the trade-off between permeability and selectivity. Thus, the quest for novel membrane materials is a primary focus for academia and industry. Nanoporous materials, such as zeolites, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs), based membranes provide better separation performance due to their ordered porous structures.

COFs, in particular, are promising for advanced gas and liquid-phase separation processes because of their crystalline nature, well-defined porosity, tunable functionalities, and versatile architectures.<sup>1</sup> Since their introduction, covalent organic framework membranes (COFMs) have witnessed rapid advancements, highlighting their significant potential in membrane-based separation technologies.<sup>2</sup> Not limited to molecular separation, recently, COFMs have also emerged as potential semiconducting materials for photonics and optoelectronic device applications.<sup>3</sup> In my talk, I will discuss two of our recent works on optical conductivity of free-standing 3D COFMs using terahertz (THz) spectroscopy and nonlinear optical (NLO) response of free-standing COFMs, along with molecular separation potentials of our in-house developed membranes.

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Dr. Biswal received a Ph.D. in the year 2017 from Academy of Scientific and Innovative Research, CSIR-National Chemical Laboratory, Pune. He was an Alexander von Humboldt fellow at Max-Planck-Institute of Solid-State Research, Stuttgart (Dec. 2017 - Aug. 2020) and Institute Post-doc fellow at Technical University Dresden, Germany (Sept. 2016 - Sept. 2017). He has also received several prestigious national, international recognitions and awards, which include Research Rising Star Award by Aseanian Membrane Society (2025), Associate of Indian Academy of Sciences (IASc) Bangalore (2024), and Head of Max Planck Partner Group appointed by Max Planck Society, Germany (2024). Dr. Biswal has expertise in the field of physical and materials chemistry. His group at NISER Bhubaneswar is developing advanced reticular materials and membranes for sustainable applications, with a target to provide clean energy, pure water, and recycle waste.

# Using nonlinear optical processes for post-synthetic modification of metal-organic frameworks and coordination polymers

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## Abstract

Nonlinear optical (NLO) phenomena offer a versatile toolkit for materials science, serving not only as sensitive probes for structural changes but also as triggers for inducing chemical transformations within crystalline solids. Processes like second-harmonic generation are invaluable for tracking structural evolution, particularly for the unequivocal detection of noncentrosymmetric phases that can emerge during phase transitions. Beyond diagnostics, NLO processes, specifically two-photon absorption (2PA), are emerging as a novel method for realizing photochemical reactions in a controlled manner. This approach opens a speculative yet exciting frontier for the post-synthetic modification of materials such as metal-organic frameworks (MOFs) and coordination polymers. This presentation will explore the prospective use of 2PA to initiate solid-state reactions like [2+2] photocycloaddition, a process typically performed via one-photon excitation (UV-Vis radiation) with renowned potential for post-synthetic MOF modifications.<sup>1</sup> These include e.g. photopolymerization in a single-crystal-to-single-crystal fashion.<sup>2</sup> However, unlike conventional one-photon excitation, which tends to indiscriminately activate all reactive sites and is often limited by surface penetration effects, 2PA is governed by different selection rules. This distinction presents a unique opportunity for site-selective chemistry; by designing crystalline architectures containing multiple photoactive components with differing 2PA cross-sections, it may be possible to selectively address and transform specific molecular fragments within the crystal lattice. Furthermore, the use of long-wavelength light for 2PA allows for homogeneous excitation throughout the bulk of a crystal, potentially leading to more uniform conversions and preserving crystal integrity. In this talk will be discussed possibilities for deliberate construction of periodic systems with regions displaying high and low photoreactivity through tailored 2PA cross-sections. The emerging concepts of site-selective photochemical transformations in materials combining multiple distinct photoreactive chromophores will be explored, highlighting how synthetic design can shape the likelihood of 2PA-induced reactions. Additionally, the prospects for achieving controllable photochemical conversions in targeted frameworks while intentionally preserving other reactive centers will be examined as a pathway toward precise modification of metal-organic materials.

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Dr. Jan K. Zaręba is an Assistant Professor at the Institute of Advanced Materials, Wrocław University of Science and Technology, Poland. His research expertise centers on nonlinear optics of MOFs and hybrid organic-inorganic perovskites. A key aspect of his work involves using nonlinear optical phenomena, such as second-harmonic generation, third-harmonic generation, and two-photon excited luminescence as tools for tracking temperature- and pressure-induced structural phase transitions. His current research activities are expanding into two-photon induced single-crystal-to-single-crystal photoreactivity. This emerging research direction is being explored within the PhotoReactMat2 project, which aims to harness nonlinear absorption processes for site-selective controlled solid-state photochemical reactions in MOFs and coordination polymers.

## How can process engineering enable the discovery/screening of MOFs for CO<sub>2</sub>

# capture

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## Abstract

In the last 20 years, significant efforts have been invested in developing adsorption processes for CO<sub>2</sub> capture. The explosion in adsorbent synthesis and molecular simulations has generated hundreds of thousands of (hypothetical & real) adsorbents, particularly MOFs. This excitement has led to an implicit assumption that the key bottleneck in developing large-scale adsorption processes is discovering the right adsorbent. Recent studies have demonstrated that an adsorbent's performance is intimately linked to the process in which it is deployed, and any meaningful screening should account for the process's complexity. Hence, screening these large databases to identify suitable candidates for scale-up is a challenging problem. The talk will have two parts.

Part 1. Process Engineering for screening & optimization [1]: Here, we will focus on recent modelling and machine learning developments that have allowed us to screen large adsorbent databases and develop achievable separation/cost targets for adsorption with other technologies. These techniques have allowed us to understand the interplay between processes and materials. We will illustrate the interplay using recent work related to the screening of adsorbents, machine-learning models for process optimization scale-up and costing.

Part 2. Quantifying water-CO<sub>2</sub> co-adsorption on MOFs [2]: Adsorptive CO<sub>2</sub> capture is inherently a water handling problem. Water in the flue gas can have significant process implications, and for a MOF to be suitable for practical applications, the co-adsorption behaviour of CO<sub>2</sub> and H<sub>2</sub>O must be quantified. Despite its importance, very few studies focus on this problem. We will illustrate co-adsorption measurements on several CO<sub>2</sub> capture MOFs and explore their impact on process outcomes.

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## Name: Arvind Rajendran

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Arvind Rajendran is a professor of Chemical Engineering at the University of Alberta. He received his PhD from ETH Zurich. He began his academic career at Nanyang Technological University in Singapore and later moved to the University of Alberta in 2012. He has co-authored over 100 papers and (co-) advised 50+ highly qualified personnel (MSc+PhD+Post-doc). His research group focuses on adsorptive gas separations with applications in CO<sub>2</sub> capture, direct air capture, oxygen purification and helium separation. Between 2016 and 2020, he served as an associate editor of the *Canadian Journal of Chemical Engineering* and as an area editor of *Adsorption*- the journal of the International Adsorption Society. Arvind serves as the secretary of the International Adsorption Society (IAS). He directs the newly established Centre for Energy and Mineral Processing (CEMP) at the University of Alberta's Faculty of Engineering.

# Development of Water-Stable Metal-Organic Frameworks for Fluorescence Sensing, Oil-Water Separation and Heterogeneous Catalysis

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## Abstract

In this lecture, I will highlight our recent research achievements in the area of applications of water-stable metal-organic frameworks (MOFs) in fluorescence sensing, oil-water separation and heterogeneous catalysis. Cleaning marine oil spills is a demanding task since it causes severe pollution. Hence, few superhydrophobic MOFs attached were developed for oil-water separation [1]. High oil absorption capacity, separation efficiency and self cleaning properties were achieved for all superhydrophobic MOF composites with foam/fabric. Fluorescence sensing of analytes is a convenient technique because of its portability, fast response and cost-effectiveness. Several MOF based fluorescent sensors have been developed with fluorescent organic ligands for detection of metal cations, anions, nitroaromatic explosives and other biologically important analytes [2]. Few of the MOF sensors have been applied for sensing of analytes in real-life samples, paper strips and living cells. In chemical, pharmaceutical and agrochemical industry, heterogeneous catalysts are widely used for several organic transformations and CO<sub>2</sub> conversion reactions to produce numerous valuable chemicals. Therefore, few MOF based heterogeneous catalysts were developed for various organic transformations and CO<sub>2</sub> fixation reactions [3]. In all cases, MOF catalysts showed high catalytic activity, reusability and broad substrate scopes.

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Dr. Shyam P. Biswas received his Ph.D. degree in 2010 from University of Ulm, Germany under the supervision of Prof. Dirk Volkmer in the area of coordination compounds and coordination polymers based on 1,2,3-triazolate ligands. He has carried out post-doctoral research works with Prof. Norbert Stock in Christian-Albrechts-University of Kiel, Germany and with Prof. Pascal Van Der Voort in University of Ghent, Belgium in the area of meta-organic frameworks (MOFs). He has joined IIT Guwahati in 2013 where he is currently working as a Professor in Department of Chemistry. His research interests include applications of water-stable MOFs in fluorescence sensing, oil-water separation and heterogeneous catalysis.

# Chemically programmed molecular diffusion in metal-organic frameworks

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## Abstract

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

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Dr. Ritesh Haldar is a Reader F at Tata Institute of Fundamental Research Hyderabad, India since 2021. His research group works on the development of gas and ion selective membranes, microfluidic catalysis and understanding of molecular diffusion in metal-organic frameworks. Prior to this, Dr. Haldar was a group leader and Alexander von Humboldt postdoctoral fellow at Karlsruhe Institute of Technology, Germany with Prof. C. Woell. Dr. Haldar earned his PhD degree (2015) from JNCASR, Bangalore under supervision of Prof. Tapas Kumar Maji.

# Metal-Organic Frameworks and Porous Organic Polymers: A New Frontier in Space Materials

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## Abstract

The next era of space exploration, including long-duration human missions and permanent off-world habitats, demands a revolution in materials science to overcome challenges of mass, volume, and efficiency. Metal-Organic Frameworks (MOFs) and Porous Organic Polymers (POPs) represent a new class of porous materials that are highly promising for these applications. MOFs and POPs hold the potential to revolutionize space exploration by providing lighter, more efficient, and more reliable systems for life support, resource utilization, thermal control, and radiation shielding. While challenges related to durability and manufacturing scalability remain, a strategic, integrated approach combining rational design, advanced manufacturing, and commercial partnerships is poised to transition these remarkable materials from the lab to a cornerstone of future space missions.<sup>1</sup>

Here, the transformative potential of these materials across critical space systems will be examined:

Atmosphere Revitalization: Acting as "molecular sponges" to selectively capture carbon dioxide and moisture, significantly reducing the energy and mass of life support systems.<sup>2</sup>

In-Situ Resource Utilization (ISRU): Serving as efficient photo-catalysts to produce water and propellants from local extraterrestrial resources.<sup>2</sup>

Passive Thermal Control: Providing a conceptual design for materials with tunable thermal expansion, a crucial capability for sensitive electronics and structural components.

Radiation Shielding: Functioning as a lightweight, passive solution for protecting astronauts from harmful neutron radiation by incorporating hydrogen-rich materials in a thin form factor.

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Dr. Renjith S. Pillai employ both computational chemistry techniques and advanced experimental tools to research and design of novel porous materials, such as Zeolites & Metal-Organic Frameworks (MOFs). Specialties: - Computational Chemistry including Force-field based simulations (Monte Carlo, Molecular Dynamics), Density Functional Theory (DFT) and ab initio techniques - Separation and Purification technologies - Adsorption and diffusion in porous materials - Modelling of electronic structure of catalysts



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

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## Abstract

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 also identified which was attributed to be due to charge-transfer across the interface. Very recently, in such hetero-structured thin films, bistable interface (switching from non-Ohmic to Ohmic conduction by thermal energy) was recognized and also, reversibly switched the Knee-voltage by light-irradiation. 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.

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Nirmalya Ballav is an Indian scientist and a faculty member at the Indian Institute of Science Education and Research Pune (IISER Pune). He is a chemist by training, widely recognized for his contributions to the field of functional materials and molecular chemistry. His research primarily focuses on metal–organic frameworks (MOFs), porous materials, and supramolecular chemistry, with an emphasis on understanding structure–property relationships and designing materials for applications such as gas storage and separation, catalysis, and energy-related processes. Prof. Ballav’s work bridges fundamental chemical principles with practical material applications, making it highly relevant to both academic research and emerging technologies.

# Engineering Earth-Abundant Metal Catalysts using Metal-Organic Frameworks for Selective Methane Functionalization

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## Abstract

The direct oxidation of methane to valuable oxygenates, such as alcohols and acetic acid, is highly challenging under mild conditions due to high C–H bond dissociation energy, facile overoxidation to CO and CO<sub>2</sub> and the intricacy of C–H activation/C–C coupling. To address this challenge, we have developed multifunctional porous metal-organic frameworks (MOFs) catalysts using earth-abundant metals for direct methane oxidation into methanol or acetic acid selectively at different reaction conditions using O<sub>2</sub>. The heterogeneous MOF-supported single-site copper(II) hydroxyl catalyst gives exceptionally high acetic acid productivity of 1,57,366  $\mu\text{mol}_{\text{CH}_3\text{CO}_2\text{H}} \text{g}_{\text{Cu}}^{-1} \text{h}^{-1}$  in 100% selectivity at 115 °C in water. Additionally, MOF nodes supported monomeric Fe<sup>III</sup>(OH)<sub>2</sub> species yields methanol or acetic acid with high productivities of 38,592  $\mu\text{mol}_{\text{CH}_3\text{OH}} \text{g}_{\text{Fe}}^{-1} \text{h}^{-1}$  and 81,043  $\mu\text{mol}_{\text{CH}_3\text{CO}_2\text{H}} \text{g}_{\text{Fe}}^{-1} \text{h}^{-1}$ , respectively. Through spectroscopic analyses, controlled experiments and computational studies, we demonstrate that the active-site isolation of mononuclear metal-hydroxyl species at the MOF nodes, their confinement within the porous framework, and their electron-deficient nature facilitate methane C–H activation via  $\sigma$ -bond metathesis, leading to the formation of liquid oxygenates in excellent selectivity. Our rational design of MOF-based base-metal catalysts and the reaction mechanism offers a sustainable route for methane valorization utilizing only O<sub>2</sub> and H<sub>2</sub>O in a single-step, alternative to the capital-intensive syngas route. In addition, we will discuss our recent advancements in abundant-metal catalyzed methane C–H borylation.

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# Excited-state intramolecular proton transfer (ESIPT) in metal organic frameworks

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## Abstract

Smart luminescent materials have taken a leading role both in photophysical science due to their versatile use as sensors and/or imaging agents.<sup>1</sup> Among different photophysical phenomena of such materials, photo-induced structural isomerism-coupled ultrafast intramolecular proton transfer in a suitable system are popularly known as excited-state intramolecular proton transfer (ESIPT), which is an interesting phenomenon in this context.<sup>2</sup> In an ESIPT process, two different excited states are formed, one from normal excitation of the parent molecule and another from the excited-state proton-transferred species. Consequently, from these two excitation states, two different emission maxima (dual emission) are observed which is the signature of ESIPT.

The ESIPT behavior has been extensively studied in various organic systems, in both experimental and theoretical aspects, mostly in solution. However, it has been observed that the metal organic frameworks (MOFs) particularly the flexible or dynamic MOFs are found very promising in the design of ESIPT active probe, for their unique structural features as well as for their potential applications in tailoring better functionality.<sup>3</sup> Sometimes the ESIPT can be observed even in solid state in case of MOFs which is not very usual.<sup>4</sup> Here the advantages and some outstanding features of MOF based ESIPT active materials along with some future prospects of such materials will be discussed.<sup>5</sup>

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Debajyoti Ghoshal did his PhD in 2005 from Indian Association for the Cultivation of Science, India. After that he worked at University of Göttingen, Germany, as an Alexander von Humboldt fellow to pursue his postdoctoral research. Presently he is a full Professor in Department of Chemistry, Jadavpur University and enthusiastically involved in teaching and research, since last twenty years. His current research focuses on functional metal organic frameworks with a special emphasis to the selective gas storage and separation, ESIPT-based sensing, proton conduction, and electrical conductivity. Concentrating on MOF design and exploring their diverse applications, he has published over 100 research papers so far, in various prestigious peer-reviewed journals.

# Task-specific Functionalization in Framework Materials for Environmental Remediation and Sustainable Catalysis

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## Abstract

As promising class of advance materials to address clean energy technologies, and environmental sustainability, metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) witnessed remarkable advances. With plentiful structures and topologies, their pore functionality engineering provide numerous advantages for targeted application. For example, pore-space-partitioning bifurcate larger channels into multiple smaller pockets for selective gas adsorption while dynamic structural alternation offers an effective mechanism for separating gas mixtures with similar properties. Alternatively, implantation of self-calibrating moiety allows fabricating high-level anticounterfeiting labels. Aiming at real-world applications, this lecture will cover the development of our approaches<sup>1-5</sup> on task specific functionalization in MOFs and COFs for tackling the global concerns like CCUS, water harvesting, acronym encryption, heterogeneous catalysis and environmental remediation (Figure 1).

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# Nanochannel-Assisted Organic Transformations in Metal–Organic Framework

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## Abstract

Atom economy, the use of catalysts and the use of safe or minimal solvents are key principles of green chemistry that appeal to chemists striving to minimize negative impacts on human health and the environment. In this work, we demonstrate the synthesis of several organic compounds—viz. cyanohydrins, cyclic carbonates, benzoxazoles, benzimidazoles, benzyldenemalononitrile and  $\alpha$ -aminonitriles—with excellent conversions using a simple metal–organic framework (MOF),  $\{\text{Mn}_2(1,4\text{-bdc})_2(\text{DMF})_2\}_n$  (**Mn-BDC**) (Scheme 1).<sup>1–3</sup> For most of these transformations, near-quantitative conversions (up to 99.9%) were achieved. The MOF catalyst exhibits remarkable robustness; our studies show that complete conversion can be maintained for up to 24 cycles during the synthesis of benzyldenemalononitriles. Theoretical calculations indicate that upon removal of coordinated DMF, the desolvated MOF undergoes an 18.2% increase in unit-cell volume, effectively opening its pore structure. This expansion likely facilitates the diffusion of small molecules into the nanochannels, enabling their activation by unsaturated Mn(II) sites (UMS). Overall, our investigations demonstrate that **Mn-BDC** is an economical, efficient, and robust catalyst that enables most reactions to proceed under solvent-free, greener conditions. Hence, catalysis with Mn-BDC can justifiably be regarded as “green.”

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Dr. Prakash Kanoo completed PhD in 2012 from JNCASR, Bangalore where he worked with Prof. Tapas Maji, a Shantiswaroop Bhatnagar awardee in Chemical Sciences in 2019. Dr. Kanoo has been awarded the prestigious JSPS fellowship in 2012 that enabled him to work with 2025 Nobel laureate Prof. Susumu Kitagawa at Kyoto University during 2012–2014. He has been awarded the UGC-DS Kothari fellowship and DST-Young Scientist Project in 2015 followed by an Early Career Research Award in 2017 by SERB. He had been an Associate Member of Royal Society of Chemistry. He joined Central University of Haryana as an Assistant Professor in the year 2016 and served there till 2024. In February 2024 he joined the Special Centre for Nanoscience, JNU, New Delhi as an Associate Professor where he is currently serving. Dr. Kanoo has published many research papers in reputed international journals and his papers are well cited. His *h* index is 23. His research interest are the design and synthesis of metal–organic frameworks and their applications in the field of adsorption, catalysis and drug delivery.

# Surface Functionalization of Hybrid Porous Materials for Next-Gen Applications (SFP Nex-Gen)

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## Abstract

Metal-organic frameworks (MOFs) have emerged as a promising platform for energy and environmental applications due to their highly tunable porosities, structural diversity, and multifunctionality. However, they face challenges related to limited chemical stability, poor electrical conductivity, and complex, often inaccessible pore structures. Nonetheless, surface modifications of MOFs can impart new hybrid materials with synergistic properties and functions, such as hydrophilicity, hydrophobicity, colloidal stability, hierarchical pores, enhanced stability and conductivity, and efficient host-guest electron/charge transfer. These attributes significantly enhance the performance of hybrid porous materials in various energy technologies, including catalysis, thermal-electro-photochemical CO<sub>2</sub> reduction, neuromorphic computing and triboelectric nanogenerators. In this presentation, I will discuss about our group recent research advances in surface functionalization and their synergistic effects. Finally, I will address the remaining challenges and limitations in the field while highlighting potential future research directions.

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# Using Molecular Building Block Approach Towards MOF Design for Sensing, Separation, and Catalysis Applications.

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## Abstract

Metal-organic frameworks have been utilized for various applications, including storage, separation, catalysis, carbon capture, and drug delivery. These properties are primarily a result of the fine-tuning of the MOF structure using suitable molecular building blocks (MBBs)—linkers and metal ions. The current discussion will focus on the design of new MOFs for environment and energy-related applications, which includes various UN SDGs such as **SDG 7**: Affordable and Clean Energy, **SDG 13**: Climate Action, and **SDG 3**: Good Health and Well-Being. My talk will discuss a lesser-known linker-design-based strategy to construct new Zr-based ultra-microporous MOF structure(s) for important separations such as CO<sub>2</sub>/N<sub>2</sub> separation, water/ethanol separation, and discriminative detection of aromatic vs. aliphatic amines. The separation of amines, in particular, is a tedious task due to their similar chemical properties. However, our design demonstrates that careful modulation of the linker design can result in a pore window size that is just right for separating aliphatic and aromatic amines. Continuing on similar lines, I will discuss another new Zr-MOF that has been designed for the selective conversion of CO<sub>2</sub> to CO. The MOF shows efficient photocatalytic conversion of CO<sub>2</sub> without the use of any noble metal or secondary photosensitizers. Operando Raman detects key intermediates (CO<sub>2</sub><sup>-</sup>, \*COOH, \*CO, formyl, and O-bound methoxy species), while DFT freeenergy profiles indicate a lower barrier via the \*OCOH pathway to \*CO relative to formyl formation, rationalising the observed CO selectivity. Lastly, another recent work on a RE-based MOF will showcase how the MOF topology can differ significantly when the same linker is used to construct both Zr- and RE-based MOFs.

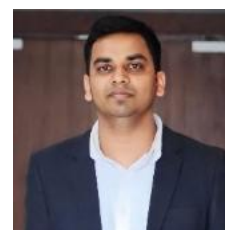
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# Bandgap Engineered Conjugated Porous Organic Polymers in Photocatalysis and Pollutant Removal

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## Abstract

Donor-acceptor (D-A) based porous organic polymers (POPs) have emerged as promising materials in photocatalysis due to their tunable electronic structures, bandgap, high surface areas, and efficient charge separation capabilities. These polymers leverage the strong intermolecular interactions between donor and acceptor units to facilitate charge transfer, thereby enhancing light absorption and catalytic efficiency. By incorporating diverse functional groups, one can tailor their bandgap and optimize redox properties for various photocatalytic applications, including hydrogen evolution, CO<sub>2</sub> reduction, and organic transformations. Also, photocatalytic degradation of toxic micropollutants has innate advantages compared to adsorptive removal, particularly converting them into non-toxic or value-added byproducts. Conjugated porous polymers are photoactive, and upon light exposure, they generate electrons/holes and various reactive oxygen species. We successfully demonstrated that triphenylamine-based D-A POPs can perform visible-light-driven oxidative hydroxylation of various phenylboronic acids to phenols with yields up to 96%<sup>[1]</sup>, selective detection of nitroaromatic micropollutants and their simultaneous photodegradation in water,<sup>[2]</sup> as well as atom refinement by two-fold single-atom substitutions (S→Se; C→N) in photocatalysis for the oxidation of thioanisole with >99% conversion and ~93% isolated yield.<sup>[3]</sup> Quinoid-locked dyes in porous polymers and conjugated polymers can degrade sulfur mustards photocatalytically.<sup>[4,5]</sup> Serendipitously, for the first time, we showed that BINOL-based POPs can photosynthesize large amounts of H<sub>2</sub>O<sub>2</sub> and degrade various micropollutants.<sup>[6,7]</sup>

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# Amine-Rich Metal–Organic Framework/Polymer Hybrid Interfaces for Non-Faradaic Capacitive Halide Sensing

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## Abstract

The continuous and selective detection of halides, particularly fluoride ( $F^-$ ), is of critical importance in biomedical and environmental monitoring. However, achieving real-time sensing in neutral aqueous media remains a major challenge due to the lack of stable, redox-independent platforms. In this work, we present a non-faradaic, capacitance-based fluoride sensor that exploits interfacial  $F^- \cdots H$  bonding chemistry at an amine-rich electroactive interface. Operating under ambient conditions, this system functions without any redox-active components, offering enhanced stability, reduced background signals, and continuous ON/OFF operation via voltammetric and impedimetric switching. The sensing interface is constructed by hybridizing polyethyleneimine (PEI) with a water-stable metal–organic framework (UiO-66-NH<sub>2</sub>) to enrich surface  $-NH/NH_2$  groups. The resulting MOF/PEI composite enables fluoride detection down to  $\sim 0.1$  ppm, far exceeding the performance of either component alone. The exceptional selectivity toward  $F^-$  arises from the unique strength of  $F^- \cdots H$  bonding, as weaker halides ( $Cl^-$ ,  $Br^-$ ,  $I^-$ ) fail to form a stable electrical double layer. Theoretical modelling confirms concentration-dependent stabilization of  $F^-$  at cationic amine sites, elucidating the molecular origin of the observed sensitivity. The sensor exhibits long-term operational stability ( $>25$  h) and maintains functionality across a wide concentration range (0.2 mM–30 mM), with successful validation in real tap and drinking water samples. This study introduces a new paradigm in non-faradaic electrochemical ion sensing, demonstrating how interfacial hydrogen-bonding and capacitance modulation can be harnessed for continuous, selective, and robust halide detection.

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Dr. Nivedita Sikdar joined GITAM university, Hyderabad campus, in 2022 as an assistant professor. She has received Alexander von Humboldt (AvH) fellowship and worked as senior scientist in Ruhr-University Bochum (RUB), Germany from 2019–2022. Before this, she was associated with University of Limerick, Ireland, as postdoctoral fellow in 2018. Dr. Sikdar received her PhD degree in Materials Science from Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), India in 2017, under Prof. Tapas Kumar Maji. Her research primarily focuses on the chemical synthesis and design of inorganic, organic, and hybrid materials to gain mechanistic insight into electrocatalytic and sensing processes. Specific areas of interest include CO<sub>2</sub> reduction, water splitting, biomass utilization and ion sensing.

# Metal–Organic Frameworks (MOFs) for Sustainable Energy and Environmental Solutions

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## Abstract

Over the past two decades, metal–organic frameworks (MOFs), a class of porous crystalline materials, have drawn significant attention. Their inherent crystallinity, ordered porosity, and molecular-level tunability have turned the concept of “designer solids” into reality. Owing to these unique features, MOFs have been extensively studied for applications ranging from gas capture and storage to catalysis, fluorescence, and chemical sensing. Our group aims to synthesise and explore MOFs to address challenges in clean energy technologies and environmental sustainability. In this talk, I will highlight recent advances in designing MOFs for the selective and sensitive detection of chemical analytes, where framework modification and nanoscale structuring, such as MOF nanosheets and nanotubes, can enhance signal response. I will also discuss the role of MOFs in electrocatalysis for overall water splitting reactions to produce green hydrogen. Finally, I will outline strategies for CO<sub>2</sub> utilisation using MOFs through thermal (photo) catalytic conversion into value-added chemicals. Overall, this illustrates how MOFs can serve as multifunctional materials at the intersection of sensing, catalysis, and sustainability, offering promising pathways toward energy-efficient and environmentally benign technologies.

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Dr. Monika pursued her Masters in Chemistry (2005-2007) and PhD in Materials Chemistry from IIT Delhi (2007-2012). She joined Institute of Nano Science and Technology, Mohali in the year 2014 as Scientist B and currently she is working there as Scientist D. Her area of research is Porous Framework materials for various applications in Energy and Environment. At present the research group focuses on the following areas: Developing new MOFs for sensing and electrocatalysis, CO<sub>2</sub> catalytic conversion to useful carbonates. They are also working on Polyoxometalate cluster based open framework materials and their various applications in energy and medicine.

# Coordination-Driven Framework Materials for Catalytic and Sensing Applications

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## Abstract

Framework materials (metal-organic frameworks, coordination polymers, and coordination polymer gels) are versatile due to their unique structural features. With active metal centers, functional ligands, and porosity, they enable efficient, sustainable heterogeneous catalysis. Their catalytic behavior includes intrinsic, induced, and hydrogen bond donor (HBD) activities. We incorporated Lewis acidic/basic sites, labile solvent molecules, metal nanoparticles, and HBD ligands to enhance performance in key organic transformations. Additionally, tunable soft coordination-driven gels were developed for catalysis, full-spectrum color display, security inks, and sensing. These materials can be tailored into flowing inks, self-healing gels, and self-sustaining shapes. The goal is to establish a fundamental link between structural features and catalytic and sensing activities.<sup>1-5</sup>

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# Advancing Porous Solids for Selective Carbon Capture and Utilization

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## Abstract

Drastic increase of CO<sub>2</sub> level in the atmosphere is a curse of technological advancement as CO<sub>2</sub> is the major contributor as greenhouse gases in current time. Porous solid materials are promising in this regard based on fast kinetics, reversibility and easy regeneration of the sorbents. In our research, we aim to develop porous solid materials, precisely metal-organic frameworks (MOFs) and polymers of intrinsic microporosity (PIMs) for carbon capture and utilization (CCSU). In my talk, I will discuss our recent development on PIMs and MOFs in CCSU. We have explored functionalization of the prototype material PIM-1 backbone, comparing simple primary amine to guanidine groups. While both performed similarly at high partial pressures of CO<sub>2</sub>, the addition of guanidine groups to the PIM-1 polymer provided enhanced CO<sub>2</sub> affinity relative to the parent and amine-functionalized materials at low CO<sub>2</sub> concentrations. Excellent performance and stability could be achieved by thermal cycling establishing PIM-guanidine as a promising candidate for scale-up for NGCC CO<sub>2</sub> capture. The second part of my talk will focus on how topology and/or morphology of zirconium MOF can be modulated through selection of appropriate modulators. I will discuss how rational structural design and morphological control of MOFs promote CO<sub>2</sub> utilization, providing insights into the development of functional materials for sustainable carbon management.

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# Mechanochemistry as a Tool for Disorder Engineering in Macromolecular Frameworks

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## Abstract

Mechanochemical synthesis exhibits enormous potential for the clean, economic, environmental-friendly and efficient route for the structural transformation of molecules and materials. Our recent work based on an attempt to design and synthesis of new phase pure Metal Organic Framework (MOF) materials by solid state hand grinding or ball mill method. Additionally, our research group also focused to do the ball mill induced mechanical engineering on the various MOFs to acquire new type of structures with unique properties. These types of approach are very rare and not attempted earlier in this area of research. We have developed a unique series of pure phase MOFs (ZnTIA-1mc, CuTIA-1mc and CoTIA-1mc) synthesized exclusively by mechanochemical (mc) grinding method (Figure 1). The same synthesis was also attempted in each case by using solvothermal procedure, which result the phase impure mixture of two different MOFs crystals. Kinetics study with the function of grinding time during the mechanosynthesis process revealed that the formation of variety of new metastable phases. Less crystallinity and short of mechanical defects in the structure of synthesized mechanochemical MOFs showed enhanced electrocatalytic activity towards oxygen evolution reaction (OER). In our next work, a novel zeolitic tertrazolate framework (ZTF-8) has been synthesized by green and facile mechanochemical ball mill method with exceptional acid/base stability. The structure of ZTF-8 adopts the zeolitic sodalite (SOD) topology with uncoordinated N-heteroatom sites and resembles with the structure of the well-known zeolitic imidazole framework ZIF-8. Directly used ZTF-8 is the unique report among all the MOFs for the selective electrochemical sensing of dopamine (DA) in the presence of highly concentrated common interferents. Additionally, ZTF-8 electrochemical sensor is the best among all the MOFs in terms of its ability to detect DA in a very wide linear range (5-550  $\mu\text{M}$ ) of concentration with excellent sensitivity. DFT study, strongly support our experimental result, revealed that the ZTF-8 framework has a higher binding energy and stronger interaction with dopamine than its isostructural ZIF-8 structure.

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# Accelerating the Discovery of Metal Organic Frameworks for Capture, Separation and Activation of Small Molecules

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Porous materials especially, coordination polymers (CP) or metal-organic frameworks (MOFs) have emerged as a special class of hybrid nanoporous materials. The variation of metal oxides and the vast choice of controllable organic linkers allow the pore size, volume and functionality of MOFs to be tailored in a rational manner for designable architectures. MOFs thus provide a wealth of opportunities for engineering new functional materials and are considered as versatile candidates for storage, separation, sensing, catalysis, drug delivery and other important applications. With ever-growing computational resources and advance in mathematical techniques, molecular simulations have become an indispensable tool for materials characterization, screening and design. At a molecular level, simulations can provide microscopic insights from the bottom-up and establish structure-function relationships. This presentation will highlight how molecular modelling combining with machine learning approach can be a powerful tool in complementing experiments and thus aid in designing of new smart porous materials for capture, activation and separation applications [1-5].

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Dr. Ravichandar Babarao is an internationally recognized materials scientist known for his contributions to porous materials, metal–organic frameworks, and energy- and sustainability-driven separations. A recipient of numerous prestigious awards including the Alexander von Humboldt Fellowship, ARC DECRA, and the Rennie Memorial Medal, his work has been widely cited and featured for its impact on clean energy, climate action, and sustainable technologies.

# Understanding Guest-Host Materials for Photocatalytic Carbon Dioxide Reduction Using NMR Crystallography

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## Abstract

Porous materials are relevant in the context of current efforts to establish a sustainable economy. For example, they are investigated as separators in electrochemical energy storage and conversion devices and as heterogeneous photo- and photoelectrocatalysts that improve the efficiency and atom economy of essential reactions like water splitting and carbon dioxide utilisation. The spatial and chemical constraints of the structured hosts enforce a shape to the adsorbed fluid phases and impose interactions at the guest-host interfaces.<sup>1</sup> If the dimension of the constraints reaches the nanometre scale, confinement effects on properties like mass and charge transport and the catalytic reactivity emerge. Recent results suggest that the complex interplay between the confinement-induced guest-host interactions and the mobility of the mass and charge carriers can lead to unexpected properties of the guest-host materials.<sup>2</sup> The lecture will provide an overview of our recent investigations on microporous metal-organic frameworks with coordinatively unsaturated sites (CUS) as photocatalysts for carbon dioxide reduction using visible light. In contrast to many oxidic semiconductors that produce a variety of species like carbon monoxide, alcohols and hydrocarbons, respectively, the investigated systems lead exclusively to formic acid. We applied an integral approach to analyse structural details, dynamic properties, and the catalytic activity by combining techniques like powder X-ray diffraction, sorption measurements, solid-state NMR, diffuse reflectance, and Mößbauer spectroscopy, and quantum chemical calculations. This allowed us to propose a reaction mechanism where the combination of preferred adsorption sites, that bind carbon dioxide in close proximity to the generated electron-hole pairs, and the protective environments, provided by the pore confinement, are essential elements for understanding the highly selective reaction pathway.

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# Harnessing hierarchical porosity in MOFs through the templated assembly of face-decorated platonic cages

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Developing innovative tools for the rational assembly of materials<sup>[1]</sup> is key in a field now fed by millions of yet to be made, hypothetical structures<sup>[2]</sup> for which simply combining the needed metal(s) and ligand(s) gives no success guarantee on the assembly of the desired product. We recently demonstrated that mastering *geometry mismatch*<sup>[3]</sup> with the use of pyridyl and imidazole based *centring Structure Directing Agents* (cSDA) allowed for the design and assembly of a series of 30+ sodalite (**sod**) based zeolite-like-MOFs (ZMOFs),<sup>[4]</sup> pseudo-polymorphs of the MIL-100/PCN-333 family with **mtn** topology. Because the discovery of hierarchically porous materials often relies on serendipity, and rational routes for their development are yet to be generalized, we further developed the cSDA approach with that goal in mind. We explored the structural diversity accessible through templating the assembly of readily accessible, face-decorated platonic metal–organic cages into hierarchically porous MOFs.<sup>[5]</sup> Archetypical MOFs were successfully synthesized through corner sharing of tetrahedral (Co-**sod**-ZMOF-539), cubic (Co-**red**-MOF-344) and octahedral (Co-**ydq**-MOF-24) cages. The potential of the approach for producing more intricate frameworks was further explored with the realization of Co-**hmc**-MOF-323 combining both tetrahedral and cubic cages. As envisioned, the physisorption isotherms and pore size distributions for these MOFs reflect both the microporosity of the platonic cages (with apparent BET area up to 5583 m<sup>2</sup>/g for Cr-**red**-MOF-344) and the mesoporous cavities (up to 5 nm wide in Co-**sod**-ZMOF-539) resulting from their predicted 3-periodic tiling. This work unlocks structural diversity deviating from typical default nets and paves the way for the systematic design of MOFs with tunable hierarchical porosity.

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Dr. Vincent Guillerm is a materials chemist specializing in the design and synthesis of porous materials, particularly metal–organic frameworks (MOFs) and related hybrid architectures. His research focuses on structure–property relationships and the development of functional porous solids for gas storage, separation, and catalysis, with contributions widely recognized in the MOF community.

# Porous Organic Materials for Energy and Environmental Sustainability

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## Abstract

Interfacial polymerization developing processable nanoporous organic thin films of crystalline covalent organic frameworks (COFs) could be promising for applications from molecular separation to energy storage.<sup>1,2</sup> In this context, we achieved a room-temperature transformation of an organic imine cage to a free-standing COF film at the aqueous-organic interface using an amine linker exchange strategy, producing highly porous and crystalline COF films in 24 h.<sup>3</sup> The COF film showed high permeance and excellent molecular sieving performance. Additionally, a 2D electrochromic COF (EC-COF) film having tunable redox functionalities was developed at the solid-liquid interface with broad absorption across the UV-to-NIR range, showing three-state anodic electrochromism, high color contrast (~60 % in the NIR), and fast switching.<sup>4</sup> A prototype device using the EC-COF film as a safety indicator for electronic circuits has been developed.<sup>4</sup> We further expand the scope of redox-active amorphous porous organic polymers in sodium-ion battery electrodes.<sup>2</sup> The key aspects of some of these findings will be presented.

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# Stimuli Responsive Magnetic Switching in Hofmann type of MOFs

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## Abstract

The development of molecular materials that can be switched between two different spin states through the application of external stimuli is of great interest owing to their potential use in molecular devices and information technology<sup>1,2</sup>. This switching behavior can be triggered by different reasons such as a charge/proton transfer, a change in the solid-state structure, or molecular orientation. When the *cooperativity* between spin centres is strong enough, a region of bistability opens, in which either of the two states can be found depending on the material's immediate past. This *memory* effect has been widely exploited in transition metal complexes for their potential application in magnetic data storage, spintronics, sensing etc. Some exciting recent discoveries<sup>3-6</sup> of spin-state switching in the Fe(II) based Hofmann type MOFs and Prussian Blue analogues (PBAs) in presence of external perturbation would be discussed in this presentation.

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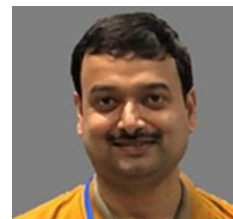
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He has published 180+ peer-reviewed journal articles, having ~7500 citations and an H-index of 49.

He currently serves as the international editorial board member of the Wiley journal *European Journal of Inorganic Chemistry*, MDPI journal *Magnetochemistry* and an associate editor of ACS journal *Crystal Growth and Design*.



# A $\pi$ -Conjugated COF as an Integrated Photoredox Catalyst for Energy/Electron Transfer–Driven Cross-Coupling Reactions

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## Abstract

Sustainable catalytic platforms are essential for advancing modern synthetic chemistry, particularly in the production of pharmaceuticals, agrochemicals, and fine chemicals. Although dual photoredox/transition-metal catalysis has transformed cross-coupling chemistry, its dependence on noble-metal photosensitizers, poor catalyst synchronization, and deactivation pathways—such as nickel-black formation—limits practicality and scalability. Semi-heterogeneous strategies offer partial improvement but still lack full recyclability. Covalent organic frameworks (COFs) have emerged as a compelling alternative due to their crystalline porosity, modular design, and intrinsic light-harvesting capacity. Their extended  $\pi$ -systems enable efficient energy and electron transport, while their structural tunability allows precise anchoring of redox-active centers. These features position COFs as highly promising materials for next-generation photocatalysis. In this talk, I will present our development of  $\pi$ -conjugated COFs as unified, recyclable photocatalysts for diverse light-mediated bond-forming reactions. Metalated COFs with engineered binding sites enable synchronized photoredox and transition-metal activity, delivering efficient C–N, C–C, and C–heteroatom cross-couplings while preventing common deactivation pathways. These frameworks consistently outperform their homogeneous counterparts and exhibit excellent durability. I will also discuss metal-free photocatalysis using olefin-linked COFs, which surpass imine-linked analogues in thioesterification, offering broad substrate scope and robust catalyst stability. Additionally, quinone-based COFs developed in our laboratory enable efficient photodecarboxylative fluorination and halogenation with wide functional-group tolerance and scalability in both batch and flow. Overall, this work demonstrates how rational COF engineering can integrate photosensitization, charge transport, and catalytic function within a single material, providing a sustainable platform for light-driven fine chemical synthesis.

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# Covalent organic frameworks for efficient organic transformations

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## Abstract

Covalent organic framework (COF) has recently emerged as a promising material for conducting organic transformations under visible light irradiation owing to their high tunability, large surface area and remarkable chemical stability. The low band gap of COF materials ensures visible light absorption which helps in effective charge transport. Utilizing the positive attributes of a framework material, we have been able to show that several challenging organic transformations can be conducted under milder conditions affording good yield of the desired products.<sup>1-2</sup> Interestingly, it sometimes shows significant improvement over their homogeneous analogues proving the utility of the extended framework in light harvesting, efficient charge separation, and charge transport. In this lecture multiple organic transformations will be highlighted involving amide formation directly from alcohol, isoindolonone formation from o-halo anilide where the COF matrix plays a critical role. Contrasting features to homogeneous catalysts and the scope of improvement in the heterogeneous framework will also be described and discussed.

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Dr. Debashis Adhikari is an associate professor at IISER Mohali. He started his career at IISER Mohali in 2016 after earning his Phd from Indiana University, Bloomington and conducting his postdoctoral research in Northwestern University, Evanston. His research interest spans on designing catalyst molecules from electronic structure understanding and studying detailed reaction mechanism. He is also interested in heterogeneous catalysis utilizing covalent organic frameworks. His group is involved in translating the small molecule reactivity to the extended frameworks that makes it more efficient employing milder reaction conditions. Debashis has published more than 90 research articles and recently became a recipient of CRSI Bronz medal.

# Application of MOF and Related Materials towards Energy Storage & Conversion

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## Abstract

The development of efficient and durable catalysts for hydrogen generation is a central challenge in the transition toward clean energy technologies. Among various chemical hydrogen storage materials, ammonia borane (AB) has attracted considerable attention due to its high hydrogen content (19.6 wt%), water solubility, and stability under ambient conditions. Despite these advantages, the catalytic hydrolysis of AB often suffers from high activation barriers and the simultaneous release of ammonia, which severely limits its practical implementation in fuel cells. Metal-organic frameworks (MOFs), have emerged as attractive platforms for designing advanced catalysts because of their high surface area, tunable pore architecture, and structural versatility. However, understanding how metal incorporation alters its pore network, stability, and catalytic activity remains an open challenge. In this talk we will discuss metal substituted MOF for AB hydrolysis, combining experimental and theoretical approaches to uncover how metal identity and pore architecture govern catalytic efficiency, stability, and ammonia mitigation. The structural and compositional integrity of the synthesized catalysts was confirmed by XRD, FTIR, TGA, SEM-EDX, and ICP-AES. XPS analysis revealed a clear difference in the chemical states of incorporated metals. To probe pore structure beyond surface area, the role of Positron Annihilation Lifetime Spectroscopy (PALS) will be discussed. Apart from that the application of MOF towards the cryogenic storage of hydrogen and gas sensing will also be discussed.

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Dr. Seemita Banerjee is a scientist at the Bhabha Atomic Research Centre (BARC), Mumbai, with research interests spanning functional materials, solid-state chemistry, and energy-related applications. Her work focuses on the synthesis and characterization of advanced inorganic and hybrid materials, with particular emphasis on structure–property relationships. She has contributed significantly to materials research through peer-reviewed publications and interdisciplinary collaborations within national research programs.

# Sustainable Chemistry with Glassy & Liquid Metal-Organic Frameworks

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## Abstract

Metal-organic frameworks (MOFs) are porous materials well-known for designability, highly ordered crystalline structure and host-guest chemistry.<sup>1,2</sup> Stemmed from these unique features, they have been extensively used for gas storage/separation, chemical conversions, pollutant removal, etc., greatly contributing to sustainable development. While crystallinity is not a prerequisite, studies on crystalline MOFs dominate the literature. Recently, Glassy and Liquid forms of MOFs have gained significant attention owing to their high degree of defect, disorder and are both fundamentally and functionally important materials.<sup>3</sup> The melting and glass formation phenomenon in MOFs have, introduced a fundamentally new category of glass-forming system.<sup>4</sup> The MOF glass and melt states partially retain the metal-ligand framework connectivity similar to the parent crystal. This offers a tool to transfer the designer framework chemistry of crystalline MOFs to their respective melt and glassy states and realize designer hybrid glasses otherwise inaccessible in addition to ease of processability.<sup>5</sup> Alternately, Porous Liquids (PLs) have recently emerged as an exciting new class of materials that merge the intrinsic, permanent porosity of solids with the dynamic fluidity of liquids, opening a design space that conventional solids or liquids alone cannot achieve.<sup>6</sup> This unusual hybrid nature has sparked wide interest because it enables properties that bridge molecular mobility with accessible free volume, offering opportunities in gas storage, separation, and catalysis.<sup>7</sup> In my talk, I will present some of our recent works on sustainable chemistry with the glassy and liquid states of MOFs.

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Prof. Sanjog S. Nagarkar is an Assistant Professor at the Department of Chemistry, Indian Institute of Technology (IIT) Bombay. He received his Ph.D. from the Indian Institute of Science Education & Research (IISER), Pune, India, under the supervision of Prof. Sujit K. Ghosh, where he developed MOF-based sensors for environmental applications. He then moved to Kyoto University, Japan, as a JSPS postdoctoral fellow to work with Nobel Laureate Prof. Susumu Kitagawa, where he developed MOF glasses for clean energy applications. At IITB, he leads the Framework Materials Lab (FML) focused on the development of various designer porous materials like Metal-organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), Porous Organic Polymers (POPs), etc., for industrially relevant applications. His group utilizes the reticular chemistry concepts to design task-specific porous solids, liquids and glasses for separation, storage and catalytic applications. Additionally, the group works extensively towards the development of greener and scalable synthetic processes for these porous materials. Prof. Nagarkar has been awarded the Dalton Horizon Prize (2025) for his contribution to hybrid MOF glass research.

# Exploring MOF/COFs as Next-Generation Materials for Room-Temperature Hydrogen Sensing

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## Abstract

Hydrogen is a clean, zero-emission energy carrier with immense potential to replace carbon-based fuels in the global transition toward sustainable energy. However, its high diffusivity and wide flammability range demand efficient and reliable hydrogen sensors to ensure safety in production, storage, and utilization. Among various sensing technologies, chemiresistive sensors are particularly attractive due to their simplicity, fast response, miniaturization capability, and cost-effectiveness. Conventional semiconducting metal oxides (SMOs) and Pd-based materials have been widely explored, yet issues such as poor selectivity, high operating temperatures, and limited long-term stability continue to hinder their practical application.

Recent developments in crystalline framework materials—namely metal–organic frameworks (MOFs) and covalent organic frameworks (COFs)—have opened new directions in hydrogen sensing. Owing to their high porosity, tunable pore architecture, and chemically designable active sites, these frameworks provide selective adsorption pathways and efficient hydrogen diffusion even at room temperature. Their modular chemistry enables incorporation of redox-active metal centers and functional linkers, imparting both sensitivity and selectivity while allowing operation in oxygen-deficient environments.

Furthermore, hybrid systems integrating MOFs/COFs with SMOs, noble metals, or carbon nanostructures combine the selective adsorption characteristics of frameworks with the excellent charge transport properties of inorganic materials. Such synergistic architectures represent a promising route toward the realization of selective, stable, and low-temperature hydrogen sensors. This presentation will highlight our recent findings on structure–property correlations highlighting design strategies, and future directions for achieving practical, room-temperature hydrogen detection technologies.

Include the Table/graphics here, if any.

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Dr. Suresh Babu Kalidindi obtained his PhD from the Indian Institute of Science (IISc), Bangalore, in 2010. Following his doctoral studies, he conducted postdoctoral research as an Alexander Humboldt fellow at Ruhr University, Germany, and later worked at the University of Liverpool as post-doc fellow. Upon returning to India, Dr. Suresh joined the Poornaprajna Institute of Scientific Research (PPISR), Bangalore, as a DST-INSPIRE faculty member. He subsequently served as a UGC-Assistant Professor at Andhra University before assuming his current role as Associate Professor at the Central Tribal University of Andhra Pradesh. Currently, Dr. Suresh and his research group focus on the hybridization of nanomaterials with porous framework materials, integrating reticular chemistry with nanoscience. This approach aims to develop new functional advanced materials with applications in clean energy, gas sensing, and nanocatalysis.





# Systematic Acceleration of Photocatalytic H<sub>2</sub>O<sub>2</sub> Generation using Conjugated Microporous Polymers

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## Abstract

The efficient utilization of solar energy to produce widely used hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) minimizes the challenges of current industrial chemical methods, allows on-site production, reduces the safety risks associated with its transport, and also the hazardous chemical waste.<sup>[1]</sup> Here, we discuss the designed approach of donor-acceptor conjugated microporous polymers (CMPs) as heterogeneous photocatalysts for systematic acceleration of photocatalytic H<sub>2</sub>O<sub>2</sub> production from natural water resources. The design involves a systematic change of donor and acceptor to realize an optimal band gap and efficient photocatalytic activity.<sup>[2]</sup> The donor-acceptor CMPs, namely TPA-BTz ( $E_g = 2.38$  eV), TPE-BTz ( $E_g = 2.59$  eV), and TPE-TTz ( $E_g = 2.41$  eV),<sup>[3]</sup> showed remarkably high photocatalytic H<sub>2</sub>O<sub>2</sub> rates in O<sub>2</sub>-saturated water (up to  $3.8 \times 10^3 \mu\text{mol g}^{-1} \text{h}^{-1}$ ), which significantly increased to  $54.7 \times 10^3 \mu\text{mol g}^{-1} \text{h}^{-1}$  in 10% benzyl alcohol/H<sub>2</sub>O (ca. 14-folds). The mechanistic scavenging experiments indicated the major role of superoxide radicals (O<sub>2</sub><sup>•-</sup>), and the production of H<sub>2</sub>O<sub>2</sub> occurs via an indirect two-electron O<sub>2</sub> reduction pathway. The transition state analysis and the reaction pathway were further supported by density functional theory (DFT) and *in situ* electron paramagnetic resonance (EPR) spectroscopy analysis. The CMPs exhibit similar photocatalytic H<sub>2</sub>O<sub>2</sub> efficiency with deionized and tap water. This study demonstrates the structure–property relationship of CMPs in photocatalytic H<sub>2</sub>O<sub>2</sub> production and highlights their potential as efficient, metal-free platforms for sustainable solar-to-chemical energy conversion.

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Dr. Venkata Suresh Mothika completed his PhD in 2016 at the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, with a thesis entitled “*Investigation on photophysical properties of nanoscale metal-organic frameworks and conjugated microporous polymers*” under the supervision of Prof. T. K. Maji. He was subsequently awarded the prestigious Alexander von Humboldt (AvH) postdoctoral fellowship and conducted research on “*conjugated microporous polymer thin film chemical sensors*” at the University of Wuppertal, Germany. He then moved to the University of York, UK, as a Newton International postdoc fellow, where he worked on redox-active, helically chiral organic mono and diradicals. In 2022, he joined the Department of Chemistry, Indian Institute of Technology Kanpur (IITK) as an Assistant Professor. Mothika’s group at IIT Kanpur is engaged in the development of porous organic polymer (POP) materials for applications in chemical sensing, capture, and photocatalysis. The recent research results were concentrated on conjugated microporous polymers (CMPs) for chemical sensing and capture of uranium (UO<sub>2</sub><sup>2+</sup>) from natural seawater and photocatalytic H<sub>2</sub>O<sub>2</sub> generation from natural water resources. We also work on  $\pi$ -conjugated persistent organic radicals, with particular emphasis on air-stable Blatter radicals. With our recent demonstration of conjugated Blatter radicals for enhanced electrical conductivities, we are actively developing a new class of Blatter radicals and their polymer thin films for applications in chiral organic electronics, spintronics, and beyond as long-term goals.

## Dual-Functional Organopolysulfide Frameworks Cathodes: Bridging Organic and



# Chalcogen Battery Chemistry

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## Abstract

Advancing toward future green energy storage calls for a shift to organic battery chemistry, which offers ecofriendly and energy-efficient alternatives to conventional toxic transition metal-based cathodes. By combining organic battery chemistry with chalcogen battery principles, we introduce Organopolysulfide Framework cathodes, which are periodic, covalently linked materials where polysulfides are directly integrated into the redoxactive organic backbone. These frameworks enable pre-designed structure and property relationships, allowing precise tuning of electrode performance while overcoming key limitations of existing sulfur-based batteries, including poor conductivity, slow charging, and sulfur dissolution. Unlike traditional sulfur cathode designs that rely on inert conductive carbon hosts, which do not store energy and often reduce practical energy density due to added inactive mass, the Organosulfide Framework itself is electrochemically active, storing charge as a cathode while improving charge transport and kinetics. Using operando Raman spectroscopy, we revealed the dual functionality of both the organic backbone and the integrated polysulfides, confirming efficient charge sharing and electronic communication within the framework. Cells with these cathodes paired with lithium metal anodes demonstrated superior performance compared to conventional lithium sulfur batteries. This Li-Organopolysulfide battery represents a new class of Metal Organopolychalcogenide Batteries, extendable to sodium, calcium, magnesium, and aluminum anodes, establishing a sustainable, high-energy, and tunable platform for nextgeneration green energy storage technologies.

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Dr. Sattwick Haldar is an Assistant Professor at IIT Tirupati, working at the interface of organic framework chemistry and sustainable energy storage. His research focuses on designing organo- and organopolysulfide frameworks as next-generation cathode materials, integrating organic and chalcogen battery chemistry to overcome limitations of conventional sulfur batteries. He has made key contributions to metal-organopolychalcogenide batteries and operando spectro-electrochemical studies, with publications in *JACS*, *Angewandte Chemie*, and *Advanced Materials*. Prior to joining IIT Tirupati, he was a postdoctoral researcher at TU Dresden and a Faraday Institution Fellow at Imperial College London.

## MOF-Derived Single-Atom-Catalysts for Energy Applications

## Abstract

Metal-organic frameworks (MOFs)-derived materials can have a range of carbon nanostructures where encapsulated metals play a crucial role in establishing the electrochemical structure-activity relationship. Single-atom-catalysts (SACs) have emerged as promising heterogeneous catalysts owing to their maximum metal utilization efficiency. These materials have been excellently utilized for various kinds of catalytic reactions, especially electrocatalysis. Transition metals (Fe, Co, Ni), atomically stabilized by N-doped carbons (M-N-C) are one of the most widely studied SACs. Oxygen reduction reaction (ORR), water electrolysis, CO<sub>2</sub> reduction or nitrate reduction are some of the developing catalysis areas where SACs are playing vital role for establishing structure-activity relationships. Their applications are broad. However, SACs are still suffering from their insufficient stability and metal loading issues. For example, Fe-N-C has highest intrinsic ORR activity, but noxious Fenton effect limits their long-term applications. Compared to SACs, dual-metal-atom catalysts coordinated with nitrogen atoms are more favorable for splitting O<sub>2</sub> bonds. Second metal atom not only tunes the electronic structure of active sites, but also synergistically boosts the catalytic performance of the catalysts. Similarly, coupling small metal nanoparticles with SACs not only enhances the metal loading but also solves the problem of instability. Herein, we have demonstrated the well-defined various SACs for highly efficient ORR and their applications in hydrogen fuel cell and metal-air batteries. X-ray absorption spectroscopy and density functional theory have been used to establish the SACs active sites and its behavior towards the activation of O<sub>2</sub> molecule at atomic level, respectively. This work may highlight interesting metal active sites for both fundamental research as well as practical energy applications.

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Dr. Arshad Aijaz is an Assistant Professor - Department of Energy & Human Sciences at Rajiv Gandhi Institute of Petroleum Technology (RGIPT) - Jais, Amethi, Uttar Pradesh. He completed his Ph.D. in 2011 from Indian Institute of Technology (IIT) Kanpur and subsequently moved to National Institute of Advanced Industrial Science and Technology (AIST) - Osaka, Japan for his first postdoctoral research work. He worked there till the end of 2014. He then worked at Ruhr University - Bochum, Germany till the joining of RGIPT (April 2017). Dr. Aijaz works mainly on MOFs, MOF-derived nanostructured materials, and their application in heterogeneous catalysis especially organic transformation and electrocatalysis. Currently, his research group is working on MOFs for organic reactions such as C-C or C-N couplings which require very harsh reaction conditions. Using MOF-derived electrocatalysts, especially single-atom-catalysts (SACs) are one of the topics, which is going in the group for the application of water splitting, oxygen reduction, selective CO<sub>2</sub> reduction, ammonia production, etc. Dr. Aijaz is receipt of several awards and fellowships which include Master of Science Gold Medal, JSPS postdoctoral fellowship, Humboldt postdoctoral fellowship, etc.

## Poster Presentations: Day 1, 12-01-2026

<b>P1</b>	Aarya Sharma	Scalable And Ultrafast Continuous Flow Synthesis of Uio-66 (Ce) MOF for Efficient Conversion of CO <sub>2</sub> Conversion to Cyclic Carbonates
<b>P2</b>	Aayush Anand	Engineering Multifunctional Mesoporous Polymer networks via Triazolinedione Click Chemistry for Environmental Remediation
<b>P3</b>	Abhijeet V. Kamble	1,1,6,6-Tetracyano hexatriene Linked Conjugated Microporous Polymer for High Photocatalytic Hydrogen Evolution
<b>P4</b>	Abhijith Das	Synthesis of novel DETA functionalized aluminium fumarate for the effective remediation of tetracycline form aqueous medium
<b>P5</b>	Abhilekha Borah	Visible-Light-Responsive g-C <sub>3</sub> N <sub>4</sub> /TiO <sub>2</sub> Heterojunctions Derived from MIL-125(Ti) for Efficient Hydrogen Evolution and Glycerol Oxidation
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<b>P9</b>	Ajay Ugale	Porosity-Driven Electrochemical Divergence in Structurally Isomeric 2D Metal-Organic Frameworks for Lithium-Ion Storage and release
<b>P10</b>	Akhil Chandran P	Design and development of redox active novel Metal-Organic Frameworks for efficient photocatalytic CO <sub>2</sub> reduction.
<b>P11</b>	Altaf Husain	Tuning Dimensionality and Linkage in Metal–Organic Frameworks for Enhanced Electrochemical Energy Storage
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<b>P13</b>	Amit Kumar	Metal-free Heptazine-based porous organic polymer for photocatalytic CO <sub>2</sub> reduction in water under non-sacrificial ambient conditions
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<b>P17</b>	Anagha H. Nair	Pioneering a Low-Cost Fluorescent Sensing Platform: A Stable

		ZIF-8 Framework for the Non-Invasive Detection of Urinary Biomarker in Cancer Diagnostics
<b>P18</b>	Anam Afaq	Design and Synthesis of Zn-based Metal Organic Frameworks (MOF) for Adsorptive Removal of Pharmaceutical Contaminants
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<b>P44</b>	Bitan Sardar	Metal-organic framework immobilized NNP-Fe pincer complex catalyzed selective monoborylation of methane
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<b>P47</b>	Chhaya Thadhani	Cobalt Catalyzed Selective Monoborylation of Methane
<b>P48</b>	Chithra K R	Plasma modified ZIF-8 incorporated PVDF membrane for efficient removal of antibiotics from water via crossflow filtration
<b>P49</b>	Debasis Pal	Post Synthetic Transmetalation and Water Induced Structural Transformation: The key Mediators in Proton Conduction by Metal-Organic Frameworks
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<b>P64</b>	Harshita Bagdwal	Unveiling the Role of Polyoxometalates in Oxygen Evolution: A pH-Resilient Molecular-to-Heterogeneous Catalytic Transition
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<b>P82</b>	Kishalay Biswas	Pore Engineering in Chemically Robust Porous Organic Polymer (POP) for Ultratrace Detection and Superior Sequestration of PFAS from Water
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<b>P84</b>	Komal Jiindal	Mechanistic Insights into Shape-Selective Molecular Recognition through Rotational Dynamics in MOFs using Ab-initio molecular dynamics
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<b>P94</b>	Meenakshi	Metalloligand-Based Metal-Organic Frameworks as Tunable Platforms for Visible-Light-Driven Photocatalysis
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<b>P107</b>	Neha Luhakhra	Wide range photoabsorption of PPy/g-CN for photocatalytic hydrogen production
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<b>P112</b>	Nitesh Kumar Das	MOF based Immunosensor For Ferritin
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<b>P115</b>	Partha Pratim Mondal	Site-memory-triggered reversible acronym encryption in a pore-partitioned MOF for ultrasensitive detection of organic pollutant over multiple platform
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<b>P138</b>	Ritu Rani	Polyimide Based Covalent Organic Frameworks (COFs) as a Fluorescence Sensor for Detection of Antibiotics and Picric Acid
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<b>P141</b>	Saandra	Hybrid Porous Material for Photocatalytic CO <sub>2</sub> Reduction
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<b>P145</b>	Satyapriya Nath	Revealing Wavelength Dependent Intrinsic Optical Properties of Covalent Organic Frameworks by Frequency and Time Domain THz Spectroscopy
<b>P146</b>	Sayantan Chongdar	Efficient Low-Overpotential Electrochemical CO <sub>2</sub> to Methanol Conversion Using Nickel-Based Hollow 0D Carbon Superstructures
<b>P147</b>	Shagun Kushwaha	Synthesis and Structure of Two Isostructural Lanthanide-Based MOFs with a Flexible Anthracene Ligand
<b>P148</b>	Shankar B.	MOF-Derived CoW-Alloy Carbon Nanotubes: A Trifunctional Electrocatalyst for Water Splitting and Zinc-Air Battery Applications
<b>P149</b>	Shanly Shajan	Metal-Organic Frameworks as Effective Nanocarriers for Targeted Anticancer Drug Delivery
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<b>P151</b>	Shovan Samanta	Correlating Phase Evolution and Optical Properties of Tin-based Metal Organic Framework Towards Reduction of CO <sub>2</sub> Using Visible Light
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<b>P169</b>	Supriti Dutta	Cationic Covalent Organic Framework for Photocatalytic Defluorinative Amination of Fluoroarenes



<b>P170</b>	Supriti Mahanta	Design and Functionality Engineering of Chemically Robust Porous Organic Polymer (POP) for efficient Sequestration of Highly Toxic $^{99}\text{TcO}_4^-$
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