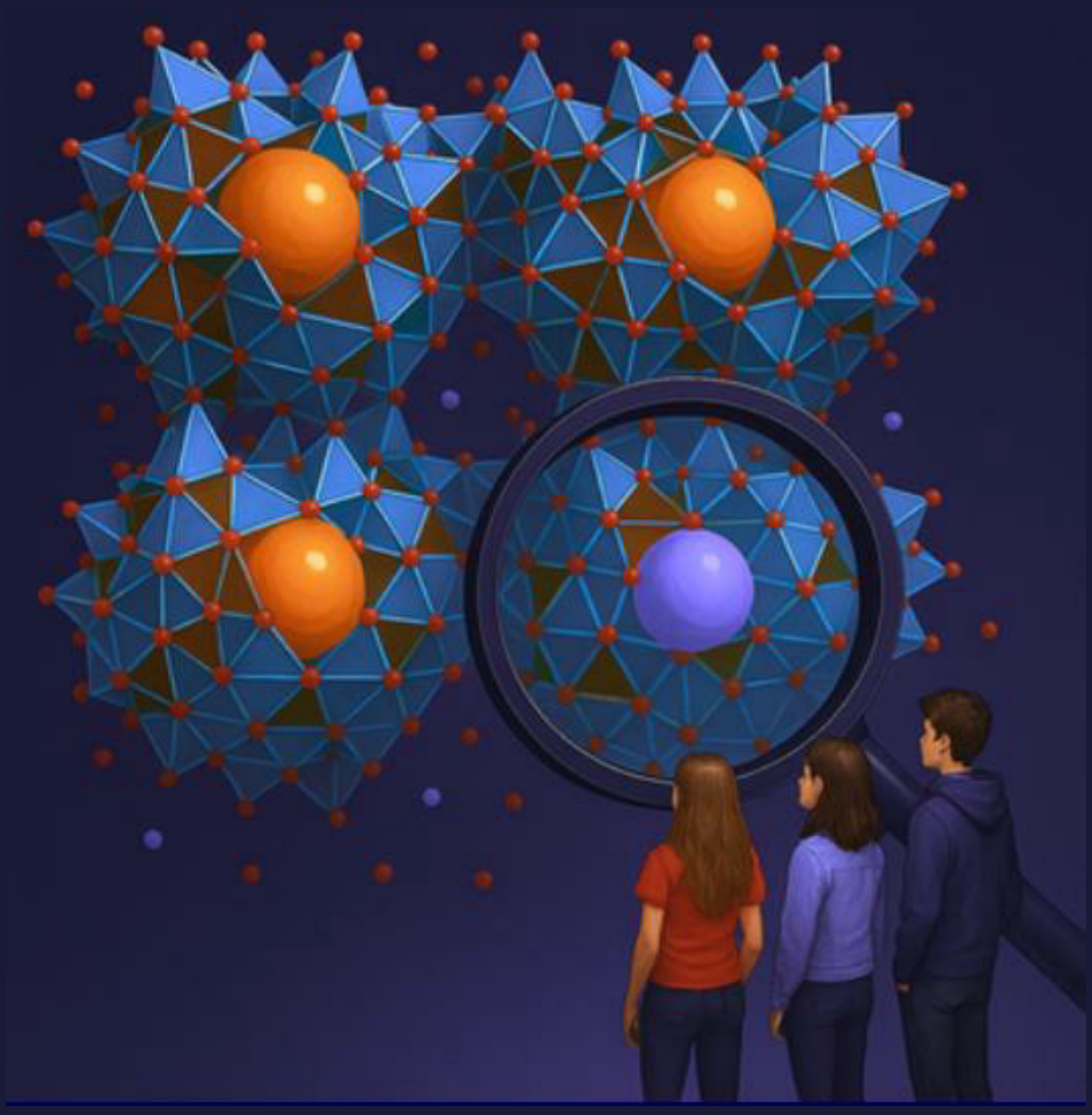
Young Investigator Forum at

12th International Symposium on the Characterization of Porous Solids (COPS XII)

2.05 - 3.05.2026
Dresden, Germany



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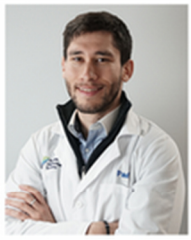

Paul Jacomi

Surface Measurement Systems, UK

Homare Arima

Kyoto University, Nishikyo, Japan

Eunji Jin

Dresden University of Technology, Germany

Registration:

Participation in the YIF is free of charge. Registration is required.

Registration form: https://tu-dresden.de/mn/chemie/ac/ac1/ressourcen/dateien/yif-cops2026/Abstract-template-YIF_COPS2026.docx

Contact:

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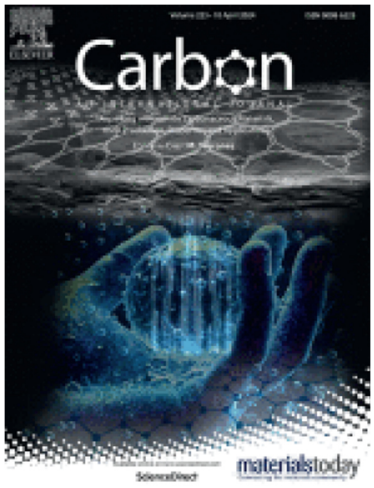


Venue & Locations:

Room S89 (Lecture hall no.1), Room 182
CHE Chemie, Bergstrasse. 66, 01069 Dresden

Venue: The conference will take place in the new buildings of the Department of Chemistry and Food Chemistry (Neubau Chemische Institute, Fachrichtung Chemie und Lebensmittelchemie, Bergstrasse 66, 01069 Dresden). These buildings are located on the TU Dresden campus.

To reach the campus from the main railway station ("Hauptbahnhof"), take bus no. 66 (direction "Freital/ Mockritz" and leave it at the station "Mommsenstrasse". Alternatively, you can also take tram no 3 (direction "Coschütz) and 8 (direction "Südvorstadt") and leave it at the station "Nürnberger Platz". You can also walk from the main railway station (ca. 20-30 minutes walking distance) for any further questions related to public transportation, see also: https://www.dvb.de/en-gb/

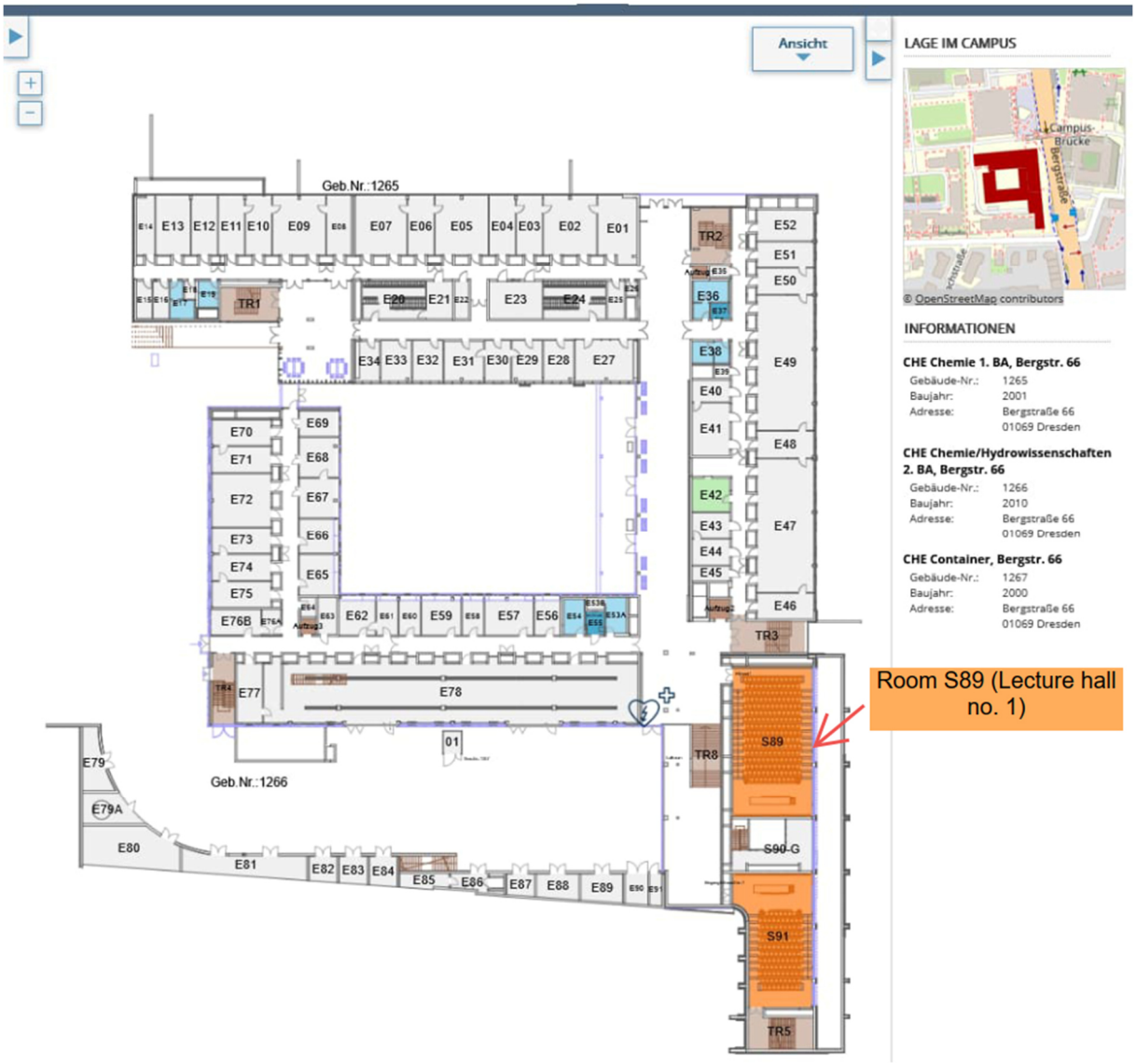
Locations: The lectures will be held in the lecture hall (room S89) on the building's ground floor.

Registration Room: Registration and Coffee can be found in Room 182

Poster Session: Room 183.

New building chemical institute

Ground Floor - Lecture hall no.1 (room S89)



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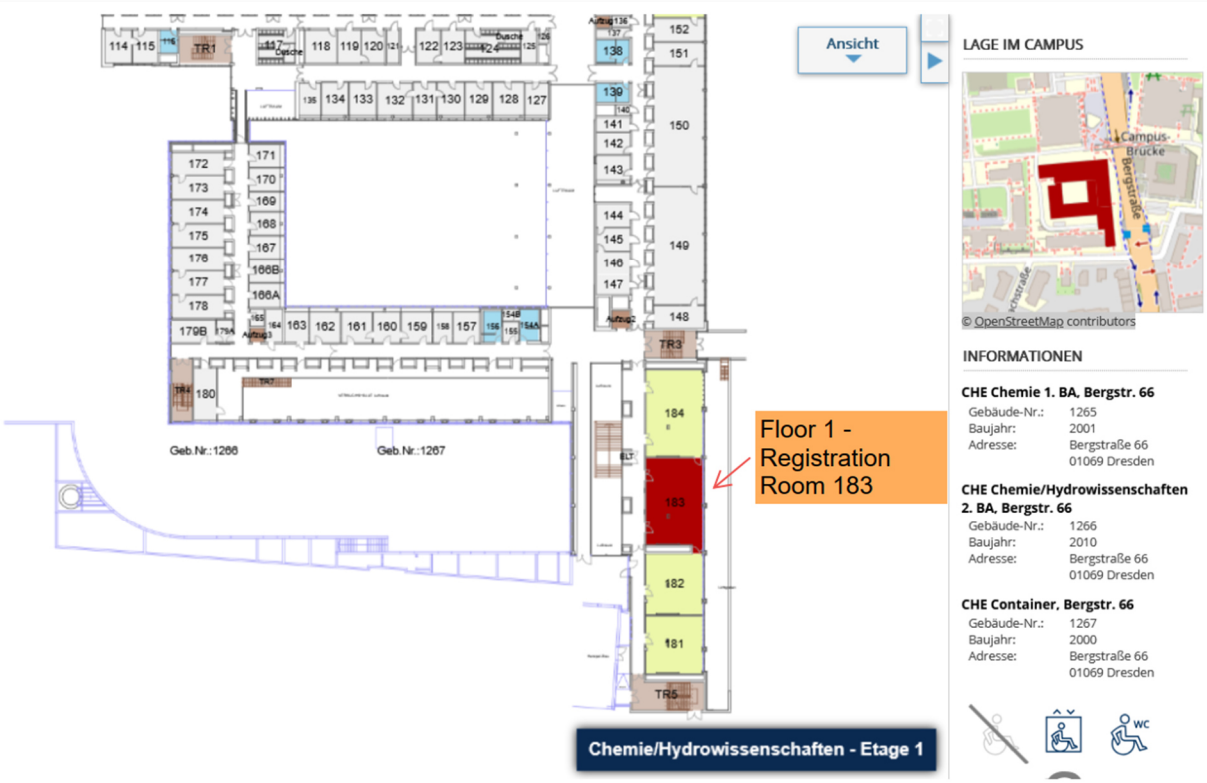
Floor 1 – Registration Room 182



Scientific Program, YIF COPS 2026

2 May 2026			
8:15 – 8:45	**Registration** (Room 182)		
08:45 - 09:00	**Welcome** (Room S89)		
Session 1: Chair: Dr. Javier Garcia Ben (Room S89)			
09:00 - 09:45	Plenary Lecture I	Matthias Thommes *Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, Germany*	Insights into the Adsorption and Phase Behaviour of Fluids in Nanoporous Materials: Towards an Advanced Textural and Surface Characterization.
09:45 - 10:00	Presentation	Adrián Gutiérrez Serpa *Universidad de La Laguna, Spain*	Advancing the Preparation of Porous Coatings based on Metal-Organic Frameworks for Solid-Phase Microextraction.
10:00 - 10:15	Presentation	Arooj Ahmed *Erlangen Center for Interface Research and Catalysis, Germany*	Creation of Surface Mesopores in Macroporous Silica *via* Partial Pseudomorphic Transformation.
10:15 - 10:30	Presentation	Rebecca E. Reber *Erlangen Center for Interface Research and Catalysis*	*In-situ* Monitoring of Metal-Organic Framework Synthesis.
10:30 - 11:50	**Coffee Break** (Room 182)		
Session 2: Chair: Dr. Eunji Jin (Room S89)			
11:50 - 11:05	Presentation	Charalampos Katsanakis *University of Southampton, UK*	2D Materials for Hydrogen Adsorption.

11:05 - 11:20	Presentation	Kornel Roztocki *Adam Mickiewicz University, Poland*	The impact of a single atom on MOF flexibility.
11:20 - 11:35	Presentation	Richard Engemann *Technische Universität Dresden, Germany*	In situ Insights into Cooperative Kinetic Enhancement via Solvent-Induced Restacking in a 2D Metal-Organic Framework.
11:35 - 11:50	Presentation	Léna Triestram, *PSL university, France*	Tools to identify and characterise phase transitions in ZIFs from molecular simulations.
11:50 - 12:05	Presentation	Preeti Bhauriyal, *Technische Universität Dresden, Germany*	Machine-Learning Prediction Of Anodic vs. Cathodic Suitability For CovalentOrganic Frameworks.
12:05 - 12:20	Presentation	Carmen Rosales Martínez *Universitat de València 1, Spain*	Defect-multifunctionalisation through multivariate modulation as a tool to enhance MOFs' environmental applications.
12:20 - 13:30	**Lunch Break** (Room 182)		
Session 3: Dr. Volodymyr Bon (Room S89)			
13:30 - 14:15	Plenary Lecture II	Camille Petit *Imperial College London, UK*	The Characterisation of Porous Solids for Application in Direct Air Capture.
14:15 - 14:30	Presentation	Paula G. Fraile *IMDEA Energy Institute, Spain*	Sustainable Production of IEF-40: A Scalable Iron-Squarate MOF for Efficient CO_2 Valorization.
14:30 - 14:45	Presentation	Sri Rezeki *Friedrich-Schiller University Jena, Germany*	Atmospheric Water Harvesting with Alkali and Transition Metal Containing Heteroatom-Rich Carbon Materials.
14:45 - 15:00	Presentation	Chloe Jacq *CNRS, France*	H_2O and CO_2 adsorption in different MOFs: experimental isotherms, heats of adsorption and their modeling.

15:00 - 15:15	Presentation	Anton Salomon *Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Germany*	Characterization of open porous metallic foams using conventional and nonconventional methods.
15:15 - 15:30	Presentation	Lei Liu *University of Science and Technology, China*	MOF-based Porous Water for CO_2 Capture
15:30 - 15:45	Presentation	Naveen Kumar *Immaterial Ltd, UK*	Decarbonising the World with monolithic MOFs.
15:45 - 16:05	**Coffee Break** (Room S89)		
16:05 - 17:15	**Roundtable Discussion:** „Future of porous materials“ Moderator: Dr. Paul Iacomi (Room S89)		
17:15 - 19:15	**Poster Session** (Room 183)		

3 May 2026			
Chair: Dr. Irena Senkovska (Room S89)			
09:00 - 09:45	Plenary Lecture III	Alexander Neimark *Rutgers University, USA*	Linking adsorption and pore structure properties of MOFs by molecular simulations.
09:45 - 10:05	**Coffee Break** (Room 182)		
Session 3. Chair: Dr. (Room S89)			
10:05 - 10:20	Presentation	Aleksandra Gerszendorf *Material Science and Engineering Centre, Poland*	A Strategy to enhance photon upconversion emisson in lanthanide MOFs.
10:20 - 10:35	Presentation	Timur Ashirov *University of Fribourg, Switzerland*	The Role of Shape-Persistent Macrocycles in Separation Applications.

10:35- 10:50	Presentation	Simon W. J. Dietzmann *Bundesanstalt für Materialforschung und -prüfung (BAM),* *Technische Universität Berlin, Germany*	A Pore or Not a Pore? Decoding Apparent Ultramicropores Through Site Specific Adsorption in Non-Graphitic Carbon and Atomically-Dispersed M-N-C Materials.
10:50 - 11:05	Presentation	Alexander E. Kurtz *Instituto de Nanociencia y Nanotecnología, Argentina*	Texture analysis of scalable green synthetized UiO -66-NH_2 MOFs with surfactants as mesoporous templates.
11:05 - 11:20	Presentation	Mohammed Shafeeullah *Technical University of Denmark, Denmark*	Thermal Evolution of Catalytically Active Nanoparticles from a 2D Zn-PorphyrinBased Metal-Organic Framework: In situ TEM Insights.
11:20 - 11:35	Presentation	Sara Talebi Deylamani *Technical University of Denmark, Denmark*	How Enzymes Reshape Porous Crystals: Direct Evidence of Nanocavity Formation in ZIF-L via Electron Microscopy.
11:35 - 12:00	**Closing remarks and Poster Prize** (Room S89)		

Plenary Lectures

Prof. Matthias Thommes

Department of Chemical and Biological Engineering, Friedrich-Alexander-Universität Erlangen, Germany

Prof. Camille Petit

Department of Chemical Engineering, Imperial College London, UK

Prof. Alexander Neimark

Department of Chemical and Biochemical Engineering, Rutgers University, USA

Insights into the Adsorption and Phase Behaviour of Fluids in Nanoporous Materials: Towards an Advanced Textural and Surface Characterization.

Prof. Dr. Matthias Thommes

Institute of Separation Science & Technology
Department of Chemical and Biological Engineering
Friedrich-Alexander University, Erlangen-Nürnberg /FAU)

Nanoporous materials (e.g. carbons, zeolites, metal organic framework materials, ordered and hierarchically structured meso-macroporous oxides etc.) have been the subject of extensive research targeted towards a wide range of applications because of their unique textural properties (e.g., increased surface area and the ability to customize the pore size and pore size distribution). In addition, unique nano-confinement effects, including shifts in the phase diagram of pore fluids and altered thermophysical properties, can be observed. In order to utilize effects of nano-confinement in various application areas (e.g., separation, catalysis, gas-energy storage), a detailed understanding of the interplay between effective fluid-fluid and fluid-(pore) wall interactions on the one hand and the effects of confined pore space and pore geometry/pore network on the other hand is required.
Within this context, we discuss important aspects associated with the adsorption-, phase- and wetting behavior of fluids in nanoporous materials and link these with recent advances in the development and application of advanced and novel adsorption methodologies for assessing key aspects of (i) their pore network characteristics (e.g., pore connectivity, characteristic parameters correlated with of pore network disorder/restrictions), and (ii) pore surface properties (e.g., hydrophobicity/hydrophilicity).

The Characterisation of Porous Solids for Application in Direct Air Capture.

Prof. Camille Petit

Department of Chemical Engineering, Imperial College London, UK

The use of adsorbents for direct air capture (DAC) of CO_2 is regarded as a promising and essential carbon dioxide removal technology to help meet the goals outlined by the 2015 Paris Agreement. It is a challenging process due to the ultra-dilute concentration of CO_2 in the air (~0.04%$_{vol}$ or 0.4 mbar) and varying ambient conditions (i.e. temperature and relative humidity), but it offers a route towards long-term carbon storage and allows the amount of CO_2 captured to be quantitatively measured.

Porous materials, particularly metal-organic frameworks (MOFs), zeolites, and porous polymers, have gained significant attention for this application. To properly assess these adsorbents at scale, adsorbent screening should be conducted using key performance indicators determined from process modeling and optimization (i.e. purity, recovery, productivity, energy consumption). To facilitate such process scale evaluation, various adsorbent properties are required, such as: equilibrium isotherms of all relevant species, heat and mass transfer coefficients, porosity, density (skeletal, particle, bed), heat capacity, and heat of adsorption.

In this presentation, we will cover the properties of porous materials to be quantitatively assessed for the application in DAC, how these properties impact the DAC process, and the techniques used to acquire them. This will be done via examples. Some of the discussion points could be more widely extended to the application of porous materials for any gas separation.

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Linking adsorption and pore structure properties of MOFs by molecular simulations.

Prof. Alexander V. Neimark

Department of Chemical and Biochemical Engineering, Rutgers University, USA

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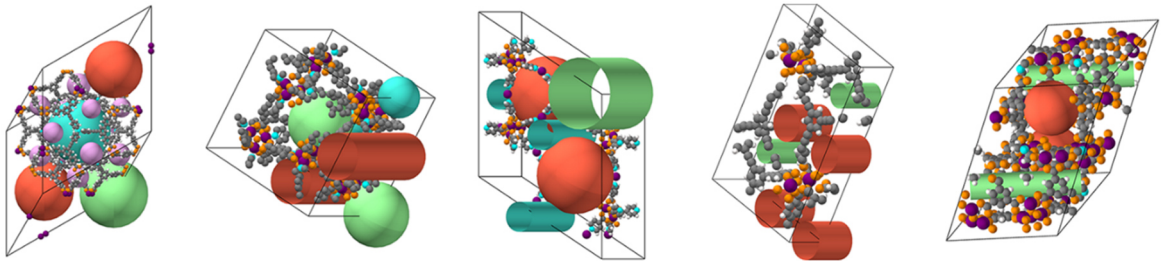
The recent Nobel Prize recognizing the inventors of Metal-Organic Frameworks (MOF) has sparked renewed overarching interest in these fascinating materials. Built of metal complexes connected by organic linkers into three-dimensional porous crystals, MOFs can selectively adsorb, separate, release, transport, or block various chemical and biological species. Their intrinsic framework flexibility enables the design of compliant molecular sieves, membranes, sensors, and actuators. The unique engineering properties of MOFs arise from the interplay of the chemistry of their building units and the morphology of their pore structure, both of which can be tailored for particular applications. Gaining a fundamental understanding of the physical mechanisms that couple adsorption, structural response, and mechanical behavior is essential for advancing the design, fabrication, quality control, and practical deployment of MOF-based materials. In this lecture, I will illustrate, through several examples from our recent research, how the advanced statistical mechanics and molecular simulation methods help elucidate the fundamental structure-property relationships and provide important practical insights of direct relevance to MOF materials engineering.



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- Parashar, Corrente, and Neimark, Unveiling Non-Monotonic Deformation of Flexible MOFs during Gas Adsorption: From Contraction and Softening to Expansion and Hardening, JCIS, 2025, 606, 88.
- Neimark, Corrente, and Coudert, Phase Transformations in MOFs Induced by Adsorbate Exchange. Langmuir, 2025, 41, 4720.

List of Abstracts (Oral & Posters):

Abstracts of Oral Presentations

Plenary Lectures

Session1

Abstracts of Posters

Abstracts of Oral Presentations

ADVANCING THE PREPARATION OF POROUS COATINGS BASED ON METAL-ORGANIC FRAMEWORKS FOR SOLID-PHASE MICROEXTRACTION

A. Gutiérrez-Serpa,[a,b] I. Negrín-Santamaría,[c] M.J. Trujillo-Rodríguez,[b,c] J. Pasán[a], and V. Pino[b,c,d]

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[b]*Unidad de Investigación de Bioanalítica y Medio Ambiente, Instituto Universitario de Enfermedades Tropicales y Salud Pública de Canarias (IUETSPC), ULL, 38206, San Cristóbal de La Laguna, Spain*

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Keywords: *metal-organic frameworks, coatings, miniaturization, extraction*

Porous materials, such as metal-organic frameworks (MOFs), have attracted special attention in extraction technologies. The outstanding properties of MOFs, such as high specific surface area, synthetic versatility, and structural tunability, have boosted their use as extraction sorbents for analytical strategies. The use of MOFs in a miniaturized extraction mode termed solid-phase microextraction (SPME) has involved a step forward in the technique, expanding its applicability. SPME is a miniaturized technique that involves the use of a microfiber coated with an active extraction phase, widely used due to its simplicity, the possibility of automation, and the high preconcentration that can be achieved. Main drawbacks of conventional SPME include low selectivity and stability of the commercial coatings, limited to organic polymers. Thus, the incorporation of MOFs as substitute coatings has noticeably improved the performance of the SPME fibers. Nevertheless, the preparation of robust MOF-based coatings is certainly challenging. This study explores an innovative approach for the preparation of robust porous SPME coatings based on MOFs over a functionalized silver support. Besides, a braided configuration support was used to increase the accessible surface area for the MOF coating. The sustainable MOF CIM-80(Al) was selected in this study, consisting of mesaconic acid and aluminum. As proof of concept, the MOF-based fiber was successfully applied for monitoring polycyclic aromatic hydrocarbons and aliphatics in human breath and car pipe exhaust by headspace SPME with gas chromatography and mass spectrometry.

Acknowledgement: This work was developed within the scope of the projects Ref. PID2023-147246OB-I00 funded by MICIU/AEI/10.13039/501100011033/ERDF, EU. M.J.T.-R. thanks her current Ramón y Cajal contract (ref. RYC2021-032502-I) at Universidad de La Laguna, contract with funding of the Spanish Ministry of Science and Innovation MCIN/AEI/10.13039/501100011033 and the European Union «NextGenerationEU»/PRTR; and both MCIN/AEI and Universidad de La Laguna for the additional funding related to the contract.

Creation of Surface Mesopores in Macroporous Silica via Partial Pseudomorphic Transformation

Arooj Ahmed[a], Carlos Cuadrado Collados[b], Tadahiro Yokosawa[c], Erdmann Spiecker[c], Matthias Thommes[b], Nicolas Vogel[d], Alexandra Inayat[a], Martin Hartmann[a]

[a] *Erlangen Center for Interface Research and Catalysis (ECRC)*
[b] *Institute of Separation Science and Technology*
[c] *Institute of Micro- and Nanostructure Research (IMN) & Center for Nanoanalysis and Electron Microscopy (CENEM)*
[d] *Institute of Interfaces and Particle Technology Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg*

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Keywords: *Porous glass beads, partial pseudomorphic transformation, hierarchical materials, C_{16}TAOH, surface structuring*

In this study, partial pseudomorphic transformation was employed to structure the pore walls of macroporous silica and to introduce surface mesopores. Cetyltrimethylammonium hydroxide (CTAOH) is used as structure directing agent (SDA) and macroporous silica (initial pore diameter ~140 nm and macropore volume ~0.96 $cm^3\ g^{-1}$) as silica source. A graded degree of partial pseudomorphic transformation between 0 to 80% was attained by adjusting the synthesis conditions (hydrothermal treatment time, silica to CTAOH ratio and concentration of CTAOH). The transformed material was analyzed by nitrogen physisorption at 77 K, water adsorption at 298 K, scanning electron microscopy (SEM), scanning transmission electron microscopy (STEM) and mercury porosimetry. The nitrogen physisorption at 77 K showed that specific surface area increased gradually from 16 $m^2\ g^{-1}$ to 107 and 907 $m^2\ g^{-1}$ and mesopore volume from 0 $cm^3\ g^{-1}$ to 0.1 and 0.82 $cm^3\ g^{-1}$ as the transformation degree increased from 10 to 80%. The creation of surface mesopores of ca. 4 nm in the macropore walls of the parent material was verified by nitrogen physisorption at 77 K and STEM. The water adsorption at 298 K exhibited the creation of ordered mesopores without the presence of substantial microporosity. Mercury porosimetry confirmed the preservation of initial macropore diameter, while SEM proved the preservation of the initial macroporous architecture and macroscopic shape of the parent material. The mentioned results revealed the pseudomorphic transformation of macroporous silica i.e., by maintaining the initial pore structure and macroscopic shape of the parent material into micellar templated silica (MTS) with hierarchical porosity which could be a potential support for e.g., catalysts in supported ionic liquids. Such macropores will provide efficient mass transfer and surface mesopores will anchor the ionic liquid film to help forming the wetting layer on the surface and result into enhanced catalytic activity.

In-situ-Monitoring of Metal-Organic Framework Synthesis

Rebecca E. Reber, Louis Rupprecht, Marcus Fischer and Martin Hartmann

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Keywords: *Ultrasound, In-Situ*

The controlled crystallization of metal–organic frameworks (MOFs) driven by the interplay of nucleation processes and growth remains a major challenge in materials chemistry. Many MOF syntheses proceed through multiphase systems in which transient intermediates and short-lived prenucleation species strongly influence the final material properties yet are difficult to probe experimentally. This complexity highlights the need for analytical approaches capable of providing robust, non-invasive, and time-resolved insight into MOF formation under realistic synthesis conditions [1].

This study demonstrates that ultrasound monitoring provides detailed insight into MOF syntheses. By sending an ultrasound pulse through the reaction mixture and analyzing both echo attenuation and sound velocity, the formation of particles can be tracked in real time. A deeper understanding of the underlying synthesis parameters ultimately enables the targeted tailoring of particle properties. This study demonstrates that ultrasound attenuation is especially responsive to the particle size of MOFs. In addition, examining the solvent systems employed for the synthesis of HKUST-1 and ZIF-8 highlights the significant role of water in determining both the crystallization mechanism and the final particle sizes of the formed MOFs [2].

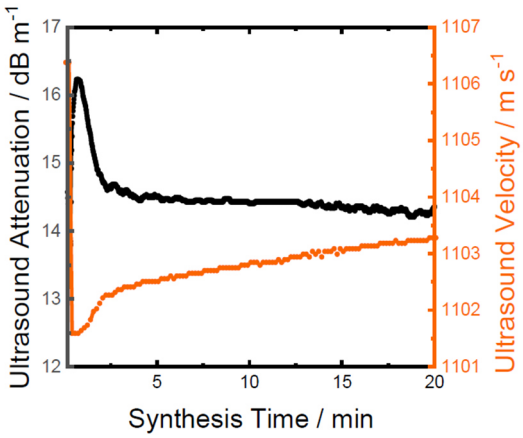

Figure 1 Exemplary progression of ultrasound velocity and attenuation of a ZIF-8 synthesis

Overall, this study demonstrates the power of ultrasound monitoring as a robust, accessible, and highly sensitive tool for in-situ tracking of MOF crystallization. More broadly, the results highlight how solvent selection can be leveraged to tune nucleation kinetics, contributing to a more systematic understanding of MOF synthesis and enabling more rational process design and optimization.

References

[1] M. Ermer, R. Reber, H. Baser, M. Fischer, W. Schwieger, M. Hartman, Crystal Growth & Design, **2023**, 23, 5355-5367.

[2] R. E. Reber, L. Rupprecht, M. Fischer, M. Hartmann, *ChemRxiv*, **2025**, submitted for publication.

2D Materials for Hydrogen Adsorption

Charalampos Katsanakis[1], Mohamed-Hassan Sayed[1] and Nuno Bimbo[1]

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Fossil fuel reserves are finite [1], and their combustion causes several environmental problems. Sustainable green hydrogen could be an excellent tool to decarbonise our economies and as such it is already used in many industrial applications such as cleaner NH_3 production [2], more sustainable hydrocracking of heavier into smaller hydrocarbons [3] and CH_3OH production [4], among others. Hydrogen has also been proposed as a clean fuel, especially in fuel cell vehicles [4]. Hydrogen has many advantageous properties if used as a fuel, including its high gravimetric energy density (120 MJ/kg), the most of any chemical fuel. However, at ambient conditions, hydrogen has insufficient volumetric energy density compared to fossil fuels[5]. Current materials lack the operational and storage requirements that are needed for hydrogen proliferation in industry. High hydrogen uptake is only possible in high-surface area materials like metal organic frameworks [6], activated carbons [7], and porous organic polymers [8] at cryogenic temperatures. There is thus a need for high surface area solid sorbents, with tuneable porosity, and hydrogen uptake at reasonable pressures and temperatures.

MXenes, a class of two-dimensional lamellar materials have excellent performance when used in Li-ion batteries and supercapacitors, due to their intercalation charge storage mechanism [9]. MXenes can host other positive ions like ammonium precursors or even amines [10-12] to increase their interlayer distance and create porosity within the materials. MXenes have also been proposed as prospective hydrogen storage materials, as the interlayer spacings can be tuned to maximise interactions with molecular hydrogen [13, 14]. In this work, a variety of organic intercalants (amines, ammonium salts, silica) and thermal treatments are employed to increase the surface area of MXenes and maximise H_2 gas uptake. The resulting materials are characterised with a range of techniques, including powder X-ray diffraction, scanning electron microscopy, elemental analysis and nitrogen adsorption. Different synthetic strategies lead to different interlayer spacings (which can be controlled depending on the intercalant), different BET surface areas and different pore size distributions. To our knowledge, the silica templating method with a high BET surface area (> 500 m^2 g^{-1}) is first demonstrated on the context of hydrogen adsorption. Hydrogen adsorption on the materials is measured under a wide range of temperatures and up to 200 bar, along with their surface properties to reveal their performance under diverse conditions and explore their potential for real-world applications.

References:

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The impact of a single atom on MOF flexibility

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Keywords: *flexibility,separation, structural transformation, in situ*

Flexible metal-organic frameworks (MOFs) are porous materials exhibiting spatiotemporal responses to environmental changes, which significantly affect their sorption properties and offer potential technological breakthroughs.[1] In this study, we investigate two isostructural thiazolo[5,4-d]thiazolate MOFs, UAM-1S and UAM-1O, which differ by a single atom, sulphur or oxygen, in the angular dicarboxylategroup.[2] Despite this subtle modification, the materials trigger distinct structural adaptation mechanisms: a continuous in UAM-1S and a discrete in UAM-1O.

Using a combination of experimental and theoretical approaches, including MicroED and DFT analysis, we reveal the factors driving different transition mechanism.[3] Appropriate treatment of UAM-1O, combined with SC-XRD analysis (**Figure 1**), revealed the structure of explosive metastable open phase, corroborating theoretical predictions. Furthermore, a timeresolved in situ powder X-ray diffraction dataset was collected under varying CO_2 at pressures exceeding the cp-op structural transition pressure at 195 K, enabling the application of the Kolmogorov–Johnson–Mehl–Avrami equation to analyze the kinetics of adsorption. Holistically, this work enhances the understanding of the key factors responsible for the time-dependent response of flexible materials, with implications for the design of dynamic materials.

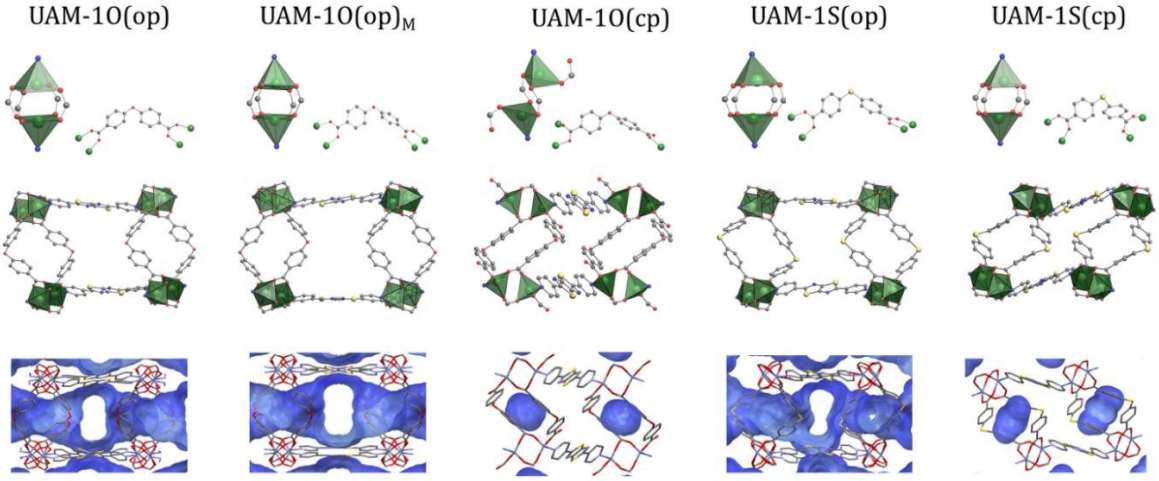

Figure 1 Comparison of single crystal structures of open pore phases and desolvated phases.

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In situ Insights into Cooperative Kinetic Enhancement via Solvent-Induced Restacking in a 2D Metal-Organic Framework

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Keywords: *MOF, ligand exchange kinetics, in situ characterization, isotope labelled ligand*

Understanding reaction kinetics at catalytically active sites is crucial for integrating catalytic 2D materials into industrial processes. This study focuses on *in situ* observation of ligand exchange kinetics and solvent-assisted structural restacking transition in the 2D paddle wheel based MOF $[Cu_2(dttc)_2]_n$ (DUT-134(Cu)[1,2]). The ligand exchange process, involving the replacement of dimethylformamide (DMF) with nitriles was investigated using fast *in situ* characterization techniques, including powder XRD and Raman spectroscopy. Bulkier substrates exhibited reduced exchange rates, consistent with enhanced steric hindrance and greater diffusion constraints.

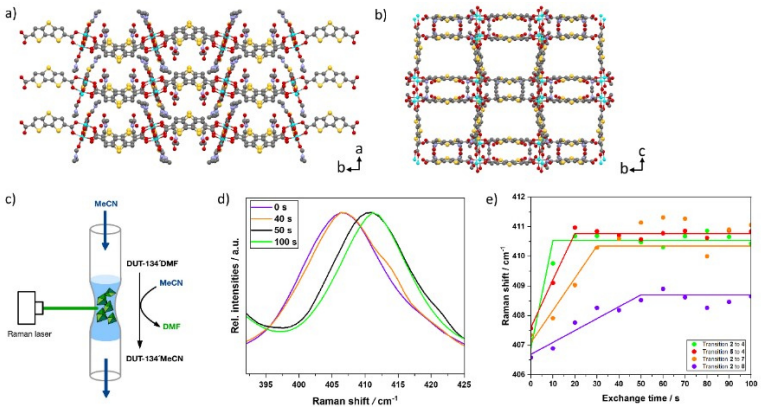

Figure 1: (a,b) Crystal structure of DUT-134; (c) Illustration of in situ Raman experiment; (d) Raman peak of Cu-O stretching band during solvent exchange; (e) Wavenumber of the Cu-O Raman band during solvent exchange of DMF to ACN (green), DMF to ACN after one cycle (red), to pentanenitrile (orange), and to heptanenitrile (purple).

Interestingly, the study revealed that the exchange of DMF with ACN induces a second-timescale structural transition to higher symmetry and a transition from AB to AA stacking mode of the layers. This structural transition dramatically accelerates the solvent exchange process through cooperative effects, offering advantages for catalytic applications. The reverse exchange from ACN to DMF proceeds more slowly and does not reverse the structural changes, but a new phase is formed with preserved AA stacking. By isotope labeling of linker molecules in combination with two complementary theoretical vibrational simulation methods, the precise assignment of Raman bands and the vibrational modes associated with the ligand-exchange process could be achieved.

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Tools to Identify and characterise phase transitions in ZIFs from molecular simulations

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Keywords: *MOFs, machine learning potential, phase transtions, polymorphs*

Zeolitic Imidazolate Frameworks (ZIFs) are a family of metal–organic frameworks composed of metal clusters bridged by imidazolate linkers. In this work, we are interested in simulating ZIFs based on Zn^{2+} ions. There exists several known topologies of this class of materials, most of them crystalline, but it is also known to feature amorphous structures which retain a high porosity. Many of these polymorphs have been characterised both experimentally[1] and in silico[2]. Working on transitions between these phases allows us to explore the mechanisms of the rearrangement of the structure during these processes. We use a Machine Learning Potential (MLP) we generated, based on the MACE architecture[3] to simulate several phases of this material as well as phase transitions. We first present the simulation protocols: a melt-quench simulation which generates atomistic glass models from the ZIF-4 crystal and a simulation of the transition between two known phases: ZIF4 and ZIF-4-cp-II. The simulated structures need to be rigorously characterised; we thus used and developed methods to identify these phases. We present a neural-network classifier based on the local SOAP descriptor[4]. Another way to classify phases is by using rings which are defined as closed loops with alternating imidazolate/cation. With these rings, we are able to see the change in topology (i.e., bond breaking or formation) as well as the change in the rings' shapes for transitions which do not involve topological changes. These tools are used as means to pinpoint phase transitions in the simulations.

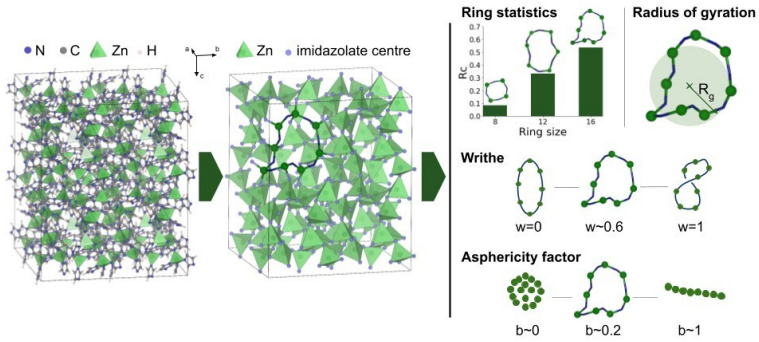

Figure 1 *: Several methods based on rings can be used to characterise phases in ZIFs*

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MACHINE-LEARNING PREDICTION OF ANODIC VS. CATHODIC SUITABILITY FOR COVALENT-ORGANIC FRAMEWORKS

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Keywords: *COFs, Metal-ion batteries, Anode and Cathode, Machine learning*

Covalent organic frameworks (COFs) are promising organic electrodes for metal-ion batteries,[1,2] but the design rules that determine whether a COF behaves as an anode or a cathode remain unclear.

Here, we develop a data-driven screening workflow that combines DFT and interpretable machine learning to classify experimentally synthesized 2D CoRE-COFs and identify high-performing candidates. We curate 137 chemically diverse COFs and compute open-circuit voltages and accessible capacities using a sequential Li^+ insertion voltage-profile protocol. Using structure- and chemistry-based descriptors extracted from experimental crystal structures, ensemble XGBoost classifiers achieve strong predictive performance (ROC–AUC up to 0.92 for voltage; ~0.82 for capacity >200 mAh g^{-1}). Feature analysis shows that anode/cathode character is primarily controlled by local coordination environments of redox-active N/O sites and proximal heteroatoms, whereas capacity is dominated by unit-cell metrics and redox-site density. Screening the full CoRECOF space yields actionable design rules and DFT-validated anode and cathode candidates for next-generation batteries.

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Defect-multifunctionalisation through multivariate modulation as a tool to enhance MOFs' environmental applications

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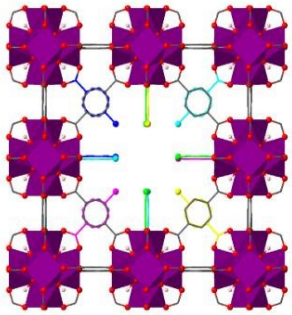
Keywords: *MTVM MOFs, Defect Multifunctionalisation, water treatment…*

Multivariate Metal–Organic Frameworks (MTV MOFs)[1] [2] are hybrid materials that incorporate multiple linkers or metals within a single crystalline structure. These porous materials have attracted significant interest due to their unique properties, which arise from synergistic effects rather than a simple combination of individual components.

While conventional multivariate MOFs (MTV MOFs) rely on the direct incorporation of multiple linkers or metals, multivariate modulation (MTVM) provides a more versatile and controllable strategy. By introducing functional diversity through modulators, MTVM enables the simultaneous tuning of framework chemistry and defect concentration, promoting cooperative effects between functionalities and enhancing porosity. This added level of control makes MTVM particularly attractive for applications where adsorption performance and selectivity are critical.

These synergistic effects enhance adsorption performance, making MTVM MOFs particularly promising for the removal of contaminants from water and air. By combining multiple functionalities within a single framework, complementary interactions with target molecules improve both selectivity and uptake.



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Sustainable Production of IEF-40: A Scalable Iron-Squarate MOF for Efficient CO_2 Valorization

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Keywords: *CO_2 valorization, MOF-based catalyst, Defect engineering, MW-assisted synthesis.*

The chemical valorization of CO_2 into value-added products is a key challenge in sustainable chemistry. In this work, we present the development of IEF-40 (or FJUT-3(Fe)), a new porous iron(III) squarate metal-organic framework (MOF).[1] By implementing a microwave-assisted (MW) synthetic protocol, we achieved space-time yields (up to 127.2 $kg \cdot m^{-3} \cdot day^{-1}$), according with the industrial scalability.

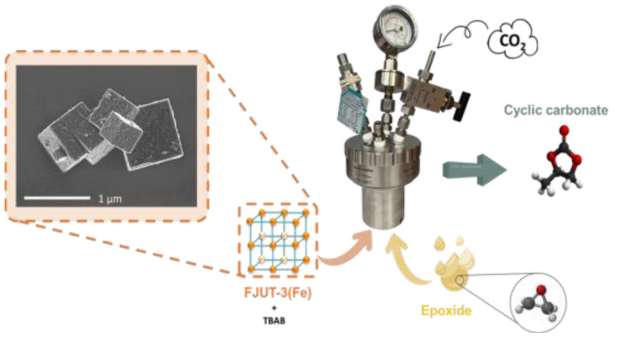

Figure 2 Catalytic performance of the material IEF-40(Fe)

The physicochemical characterization confirms that IEF -40 is isostructural to FJUT-3(Co).[2] By replacing Co(II) with Fe(III), we developed a more sustainable and low-cost alternative. XPS analysis confirmed the presence of Fe(III), while TGA enabled quantification of a significant degree of missing-cluster defects (ca. 25%). Notably, the use of MW radiation introduces structural defects that modify textural properties, leading to the coexistence of microporosity and induced mesoporosity. These features enhance access to the active Fe(III) sites without compromising framework stability, providing an efficient pathway for CO_2 valorization under mild conditions.[3] The catalytic performance of IEF-40 was evaluated in the solvent-free cycloaddition of CO_2 to cyclic carbonates.[1] Under mild conditions (35 °C, 1 bar CO_2), the catalyst achieved conversions of up to 89% and TON > 140, maintaining its performance over four cycles. These results are competitive with benchmark catalysts requiring harsher conditions. Importantly, MW synthesis reduced reaction time by 96% and enabled reproducible gram-scale production.[4] The correlation among synthetic conditions, defects, and activity underscores the importance of defect engineering in developing scalable MOF-based CO_2 catalysts.

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ATMOSPHERIC WATER HARVESTING WITH ALKALI AND TRANSITION METAL CONTAINING HETEROATOM-RICH CARBON MATERIALS

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Keywords: *Carbon, heteroatom, metals, adsorption, atmospheric water harvesting*

Global freshwater resources are under increasing pressure caused by population growth, industrial development, agricultural demand, and climate change. According to global water assessments, billions of people face water scarcity, especially in arid regions.[1] Moreover, the ability to harvest water in humid and foggy areas is necessary in more rural environments, such as on mountains or coastal regions, and in natural disaster production technologies, including desalination, effluent recycling, and atmospheric water harvesting (AWH).[2] The earth's atmosphere holds approximately 12900 km³ of water vapor worldwide.[3] In contrast to surface water, atmospheric moisture is continually replenished through the hydrological cycle, making it a renewable and widely distributed resource.[4] AWH is a technology that adsorbs water vapor from the atmosphere and desorbs it into the liquid phase using solar heat or other forms of energy inputs. Among the various sorbents explored for AWH technology, heteroatom-rich carbon materials exhibit a remarkable ability to capture water molecules at low humidities due to their numerous functional groups, including nitrogen and oxygen. These functional groups can further coordinate with alkali and transition metals, thereby enhancing water uptake and improving their thermal and chemical stability.[5]

For this purpose, heteroatom-rich carbon materials are functionalized with alkali or transition metals via adsorption or cation-exchange method at varying metal concentrations. Afterwards, a series of characterization methods was applied to evaluate the performance of these materials for the AWH application, particularly static and dynamic water adsorption. As a result, the heteroatom-rich carbon-functionalized transition-metal material is shown to be a potential water harvester for arid regions. It exhibits water adsorption capacities of ~0.13 g g^{-1} and ~0.24 g g^{-1} at relative humidity (RH) values of 5 % and 90 %, respectively, and a fast adsorption of ~8 min at 20 % RH to adsorb ~0.1 g g^{-1}. LTA zeolite used as a reference material has similar water uptake of ~0.19 g g^{-1} and ~0.26 g g^{-1} at RH values of 5 % and 90 %, respectively, and needs longer (~18 min at 20 % RH) to adsorb ~0.2 g g^{-1}. Moreover, dynamic water adsorption demonstrated the material's high stability over at least 50 adsorption/desorption cycles. Additionally, heteroatom-rich carbon-functionalized alkali metal gives promising results across all RH levels. It adsorbs water at capacities of ~0.3 g g^{-1} at 20 % RH, ~ 0.7 g g^{-1} at 60 % RH, and ~1.5 g g^{-1} at 90 % RH. Dynamic water adsorption demonstrates the chemical stability of this material over 80 cycles of adsorption and desorption, yielding 7.2 L kg^{-1} day^{-1} of water at

90 % RH (100 % recovery) and 2.4 L kg^{-1} day^{-1} of water at 20 % RH (50 % recovery). The findings presented herein reveal the promising potential of heteroatom-rich carbon functionalized with alkali and transition metals for the AWH system compared with other AWH porous carbon-based materials, such as DUT-67, Al-fumarate, MOF-801, UiO-66, MCM-41, CAU-10-H, and LTA, providing a solid foundation for further investigations in this field.[6]

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H_2O and CO_2 adsorption in different MOFs: experimental isotherms, heats of adsorption and their modeling

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Keywords: *water, CO_2 capture, modeling, MOFs, enthalpy of adsorption, water isotherm*

Carbon capture from flue gas or air presents unique challenges, as it is often accompanied by significant amounts of water. Amongst many adsorbents considered for capturing CO_2, MOFs are regarded as potential candidates. This family of adsorbents presents a wide range of water adsorption behavior [1] which can be very complex to predict numerically and can more or less compete with CO_2. Because water plays a critical role in the process, accurately representing its isotherms is essential to simulate CO_2 capture properly. For that, an understanding of underlying adsorption mechanisms is crucial, and the measurement of adsorption enthalpy – as done in this work thanks to a home-made calorimetric/manometric setup – brings important information. As a typical example, our methodology is applied to Al-Fumarate which presents the so-called "S" shaped water isotherm (see Fig. 1), and high adsorption enthalpies at low loading followed by a plateau. It is shown that the modified Do and Do model [2,3] initially developed for water adsorption on activated carbons to account for the successive water adsorption mechanisms - strong interaction of the first water molecules adsorbed with specific sites followed by cluster formation – allows a good and temperature-consistent water adsorption modeling. Additionally, modeling of CO_2 adsorption was also performed on Al-Fumarate in good agreement with calorimetric experiments and the methodology was transferred to other MOFs such as CALF20.

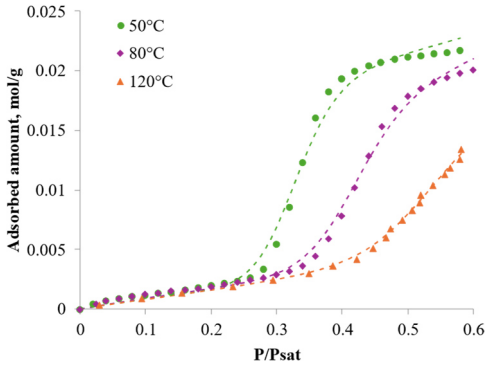

***Fig. 1**: Water isotherms of Al-Fumarate and corresponding modeling (dashed lines)*

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Characterization of open porous metallic foams using conventional and non- conventional methods

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Keywords: *metal foams, powder metallurgy, substrate, catalysis, electrodes, alloys, analysis*

Metal foams are excellent substrate materials for energy and chemical technology. However, depending on the intended field of use, the structure and surface of the foams have to be adapted and modified to yield the best performance. Powder metallurgical deposition of catalytically active coatings using different methods like dry and wet powder spraying, the doctor blade technique or dispensing result in different foam strut morphologies, surface structures, and even graded foam structures. Surface treatment and surface alloying can be applied either as a single-step process or as complementary preparation steps to modify surface properties, including wetting behavior, or to activate metal foams for catalytic applications. The process chain of surface treatment, alloying and heat treatment as the final, decisive step will be covered and connected with applications of metal foams in areas like water electrolysis or water treatment, filtration and general catalysis.

Since the respective application of a metal foam requires customised properties, the production process is accompanied by different analyses and characterization methods to verify certain features after key process steps. The success of the deposition and alloying procedure can be tested using XRF and XRD, the latter method sometimes requiring sample preparation. Furthermore, the effect of the sintering atmosphere on surface contamination can be systematically evaluated using inert gas fusion and combustion analysis (ONHCS analysis), which is critical for applications that demand either contaminant-free surfaces or intentionally pre-oxidized and otherwise pre-treated struts. The macroscopic structure and gradation of the foam can be visualized by optical microcopy to distinguish rather active, permeable or elastic parts of the foam structure from their equally important passive, impenetrable or rigid counterparts. Electron microscopy in combination with EDS is applied to investigate microstructure influences and the local chemical composition. The BET analysis highlights how the interplay between the specific deposition method, alloying strategy, and post-treatment procedures influences the active surface area of metal foams, which is a key parameter for catalytic activity [1]. Using a recently acquired tensiometer, the Wilhelmy Plate method is successfully applied to characterize metal foams having different compositions, varying porosities and differently coated surfaces in terms of their wetting behaviour. All of the above mentioned methods will be presented with reference to recent and ongoing projects to emphasize their applicability.

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MOF-BASED POROUS WATER FOR CO_2 CAPTURE

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Keywords: *porous liquid, CO_2 adsorption, hydrophobic MOF, pressure-swing adsorption.*

Type III porous liquids based on metal-organic frameworks (MOFs) exhibit permanent porosity and fluidity, with their unique applications (e.g., CO_2 capture) attracting considerable attention [1]. Nevertheless, the preparation of type III porous liquids often requires organic solvents. The high cost and potential risks related to the solvents hinder the industrial application of the porous liquids. Recently, porous water based on MOFs was proposed [2,3]; however, its synthesis and applications remain largely unexplored. Herein, we synthesized a hydrophobic MOF and subsequently prepared it into a type-III porous liquid using water as a solvent (PW). At a MOF concentration of 10 wt.%, the PW exhibited adsorption capacities of 0.36, 1.13, and 1.8 mmol/mL at 2, 5, and 10 bar, respectively (15 vol.% CO_2 balanced with N_2, simulated to the flue gas from coal-fired power plants). The hydrophobic MOF could retain its internal porosity in water, since the PW retained a CO_2 adsorption capacity of 0.97 mmol/mL (10 vol.% CO_2 balanced with N_2, 10 bar) after 3 h of He purging at 10 bar. Additionally, PW retained a capacity of 0.87 mmol/mL after preparation for five days. The prepared PW could be used in the temperature-vacuum swing adsorption (TVSA), for it could be regenerated at 318 K under vacuum for 3 h and showed good adsorption stability for five cycles. More interesting, the PW could be used in the pressure-swing adsorption process, since it showed an excellent cyclic adsorption stability of 1.67±0.05 mmol/mL after 17 consecutive cycles (adsorption: 10 bar, 15 vol.% CO_2 balanced with N_2; desorption: 1 bar, He). Compared to TVSA, PSA required lower energy consumption and shorter operation time. Furthermore, XRD and SEM revealed no significant crystalline or morphology changes in the MOF after water immersion, indicating that the decline in adsorption capacity was attributed to water invasion into the pores inside the MOF and, therefore, the capacity loss of the MOF was reversible. Current work points a novel direction for developing sustainable, low-cost, highly efficient, and low-energy consumption adsorption systems for CO_2 capture.

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Decarbonising the World with monolithic MOFs

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Keywords: *carbon capture, MOF, monolith…*

Immaterial Ltd accelerates the global energy transition through densified monolithic metal-organic frameworks (m-MOFs). Our technology combines the tunable pore size and chemistry of MOFs with the high-density conformation of monoliths, overcoming a key limitation that has historically prevented MOFs from industrial deployment. Specifically, our proprietary sol-gel densification process minimises non-adsorbing interstitial space between MOF particles that is inherent to powders and conventional pellets, thereby maximising packing density, module efficiency, and overall process performance while preserving the intrinsic porosity of the framework. This structural advantage translates directly into performance gains. Immaterial's m-MOFs deliver 3-4× higher volumetric adsorption capacities compared to mechanically densified pellets while retaining the high gravimetric performance of conventional MOF powders [1]. At the same time, the monolithic architecture provides superior mechanical stability, structural integrity, and handling robustness, all of which are prerequisites for long-term industrial operation.

Immaterial has successfully scaled the production of m-MOFs from laboratory prototypes to industrial manufacturing at 20 tonnes per year. This capability enables direct deployment across sectors requiring durable, high-performance adsorption materials, including carbon capture, direct air capture, hydrogen storage, and water harvesting. Our priority on carbon capture represents one of the most urgent challenges in reducing the carbon footprint of existing energy systems. Conventional CO_2 capture technologies, such as liquid amines, face fundamental limitations including high regeneration energy demand, corrosion, solvent degradation, and elevated operating costs [2]. In this context, Immaterial's m-MOFs enable more energy-efficient CO_2 capture and have the potential to outperform incumbent technologies by an order of magnitude on a materials basis. Supported by advanced, in-house characterisation and process optimisation capabilities, Immaterial aims to deliver a low-cost, scalable carbon capture solution that directly contributes to achieving the 2050 Net-Zero target.

Figure 1. *Picture of m-MOFs developed by Immaterial Ltd.*

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A Strategy to enhance photon upconversion emisson in lanthanide MOFs

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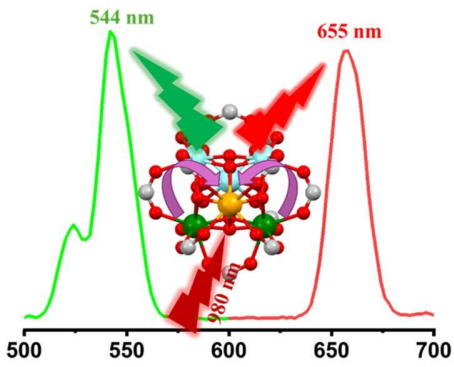
Keywords: *MOF, Lanthanides, upconversion emission, multinuclear cluster*

Lanthanide-based metal-organic frameworks (LnOFs) show promise in optical applications due to their characteristic structural features.[1] UC emission has been studied in inorganic nanoparticles, leading to various applications.[2,3] However, the use of a similar UC principle in MOFs remains limited, likely due to large Ln···Ln distances in the lattice and quenching effect.[4]

We propose a strategy to enhance UC emission by engineering multinuclear metal cluster-based MOFs. Doping clusters with optimal Yb/Er ratios ensure close Ln ion proximity in the lattice and an effective energy transfer. Comparing cluster and non-cluster MOFs revealed the critical role of cluster structures in providing more efficient energy transfer and boosting UC emission, showing potential for further advancements in the MOF field.

Two material series (cluster and non-cluster) were synthesized via solvothermal methods using H_2BPDC linker, with Yb^{3+} as a sensitizer and Er^{3+} as an emitter. UC emission measurement showed Er^{3+} emission peaks only in cluster MOFs, proving the importance of cluster structure. Structures were analyzed using PXRD, SEM-EDX, TGA, IR, and ICP-OES. Apart from this, cluster MOFs using different linkers have been investigated to understand the role of the linker on upconversion property. Through this investigation of the linker effect, the trend of UC intensity increased upon increasing conjugation, which can be excellent for tuning the UC efficiency for optical applications.



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THE ROLE OF SHAPE-PERSISTENT MACROCYCLES IN SEPARATION APPLICATIONS

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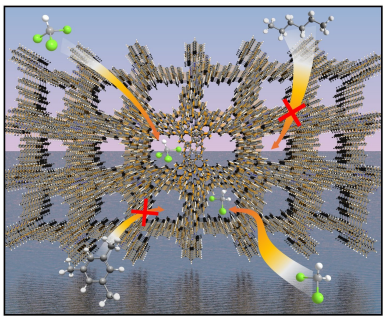
Keywords: *cyclotetrabenzoins, macrocyclic porous organicpolymers, solvent separation, host– guest chemistry, naphthalene macrocycles*

Efficient recovery and separation of pollutants, including organic solvents, are vital for sustainable chemical processes. Here, I will present a series of shape-persistent macrocyclic molecules for the selective isolation of pollutants, highlighting the recent *np*-POP made via solvothermal condensation of a cyclotetrabenzil naphthalene octaketone macrocycle with 1,2,4,5tetraaminobenzene, alongside a small-molecule model. Single-crystal co-crystallization confirmed size-selective inclusion of guest solvents. The *np*-POP features a hierarchical pore network and a BET surface area of 579 $m^2 g^{-1}$. Solvent uptake correlates strongly with kinetic diameter: acetonitrile and dichloromethane (<0.6 nm) reach >7 mmol g^{-1}. In mixed xylene isomer tests, total uptake was ~34 wt %, with o-xylene ~10 wt % lower than m- and p-xylene, demonstrating clear size/shape-based separation. These results highlight *np*-POP's potential for energy-efficient solvent recovery and fine-chemical separations.



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A Pore or Not a Pore? Decoding Apparent Ultramicropores Through Site-Specific Adsorption in Non-Graphitic Carbon and Atomically-Dispersed M-N-C Materials

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Keywords: *gas sorption, pore size distribution, adsorption*

Current research in electrochemical energy conversion and storage focuses on optimizing the performance and understanding structure–property relations of functional carbon materials, including activated carbons, supercapacitor electrodes, battery anodes, and atomically dispersed metal and nitrogen co-doped carbons (M-N-Cs) catalysts. Gas-sorption porosimetry with classical density functional theory based pore size distributions (PSDs) is a key tool in this field.[1-3] PSDs often show ultramicropores smaller than the probe molecules' intercalation limits, indicating computational artefacts.[4] Yet, such features may also signal strong, localized adsorption sites. In this work, defined in-plane adsorption sites were created by pyrolytic ion-template synthesis.[5-10] ZIF-8 containing tetrapyrrolic Zn–N4 units was pyrolyzed and subsequently Zn-leached to yield nitrogen-doped carbons (NDCs) with H2N4 sites while preserving the morphology of the Zn-N-C. These H2N4 motifs can act as solid-state porphyrins with ~0.4 nm cavities and explain apparent ultramicropores through preferential probe-molecule adsorption.[10] Quantum-chemical adsorption energies and Langmuir analysis support this interpretation. Identifying such specific adsorption sites not only clarifies artefacts in porosity analysis but also provides valuable insights for advancing electrochemical applications such as electrocatalysis and battery materials.

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TEXTURE ANALYSIS OF SCALABLE GREEN SYNTHETIZED UiO-66-NH_2 MOFs WITH SURFACTANTS AS MESOPOROUS TEMPLATES

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Keywords: *MOF, hierarchical porosity, green synthesis*

Metal-organic frameworks (MOFs) are a recently discovered class of porous materials with promising applications in gas storage, catalysis, adsorption and other fields. Though there are reports of superlative properties of these materials, the majority of synthesis methods doesn't comply with industry requirements and make the gap between MOFs and the market difficult to bridge [1]. Spray-drying is a well-known industrial technique that can be combined with green synthesis methods to obtain MOFs in a high throughput scalable fashion [2]. Additionally, mass transport is another issue for the application of MOFs due to the slow diffusion (specially in liquid phase) in the microporous texture of most MOFs. The use of soft templates during synthesis can introduce meso and macropores to obtain hierarchically porous materials [3].

This work evaluates the use of different surfactants in aqueous spray-drying synthesis of UiO-66NH_2 MOF and its influence in the product texture properties. The obtained micron-sized particles were characterized with powder X-ray diffraction, transmission electron microscopy and nitrogen sorption. Apparent surface area was calculated using the Brunauer-Emmett-Teller equation and micro and mesopores distribution were obtained with Horvath-Kawazoe and Barrett-JoynerHalenda methods respectively. Micropore volume was calculated with the Dubinin–Radushkevich equation and total pore volume was obtained with Gurvich rule.

Results showed it is possible to introduce mesoporosity with surfactants and that the synthesis technique itself introduces mesoporosity into the particles through small crystals aggregation. Isotherms with distinct hysteresis loops were obtained, indicating the presence of different types of mesoporous structures. These results demonstrate this green synthesis method is suitable for large scale hierarchically porous UiO-66-NH_2 production.

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Thermal Evolution of Catalytically Active Nanoparticles from a 2D Zn-Porphyrin-Based Metal–Organic Framework: In-situ TEM Insights

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Keywords: *2D MOFs, in-situ TEM, pyrolysis, nanocatalysts, ZnO*

Pyrolysis of metal–organic frameworks (MOFs) enables the synthesis of catalytically active nanoparticles (i.e., nanocatalysts) embedded in graphitic carbon, showing promising results in oxygen reduction (ORR) and oxygen evolution (OER) reactions. [1] Such nanocatalysts, derived from two-dimensional (2D) MOFs, often exhibit superior catalytic performance than their three-dimensional counterparts due to their higher surface area. However, thermal degradation pathways and mechanisms governing the formation of nanocatalysts from 2D Zn-porphyrin-based MOFs are not yet fully understood.

Here, we investigated the temperature-dependent transformation (pyrolysis) of the 2D porphyrin paddlewheel framework PPF-1 (Zn-TCPP-based) into ZnO nanoparticles,[2] using in-situ transmission electron microscopy (TEM) heating. PPF-1 is a known 2D porphyrinic MOF accessible as ultrathin nanosheets, providing a model platform to study framework-to-oxide conversion.

Prior to thermal experiments, powder X-ray diffraction (PXRD) and ex-situ TEM confirmed phase purity and short-range order of PPF-1 under ambient conditions. To ensure that structural changes were thermal rather than electron-beam-induced, we

established critical low-dose TEM imaging conditions via electron-diffraction (ED) intensity tracking, guided by best practices for beam-sensitive MOFs.[3]

In-situ TEM heating revealed the onset of ZnO nucleation above ~500 °C, followed by a temperature-dependent systematic increase in particle size. At ~800 °C, the nanoparticles exhibited pronounced HRTEM lattice fringes, allowing precise phase identification and crystallographic characterization. Correlating temperature-dependent nucleation/ripening kinetics with microstructural development provided direct insight into the formation mechanism.

We will discuss the mechanisms of thermal degradation, nucleation, and growth will and thereby the potential of controlled MOF pyrolysis as a tunable route to produce structurally well-defined nanocatalysts.

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How Enzymes Reshape Porous Crystals: Direct Evidence of Nanocavity Formation in ZIF-L via Electron Microscopy

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Keywords: *Enzyme entrapment, MOFs, Electron microscope, Biocatalysts*

Metal-organic frameworks (MOFs) are advanced porous crystalline materials with high chemical and thermal stability that enable applications in separation technologies, gas storage, catalysis, and biomolecule immobilization[1]. Their structural tunability provides opportunities to design frameworks with tailored pore environments for enzyme–MOF nanocomposites[2]. However, controlling enzyme distribution within MOFs and understanding the underlying enzyme–MOF interactions at the nanoscale remain major challenges. Advanced electron microscopy techniques could therefore offer valuable insights into the complex structure of enzyme-MOF nanocomposites and link structural modifications to overall functionality.

In this work, we studied the entrapment of *Persephonella marina* carbonic anhydrase (PmCA) within leaf-shaped ZIF (ZIF-L), a two-dimensional zeolitic imidazolate framework, to explore how host–guest interactions affect both enzyme activity and framework structure. Using a mild, enzyme-compatible synthesis condition, we achieved successful entrapment of PmCA within ZIF- L and confirmed that the enzyme retains its catalytic activity after encapsulation. For detailed structural characterization, Fourier-transform infrared spectroscopy (FTIR), scanning electron microscope (SEM), and X-ray diffraction (XRD) were used to confirm the incorporation of PmCA within the ZIF-L crystal, while low-dose scanning/transmission electron microscopy (S/TEM) techniques provided insight into the localization and distribution of enzymes at the nanoscale. In addition, energy-dispersive X-ray spectroscopy (STEM-EDS) further confirmed the presence of immobilized enzymes within the MOF crystal.

Our results revealed that while ZIF-L preserves its overall crystallinity, the presence of PmCA induces the formation of nanocavities (~5 nm), closely matching the size of the enzyme. This suggests an adaptive response of the host framework during synthesis, with local restructuring to accommodate the enzyme. By complementing morphological data with functional assays, we showed that the immobilized PmCA retains its enzymatic activity, supporting the capacity of enzyme@ZIF-L composites for CO2 hydration applications[3]. These findings provide direct insight into enzyme-induced framework restructuring and offer a foundation for the rational design of MOF-based biocatalytic systems.

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Abstracts of Posters

ORDERED MESOPOROUS CARBON CMK-3 FROM LIGNIN: A TEMPLATE-BASED APPROACH WITH COPPER FUNCTIONALIZATION

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Keywords: *mesoporous carbon, CMK-3, hard templating, lignin.*

The Lignin is an abundant natural aromatic polymer and a major component of lignocellulosic biomass. In the paper industry, it is generated in large quantities as a byproduct.[1][2] Because of its high carbon content and renewable character, lignin can be valorized into value added carbon materials, such as porous carbons and carbon fibers, presenting a sustainable pathway for carbon production.[1][3][4] In this work, the primary objective is the synthesis and detailed characterization of lignin derived ordered mesoporous carbon. Specifically, an ordered micro-/mesoporous CMK- 3-type carbon is used, offering uniform mesopores, high surface area, and enhanced mass transport, which are advantageous for electrocatalytic applications.[5] This material is synthesized using an combination of hard templating and CO_2 activation approaches and loaded with Cu particles via incipient wet impregnation, serving as a state-of-the-art electrocatalyst for electrocatalytic nitrate reduction (NORR). Comprehensive characterization demonstrates that the material retains some of the SBA-15 derived mesostructure. Small angle X-ray scattering (SAXS) reveals a somewhat weaker (100) diffraction peak than sucrose derived CMK-3, but pore size analysis indicates a predominantly mesoporous structure with an average pore width of 5.6 nm. Scanning electron microscopy (SEM) confirms a rod like morphology, though some particles deviate from ideal shape, likely due to incomplete infiltration. Following CO_2 activation, the micropore volume increases from 0.18 $cm^3\ g^{-1}$ to 0.23 $cm^3\ g^{-1}$, while the average micropore width remains around 0.349 nm. X ray diffraction (XRD) verifies the presence of metallic Cu nanoparticles. Although the material is primarily developed for its structural and porous properties, preliminary electrochemical tests by cyclic voltammetry demonstrate activity in NORR, suggesting that the composite could also serve as a potential electrocatalyst. Finally, this methodology is being extended to other types of lignin (e.g., Kraft lignin). The impregnation protocol is optimized for each lignin variant to establish a reproducible strategy for synthesizing mesoporous carbon–lignin composites with well controlled structural and textural characteristics.

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Semiconductive MOFs for Energy Conversion of High-energy Rays

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Keywords: *Semiconductive MOFs, X-ray detection, Structure-property design.*

Increasing demands in radiation detection technologies compel researchers to break new ground in solid-state sensing materials. Traditional ionizing radiation detectors are generally inorganic or organic. Inorganics boast excellent absorption and stability, while organics offer superior flexibility and processability. Yet, both are constrained by their inherent flaws. The path forward demands investigation into novel materials that successfully blend the advantages of both groups.

Metal-Organic Frameworks (MOFs), an emerging class of inorganic-organic hybrid materials, represents a highly promising solution. They show great potential for energy conversion due to their unique combination of high energy photon absorption, radiation sensitivity, detection efficiency, and stability. The key to developing alternative ionizing radiation detectors lies in the systematic design of MOFs via the coordination chemistry of metal centers and organic ligands. Furthermore, pore engineering can strategically leverage MOFs' porous characteristics for diverse applications. By optimizing the metal center, researchers can significantly enhance the radiation cross-section and thus improve energy conversion efficiency. Meanwhile, the framework's tunable structure, formed by organic ligand self-assembly, ensures the high charge carrier mobility required for effective signal collection.

Our research interests center on the design synthesis, and exploration of semiconductive framework materials for X-ray energy conversion applications, with a particular emphasis on elucidating the structure-property relationships of semiconductive frameworks, especially their charge-carrier behavior under high-energy radiation.

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Quantifying Percolation and Pore Connectivity in ZIF-8/6FDA-DAM Mixed Matrix Membranes

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Keywords: *MOFs, polymer, MWCO, CO2, carbon capture, separation, filtration, sustainability*

Addressing the urgency of global climate change requires transformative advances in separation technologies, especially in energy-intensive sectors such as petroleum refining, plastics production, and bulk chemicals. Thermally driven processes (e.g., distillation) remain dominant, yet impose substantial energy and carbon footprint, estimated to consume 10–15% of global energy. [1] Mixed-matrix membranes (MMMs), hybrids of process-robust polymers and nanoporous fillers such as metal–organic frameworks (MOFs), offer a promising pathway to lower the energy intensity of separations. However, conventional fillers often require high loadings to achieve percolation, increasing the risk of agglomeration and non-selective defects that degrade membrane performance and reliability.

Here we introduce an advanced characterization methodology tailored for MMMs combining branched Zeolitic Imidazolate Framework-8 (branched ZIF-8, BZ) particles embedded in 6FDA- DAM polyimide. The self–interconnected morphologies of BZ facilitate the formation of percolative networks at low filler concentrations, [2] offering a route to enhance selectivity and permeance without compromising mechanical integrity. Our approach combines gas permeation and SEM analysis to verify pinhole, defect-free morphology and uniform filler dispersion in the MMMs. The branched ZIF-8 phase is then selectively removed, producing a MOF-templated, pore network within the polymer. Finally, a molecular weight cut-off [3] (MWCO) protocol using size- varied PEG probes is employed to map pore connectivity, tortuosity, and effective size-exclusion thresholds. This chemical top-down perspective is complemented by SEM/TEM (filler distribution, interface quality, and network continuity), IR spectroscopy (polymer–filler interactions, removal of the MOF phase), and XRD (crystallinity, ZIF 8 phase integrity).

Beyond structural characterization, the methodology is used to assess the functional viability of etched membranes, with potential implications for the up-cycling aged or performance-degraded MMMs. By establishing structure–transport correlations and quantifying the onset/quality of percolation at sub-critical loadings, the findings contribute to the broader development of next- generation, life-cycle optimized separation technologies essential for enabling low-carbon, energy- efficient industrial processes.

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Electroactive metal-organic frameworks enable unidirectional supercapacitors and logic gates (MOF-CAPode)

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Keywords: *MOF, supercapacitor, CAPode, logic gate, electrochemistry*

CAPodes are innovative supercapacitor analogues of diodes designed for unidirectional charge storage.[1] The novel devices comprise two different electroactive metal-organic frameworks (MOFs) with characteristic redox potentials acting as positive (p-MOF) and negative electrodes (n- MOF), respectively. The first proof-of-concept devices presented here make use of the Chichibabin-like diradicaloid formation upon oxidation of the *N,N,N′,N′*-benzidinetetrabenzoate linker in Zr-based DUT-65/66[2] MOFs and the Thiele-like *N,N,N′,N′*-(1,4-phenylenebis- (azanetriyl))-tetrabenzoate in Zr-based DUT-232/233 MOFs (Fig. 1A) at high oxidation potentials as a positive electrode paired with the highly reversible two-step reduction in [Zn(ndi)]n (ndi = 1,4- bis[(3,5-dimethyl)-pyrazol- 4-yl]naphthalene-diimide).[3] Unidirectional charging behavior of the MOF-CAPode is reflected in high faradaic current in one polarization direction and only small double-layer current when the polarization is reversed (Fig. 1B). Optimizations based on CV measurements leads to rectification ratios for the DUT-232|TBAPF$_6$(ACN)|[Zn(ndi)]$_n$ based CAPode of RRI = 23 and RRII = 94%. The integration of the MOF-CAPode into ionotronic logic gates (AND, OR) was achieved with near lossless operation over a wide range of input voltages and frequencies (Fig. 1E).

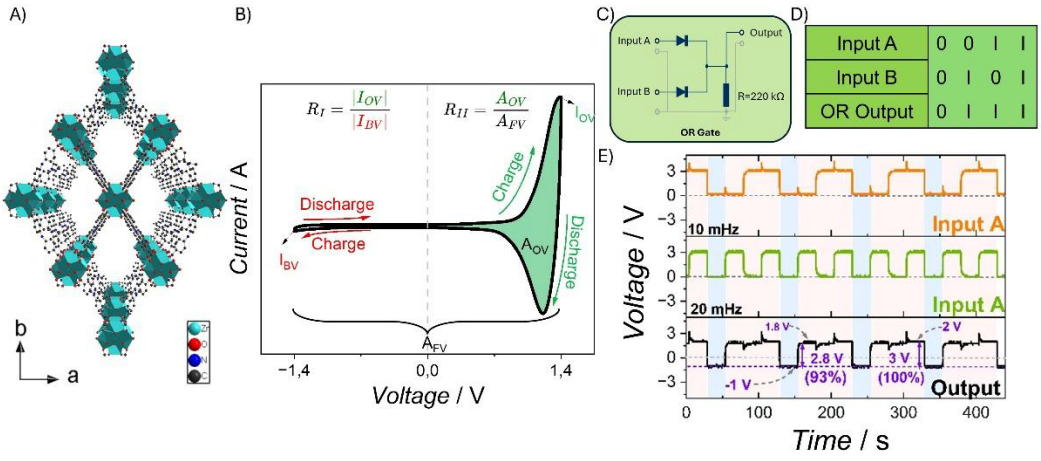

Figure 1. A) Crystal structure of DUT-232 along the c-axis (Zr blue, O red, N blue, C gray, H omitted). B) Cyclovoltammetric (CV) measurement of DUT-232|TBAPF$_6$(ACN)|[Zn(ndi)]$_n$ system. C) OR gate circuit diagram. D) OR gate truth table. E) Input and output signals for logic gate operation of two DUT-232|TBAPF$_6$(ACN)|[Zn(ndi)]$_n$ devices in OR gate circuit.

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Precisely Controlled 2D Monolayer Engineering based on Metal-Organic Polyhedron and Applications

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Keywords: *Two-dimensional materials, Metal-organic polyhedron, 2D Monolayer Materials*

Two-dimensional materials (2DMs) such as graphene, hexagonal boron nitride, MXenes, metal-organic frameworks, and covalent-organic frameworks have attracted growing interest due to their unique physical and chemical properties and their potential applications ranging from electronics to energy and medicine.[1,2] In particular, an emerging direction involves constructing 2D systems from discrete 0D molecular building blocks, such as graphullrene and polyamide nanofilms incorporating aligned macrocycles.[3,4] These materials combine the functional diversity of 0D molecules with the extended architectures of 2D frameworks, offering enhanced structural tunability and multifunctionality.

In this project, we aim to develop advanced 2D monolayers through the bottom-up assembly of metal-organic polyhedra (MOPs) and flexible *N*-donor ligands. MOPs are shape-persistent cages composed of metal nodes and multitopic organic linkers, featuring well-defined porosity, modular functionality, and addressable exterior coordination sites.[5] These characteristics enable programmable assembly and render MOPs highly processable for achieving molecular-scale alignment in 2D architectures. We synthesized alkyl-functionalized Rh- and Ru-based cuboctahedral MOPs and explored their assembly into monolayers using Langmuir Blodgett (LB) and customized Langmuir-type deposition (LD) techniques. The fabricated MOP monolayers were characterized using atomic force microscopy (AFM) and transmission electron microscopy (TEM). For further investigation, we plan to incorporate pillar molecules after dispersing the MOPs on the water surface, enabling the study of metal-nitrogen (M-N) bond formation in the resulting 2D monolayers. Raman and UV-Vis spectroscopy will be employed to probe these interactions. Ultimately, we anticipate achieving precise control over monolayer thickness, pore size, and structural flexibility. Such tunability is expected to open opportunities in gas separation, molecular storage, and selective catalysis, where adjustable channels and exposed metal sites offer distinct advantages over traditional 2DMs.

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Combining differential scanning calorimetry and adsorption to deepen the understanding of MOF adsorption thermodynamics

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Keywords: *flexible MOFs, calorimetry, adsorption, characterization.*

While most metal–organic frameworks (MOFs) show rigid structures, some—known as flexible MOFs—undergo reversible structural transformations, often involving notable changes in pore size, shape, or volume in response to external stimuli.[1] These structural adaptations, such as transitions between narrow-pore and large-pore phases, gradual swelling, or gate-opening/gate- closing motions, are typically triggered by guest adsorption or desorption.[2]

The thermodynamics underlying adsorption/desorption processes are often quite complex and usually require theoretical calculations or mathematical equations.[3] This complexity increases in flexible MOFs due to the overlap of adsorption–desorption phenomena and structural transformations of the framework itself. Although these two contributions are generally opposite in sign, they are strongly linked and cannot occur independently: adsorption is generally exothermic and desorption endothermic, whereas the structural transitions of flexible MOFs show the opposite trend—pore expansion (commonly associated with adsorption) is endothermic, and pore contraction (usually associated with desorption) is exothermic.

Experimentally, separate the different energetic contributions involved in a guest-induced transformation in flexible MOF—such as the heat of adsorption and the latent heat of the structural transition—is highly challenging. In this work, we combine two complementary techniques to address this issue and successfully separate the thermal signatures of both processes: high-pressure (HP) adsorption and variable-pressure differential scanning calorimetry (VP-DSC). As a result, we were able to experimentally estimate the adsorption heat associated with each individual contribution.

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Advanced characterization of nanoporous materials using a novel *in-situ* vapor sorption calorimetry method

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Keywords: *adsorption calorimetry, surface chemistry, characterization*

Porous materials play a key role in separation and catalysis processes. Ongoing advances in material science lead to new emerging nanoporous materials, that offer great potential for optimizing applications in many areas, including separation, catalysis, as well as gas- and energy storage. Within this context, a reliable and comprehensive textural and surface characterization of these materials is essential to understand their properties and to identify key structure-property- performance relationships. In addition to the assessment of textural properties—such as surface area, pore size/volume distribution, and pore network characteristics—a reliable determination of surface properties, including the hydrophilicity and hydrophobicity, is crucial here. To address these challenges, we developed a novel high-precision manometric *in-situ* vapor adsorption calorimetry apparatus, which is based on a combination of a high-precision 3D-Calvet calorimeter paired with a novel vapor sorption apparatus capable of high, homogenous manifold temperatures. Depending on the chosen adsorptive (vapor), the manifold can be heated up to > 100 °C to completely prevent any vapor (e.g., water) adsorption on the manifold tubing [1], which ensures both highly accurate water adsorption and heat data. It enables our setup to accurately and simultaneously measure the adsorbed amount and the resulting, corresponding heat of adsorption for each adsorption isotherm data point (for a given pressure). We have successfully validated our system by performing water adsorption experiments (at 308 K) using a well-known microporous carbon reference material (BAM-P109), which was utilized in an international round robin to obtain a water adsorption reference isotherm [2,3]. Furthermore, the obtained adsorption heat data showed good agreement with published literature data [4].

The obtained heat of adsorption as a function of coverage yields information on surface heterogeneity, surface chemistry and site energy distribution. Moreover, we demonstrate that by coupling *in-situ* adsorption heat data with the results of an advanced textural characterization (based on argon adsorption at 87 K coupled with methods of statistical mechanics such as density functional theory), it is possible to assess pore surface characteristics and wetting behavior of adsorptives on the pore walls and correlate this information with the underlying pore size distribution of the adsorbent. We present results obtained from water adsorption experiments utilizing pristine mesoporous silica materials with well-defined pore structures such as SBA-15, controlled pore glass (CPG) and functionalized silicas (SBA-15 and CPG) with varying degrees of TMS (trimethylsilanol) and C18 groups. Such adsorbents have potential applications as stationary phase materials in liquid chromatography

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CO2 Capture performance of Tailored Metal-Organic Framework

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Keywords: *MOF synthesis, modification, CO_2 adsorption*

Metal–Organic Frameworks (MOFs) have gained broad applicability across numerous fields owing to their highly ordered structures, large surface areas, and exceptional tunability. Advances in MOF chemistry now enable rational and systematic modulation of structural features to tailor materials for specific performance requirements. Consequently, MOFs have become strong candidates for CO^2 capture, as their tunable structures and adjustable porosity allow for significant enhancements in CO_2 uptake and selectivity [1]. One widely adopted strategy to further boost CO_2 adsorption involves functionalizing the organic linkers with additional functional groups, such as amines, which can substantially increase the materials's affinity for CO_2.

This functionalization concept has been effectively demonstrated in a series of triazolate-based MOFs, including CALF-20, CALF-15, and NICS-24 [2]. Notably, the introduction of additional amine groups in NICS-24 enhances its CO_2 capture performance compared to CALF-15, with both materials outperforming CALF-20 under low-concentration CO2 conditions.

To build on these improvements, we propose further optimizing NICS-24 by introducing selected linkers into the synthesis (Figure 1). This targeted modification aims to systematically adjust pore size and volume, as well as refine host-guest interactions, thereby enabling enhanced sorption capacity, faster adsorption kinetics, and improved regeneration efficiency.

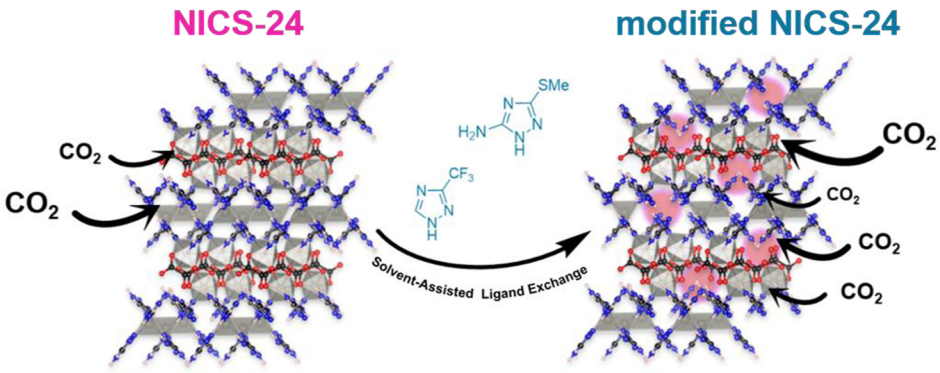

Figure 1. Linkers used for the fine-tuning strategy applied on NICS-24.

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A novel methodology for quantitative liquid-phase adsorption measurements

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Keywords: *adsorption, characterization, liquid-phase, porous materials*

Liquid phase adsorption technology plays a crucial role in separating, purifying, and extracting liquids or dissolved species in key industries such as petrochemical, water treatment, and pharmaceutical. Despite its importance, the evaluation of the adsorption capacity of materials in the liquid phase remains a challenge. Conventional methods are laborious, time-consuming, and manual, mainly due to the lack of standardization and automated equipment. Overcoming this limitation and bringing liquid phase adsorption methods to the laboratory instrumentation market offers considerable potential for SMEs and can drive the discovery of new industrial materials.

Porous materials, including metal-organic frameworks (MOFs), are highly selective adsorbents with the potential to transform separation technologies. To fully leverage their capabilities, industrial R&D, research centers, and universities must develop new strategies for the characterization of liquid-phase adsorption.

This work proposes a novel advanced methodology to perform quantitative and precise measurements of liquid phase adsorption. To illustrate its applicability, the adsorption capacities of three different porous materials were studied: NoritRox0.8 carbon, the MOF HKUST-1, and the BasoliteA100 composite, using naphthalene, toluene, and bisphenol A as adsorbed molecules.

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INFLUENCE OF V AND SI INCORPORATION ON THE PHYSICO-CHEMICAL PROPERTIES OF VAP(S)O-5 FOR SELECTIVE METHANOL OXIDATION TO GREEN OXYGENATES

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Keywords: *heterogenious catalysis, methanol oxidation, zeolites, physico-chemical characterization, catalytic testing*

The selective oxidation of methanol offers a green route for the production of industrially relevant chemicals such as dimethoxymethane (DMM), dimethyl ether (DME) and methyl formate (MF), which are used as fuel additives, green solvents and intermediates for further processing. Current industrial processes require either multiple steps, high temperatures, or elevated pressures. In contrast, the controlled selective oxidation of methanol using bifunctional catalysts containing both redox and acid sites can reduce equipment complexity and energy demand. To enhance the yield of DMM and MF while preventing overoxidation to unwanted products, the amount and distribution of active sites in the catalyst must be precisely controlled. [1, 2] The hydrothermal synthesis of V-substituted, microporous alumino- and silicoaluminophosphates enables the adjustment of composition and thus the type and concentration of active species in the catalyst.

In order to evaluate the influence of the synthesis gel composition on catalyst structure and activity, various VAPO and VAPSO samples were prepared by varying the amounts of vanadium and silicon precursors during gel preparation. The gel was formulated with an increased template concentration to induce mesoporosity and facilitate the incorporation of vanadium into the framework, resulting in an overall gel composition of Al2O3 : P2O5 : x SiO_2 : y V2O5 : 1,35 Et3N : 40 H_2O, with x = 0 – 0.6 and y = 0 – 0.1. Crystallization was carried out in a stainless-steel autoclave with a PTFE liner at 180°C for 24 h. The synthesized and calcined samples were characterized via XRD, N2-sorption, UV-Vis DRS, TPR, SEM/EDX, and elemental analysis. Catalytic performance in selective methanol oxidation was evaluated using a fixed-bed reactor setup containing a defined particle fraction. The products were analyzed by GC-TCD/FID and MS.

In this contribution, first results of the physico-chemical characterization are presented, including the structural and morphological properties of the catalysts as well as information on the crystallinity and porosity of the samples. The results reveal a strong interplay between synthesis gel composition, crystallinity and the coordination of vanadia species in the analyzed materials. Furthermore, a catalytic screening using a WHSV of 1000 $kg \cdot s/m^3$ and a methanol-to-oxygen feed ratio of 1, conducted under varying temperatures, will be presented and discussed.

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Pore Size Analysis of Mesoporous Silica Materials by Advanced NMR Relaxometry and Gas Adsorption

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Keywords: *NMR Relaxometry, Pore Size Analysis*

During the last decades, major progress has been made in the synthesis of nanoporous materials, allowing the tailoring of nanoporous materials for targeted applications in various fields such as separation, catalysis, gas and energy storage. To increase the efficiency of these processes, it is necessary to tune the selectivity of the porous material to certain compounds of interest. Textural properties, such as the specific surface area and pore size may affect the process efficiency. Therefore, valid textural characterization methodologies are essential for both surface area assessment and pore size analysis. In this context, gas adsorption is widely used; however, its application is limited to dry materials, i.e., gas adsorption cannot determine effective textural properties of wet porous materials utilized in liquid phase processes such as chromatography and catalysis. Hence, novel methodologies for textural characterization of solvated porous materials are required. Within this context, we have recently shown that NMR relaxometry is promising for surface area assessment of solvated nonporous and nanoporous silica and carbon [1]. Within this work, we expand the applicability of NMR relaxometry for reliable pore size analysis.

Pore size analysis by NMR relaxometry is based on the fact that different liquid regimes may exhibit different relaxation times if diffusion is slower than their relaxation resulting in relaxation time distributions. Deciphering the exponential magnetization decay curve measured from a low- field 1H NMR spin-spin relaxation measurement into a reliable relaxation time distribution remains one of the key challenges. This requires a trustworthy solution of the Fredholm integral of the first kind with Tikhonov regularization or other fitting algorithms, respectively.

Using the Two-Fraction-Fast-Exchange model developed by Brownstein and Tarr [2], one can convert a relaxation time distribution to a pore size distribution. The application of NMR relaxometry for pore size analysis was pioneered in the 80s and 90s by Smith and co-workers [3]. However, a rigorous validation of NMR relaxometry for pore size analysis was not possible at that time due to a lack of well-defined model materials as well as limitations in adsorption characterization. This study therefore presents a systematic study to investigate the effect of confinement on the NMR relaxation behavior using nanoporous model materials with well-defined pore structure. The NMR relaxometry results are compared with benchmark pore size data determined with Ar 87 K adsorption.[4] Recent investigations successfully correlated qualitatively the results from NMR relaxometry with the intrinsic width of the pore size distribution by comparing ordered mesoporous silica molecular sieves (KIT-6 and SBA-15) exhibiting narrow pore size distributions with a disordered mesoporous silica. This shows for the first time the applicability of NMR relaxation for advancing liquid phase textural characterization.

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PREDICTION OF DIFFUSION IN MOFS FROM POTENTIAL ENERGY SURFACE

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Keywords: *Metal-organic framework, diffusion, potential energy surface, deep learning*

The separation of radioactive krypton from xenon is a critical environmental challenge in nuclear waste management. Metal-organic frameworks (MOFs), a family of porous materials which has shown potential for gas storage and separation, offer a promising solution.

As data-based methods are showing increasing power in accelerating materials discovery, we developed a deep learning model to predict gas diffusion coefficients in MOFs. We constructed a database by performing molecular dynamics (MD) simulations on over 8,000 structures from the CoRE MOF 2024 database [1]. From these trajectories, we calculated diffusion coefficients, only retaining results with reliable diffusive regimes, thus creating the first large-scale database of diffusion properties in nanoporous materials. [2] To avoid the inherent bias in geometric & energetic descriptor selection, we used the Moxel package [3] to generate 3D voxelized images of the potential energy surface (PES) for each structure. These 3D representations served as input for a retentive network (RetNet) [4]. We present a workflow that accurately predicts diffusion coefficients orders of magnitude faster than traditional methods, accelerating high-throughput computational screenings of materials.

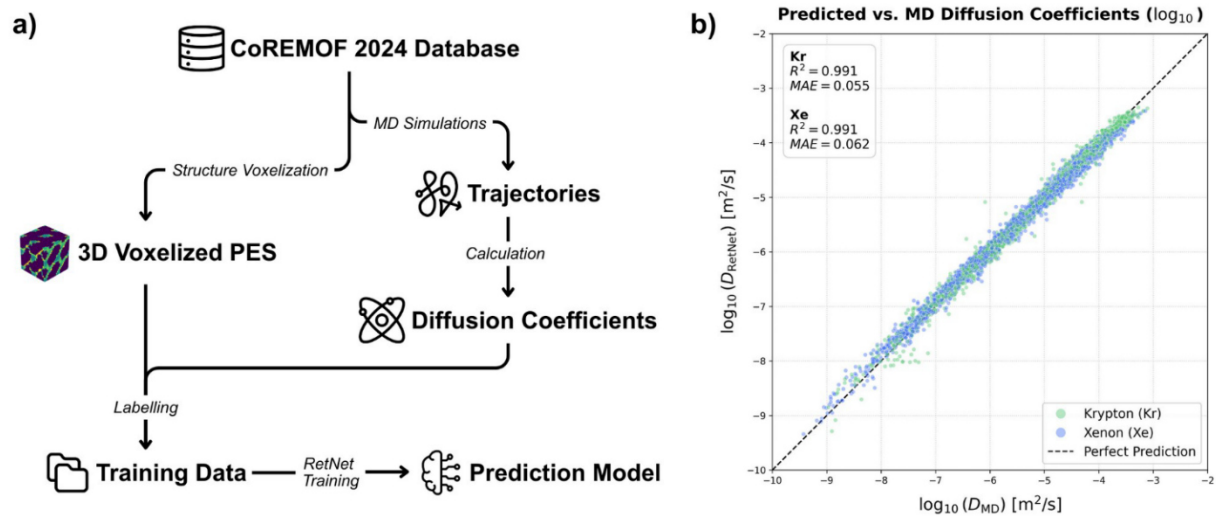

***Figure**: a) High-throughput screening workflow b) Parity plot comparing MD simulations and RetNet predictions*

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Photocatalytic performance of TiO2/MOF composites for hydrogen photo-production and pollutant photo-degradation in natural seawater

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Keywords: *TiO2, nanotube, MOF, degradation*

NH_2-MIL-125 (Ti) is a titanium-based metal–organic framework known for its stable, porous crystalline structure and enhanced photoactive properties. Built from titanium-oxo clusters linked with 2-aminoterephthalic acid, the framework incorporates amino groups that both strengthen the structure and narrow its band gap, enabling the absorption of visible light. These features make NH_2-MIL-125 (Ti) effective in applications such as photocatalytic degradation of organic pollutants, CO_2 reduction, and hydrogen generation.

In this study, a series of hybrid TiO_2 nanotube thin films decorated with NH_2-MIL-125 (Ti/Co) was developed. These TiO_2/MOF composites exhibit high activity in photoelectrocatalytic hydrogen production while simultaneously degrading seawater contaminants such as phenol under UV-Vis irradiation. The materials were tested using real seawater collected from the Baltic Sea, the Mediterranean Sea, and the Atlantic Ocean to reflect natural environmental conditions.

Comprehensive characterization including action spectra, UV-Vis and photoluminescence spectroscopy, FTIR, XRD, XPS, BET surface area measurements, and CO_2 sorption analysis allowed the properties of the prepared materials to be correlated with their performance and provided insight into the photocatalytic mechanism

Tailored Porosity in Mesoporous Hard Carbon Anodes via Soft Templating: Impact on Na-Ion Migration during (De)Sodiation

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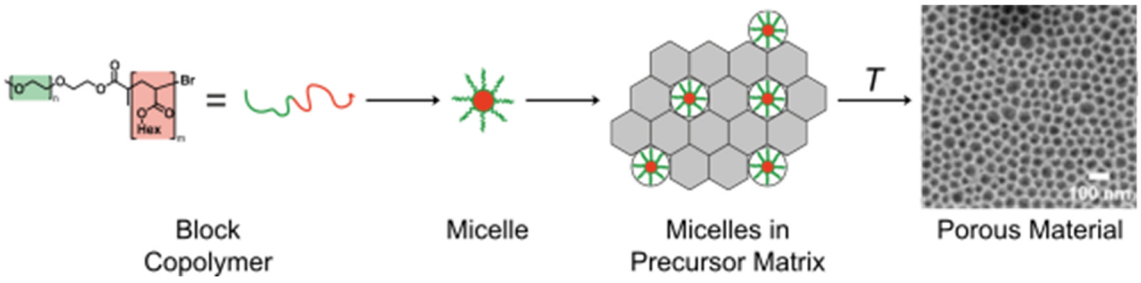
Keywords: H*ard Carbon, Sodium Ion Battery, Porosity Tuning*

Sodium-ion batteries (SIBs) are a promising alternative to lithium-based battery systems due to the high natural abundance and low cost of sodium salts. Hard carbon (HC), the most common anode material, is a non-graphitic carbon composed of small, disordered graphene layers and intrinsic microporosity arising from its turbostratic structure. The electrochemical performance of HC - particularly sodium storage capacity and ion transport - strongly depends on structural parameters such as interlayer spacing, defect density, and pore architecture. However, existing research investigates only a small range of pore sizes predominantly in the micropore region, to achieve higher capacities, but there are only few and mechanistic studies rather than systematic variation to elucidate their structure-performance correlation.[1,2]

In this work, we introduce well-defined spherical pores into resorcinol-based HC via soft templating using synthesized poly(ethylene oxide)-block-poly(hexyl acrylate) (PEOn-b-PHAm) block copolymers. This method enables controlled tuning of the mesopore size and wall thickness by adjusting block lengths and polymer concentration. We correlate the resulting pore network with sodium ion transport and storage characteristics. Structural and porosity analyses will be conducted using scanning electron microscopy (SEM), physisorption, and X-ray reflectivity (XRR). Future work will include the study of sodium migration and (de)sodiation processes which will be examined through electrochemical impedance spectroscopy (EIS), galvanostatic intermittent titration technique (GITT), and time-of-flight secondary ion mass spectrometry (ToF- SIMS). By systematically varying HC pore structures and assessing their impact on ion transport, this study aims to provide detailed insight into the role of porosity in determining HC anode performance, enabling the targeted design of high-capacity anodes for next-generation SIBs.



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TUNING GAS ACCESSIBILITY IN CARBON–IONIC LIQUID HYBRIDS THROUGH NITROGEN DOPING

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Keywords: *activated carbon, ionic liquids, gas adsorption, nitrogen doping*

Interfaces formed between porous carbon materials and ionic liquids (ILs) play a crucial role in catalysis, gas separation, and electrochemical energy storage and conversion. How gases interact with carbon surfaces in the presence of ILs strongly depends on the structure of the pores of the carbon and on the location of the IL within the pores.[1] Understanding this interaction makes it possible to design materials with optimized surface properties and controlled solid–liquid–gas interactions. This study investigates how nitrogen doping influences gas adsorption at the interface between pores of carbon and ionic liquids. Two nitrogen-doped CO_2-activated carbons with different pore sizes (NAC30 and NAC120) were synthesized and functionalized with EMIM TFSI and P4448 eFAP at varying loadings. The hybrid materials were characterized primarily by N_2 and CO_2 physisorption to quantify remaining pore volume and distribution of the IL. XRD and XPS provided supporting information on the structural properties and on how the ILs are positioned inside the carbon matrix. The results indicate that the position of the ionic liquids within the pores is influenced by pore size, nitrogen doping, and loading amount of IL. In NAC30 with smaller micropores, EMIM TFSI leads to complete pore filling, whereas P4448 eFAP forms closed porosity by obstructing the pore entrances. In contrast, NAC120 with larger micropores, both EMIM TFSI and P4448 eFAP composites retain open porosity. Notably, the undoped versions of the P4448 eFAP composites show closed porosity, highlighting that nitrogen doping influences the pore surface and can control IL distribution within the pore structure and consequently tune gas accessibility. Overall, the study demonstrates that nitrogen functionalities play a key role in modulating the spatial arrangement of ILs within the pore structure and in influencing gas–solid–liquid interfaces for applications such as electrocatalysis and energy storage.

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STRUCTURAL CONTROL OF PHOTOCONDUCTIVITY IN A FLEXIBLE TITANIUM-ORGANIC FRAMEWORKS

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Keywords: *flexibility, Ti-MOFs, photoconductivity*

The softness of metal-organic frameworks (MOFs) is a characteristic that differentiates them from other naturally occurring porous materials. This flexibility allows for the structured reorganization of the framework's components, enabling access to different states and properties in response to environmental changes.[1,2] In this context, the design of the organic ligand is fundamental to give the resulting material the desired structural and physicochemical properties.

Our work expands flexibility to titanium-based frameworks and shows controlled charge transport in porous molecular crystals. MUV-35 is a two-fold catenated TiMn2-based MOF with a rare site-c topology that can reversibly fold, reducing its volume by ~40% through a single-crystal transformation driven by linker conformations (Figure 1). This process is strongly thermodynamically favored (≈300 kJ·mol^{-1}) due to a network of non-covalent interactions that promotes solvent loss. The structural change enables charge-transport pathways, yielding photocurrents of 2.5 × 10^{-3} S·m^{-1} under visible light with an ON/OFF ratio of four orders of magnitude. Notably, this high conductivity is achieved together with a large porosity (~1000 m^2·g^{-1}). These findings provide a molecular strategy to enhance charge mobility in Ti-MOFs, with potential impact on photocatalysis and related semiconductor research.[3]

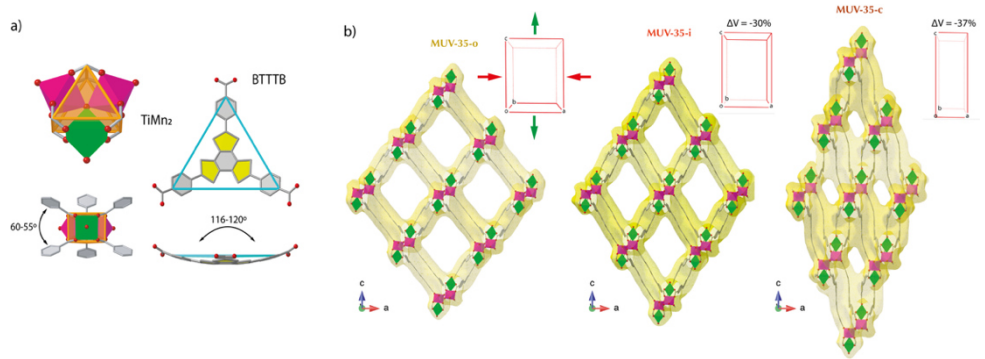

***Figure 1**. a) Structure of the 6-c trigonal prismatic $TiMn_2$ clusters and the 3-c BTTTB linkers, highlighting their internal geometry; b) From left to right: open (o), intermediate (i) and closed (c) structures of MUV-35 viewed along the b-axis.*

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Impact of Pore Structure and Particle Size on DMAP-Functionalized Silica Catalysts

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Keywords: *heterogeneous Organocatalysis, Physisorption, Porous Silica, DMAP*

4-Dimethylaminopyridine (DMAP) and its structurally related compounds are well known for their superior organocatalytic properties in a wide range of acetylation reactions, such as esterification.[1] The immobilization of DMAP motifs on the surface of a mesoporous silica carrier material enables its utilization for heterogeneous catalysis. The influence of the mesoporous size is a crucial parameter, as shown by Trommer et al.[2], but other relevant parameters, including the pore connectivity and pore size distribution, are still a matter of research. In this study, we addressed these questions by synthesizing mesoporous silica materials with variable mesoporosity, immobilized a DMAP organocatalyst, and studied the influence of the porosity parameters on catalytic properties in the acetylation of 1-phenylethanol

To answer this question, the pore system of commercially available spherical silica particles (LiChrospher Si60 (5 µm)), in which 6 nm mesopores are partially connected through small neck pores (3 nm). Thus, the mesopore space, featuring this potentially hindered connection, was modified by two different processes. In the first process, the pore connectivity was improved by etching. In contrast, in the second procedure, the sample underwent a pseudomorphic transformation (PMT)[3], which modified the pore space to yield a defined MCM-41-like pore system (cylindrical channels of ca. 3-4 nm). By immobilizing DMAP on the surface of the pore system in a two-step synthesis, the impact of the surface treatments on DMAP's catalytic activity was analyzed. The success of the surface modifications and each functionalization step was monitored by N2 physisorption and IR measurements; additionally, the catalytic load was determined by elementary analysis. The catalytic performance was tested in batch catalysis.

In comparison to the commercially available LiChrospher particles with suboptimal pore connectivity, the enhanced pore connectivity resulting from etching leads to an improved catalytic performance. Surprisingly, the ordered MCM-41-type pore system with small pores and a narrow pore size distribution (4 nm, PMT sample) exhibits enhanced catalytic performance compared to the LiChrospher particles, which was not anticipated based on the observations reported by Trommer et al.[2]. These results indicate that the pore connectivity and especially the order or pore-size distribution of the pore system of mesoporous silica carrier materials may play a crucial role if used in catalytic applications.

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Precise intermolecular distance control of fluorenones in a Zr-/Hf-MOF for sensing applications

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Keywords: zirconium MOFs, VOC adsorption, flexibility, solvatochromism

Volatile organic compounds (VOCs), particularly ketones, represent a significant class of airborne pollutants emitted by industrial processes. Owing to their toxicity and role in atmospheric degradation, their capture and separation are of critical environmental and public health importance.[1] Highly selective metal–organic frameworks (MOFs) have emerged as promising materials for VOC remediation due to their tunable physicochemical characteristics, including high specific surface areas, adjustable pore architectures, and customizable surface functionalities.[2] In this study, we report a new flexible, Zr/Hf-based MOF incorporating a fluorenone-functionalized linker (DUT-207, DUT = Dresden University of Technology). The Zr/Hf nodes impart superior chemical, mechanical, and thermal robustness, while the fluorenone moiety contributes solvatochromic properties across diverse solvent environments. Single-crystal X-ray diffraction revealed that the combination of a tetratopic linker with a 10-connected Zr/Hf cluster leads to an atypical MOF topology (Figure 1).[3] The secondary building units (SBUs) are linked by six ligands, two of which coordinate to the same cluster via double bidentate carboxylate groups, effectively converting the tetratopic linker into a tritopic node. Partial desolvation of the structure triggers an unprecedented phase transformation for Zr-/Hf-clusters where the 0D SBUs irreversibly fuse to 1D chains, followed by a second transition upon further solvent removal. Each of the three obtained phases exhibits well-defined intermolecular distances between the fluorenone units, enabling precise tuning of the physicochemical properties. Remarkably, the desolvated DUT-207 framework is largely inaccessible to most gases and vapors, yet it exhibits exceptional affinity and selectivity toward ketones. Furthermore, DUT-207 demonstrates distinct solvatochromic responses in the presence of aforementioned vapors, suggesting its dual functionality as both an efficient adsorbent and a potential chemical sensor.

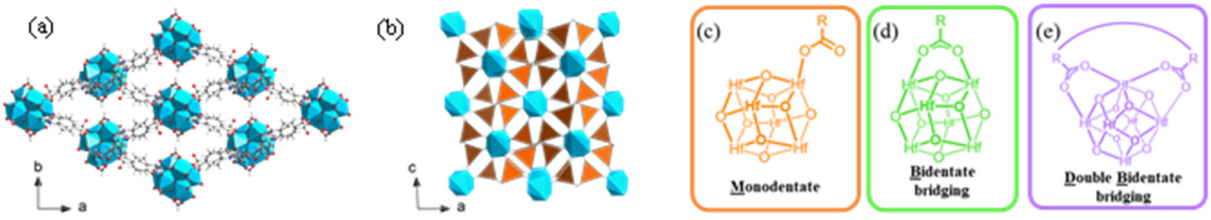

Fig. 1. (a) Crystal structure of DUT-207-I (as synthesized), view along c-axis. (b) Topological deconstruction of the MOF (3,8-c net, 3,8T220). Cyan – Zr/Hf, red – O, blue – N, grey – C, white – H. (c), (d) and (e) monodentate, bidentate and double bidentate bridging modes respectively.

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Thermodynamic-driven CH4/H2 Separation by Stable MOFs

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Keywords: *Metal organic framework, separation, green house gas.*

As a primary green energy carrier, hydrogen contributes to initiatives for attaining carbon neutrality in power generation and transportation by burning only water vapor and avoiding emissions of long-lived greenhouse gases.[1] Hydrogen recovery from natural gas pipelines after co-transport and hydrogen purification following steam methane reforming are two crucial applications in the hydrogen supply chain that depend on the effective separation of methane from hydrogen. The main technologies for hydrogen purification are pressure swing adsorption (PSA), cryogenic distillation, metal hydrides, membrane separation.[2] Conventional methods of separation need a lot of energy. Adsorption-based or membrane-based separations using the porous materials plays a crucial role as energy efficient alternatives for making the hydrogen transport economically competitive. There are various materials which are commercially available that can work in this process such as activated carbon, silica gel, zeolites. But these materials have some drawbacks; selectivity, performance. Over the last ten years, research has demonstrated that a family of adsorbents called metal-organic frameworks (MOFs) can offer improved performance, selectivity, and reduced energy costs.[3] In order to examine a wide range of MOFs for physisorption-based CH_4/H_2 separation under practical operating circumstances, atomistic simulation has been used in this work. In this pre-screening step, a number of MOFs were shown to have better separation performance than commercial adsorbents such as activated carbon and Zeolite 13X. Consequently, robust, scalable, and cost-effective Al and Fe based MOFs have been synthesized and characterized. Their experimental CH_4/H_2 breakthrough separation has been studied and their performances were compared to the predicted one. Furthermore, the practical feasibility of the materials for PSA was confirmed by evaluating the diffusion kinetics of CH_4 and H_2 in a selection of high-performing MOFs using molecular dynamics simulations. All things considered, this study suggests a number of useful MOFs as potential adsorbents for effective hydrogen separation. In this communication, our joint experimental-computational study will be further detailed before shedding light on the major findings related to the aforementioned MOFs and how each of them can outperform when it comes to compares working capacities and selectivity.

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Exploring Mixed-Metal Incorporation in 2D Layered Metal–Organic Frameworks

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Keywords: *2D MOFs, heterometallic MOFs*

Two-dimensional metal–organic frameworks (2D MOFs) combine high surface areas, short electron transport pathways, and abundant active sites, making them attractive for various functional applications. Among the different design strategies, incorporating more than one type of metal center into a cluster has become particularly appealing, as heterometallic MOFs enable electronic and geometric tuning at the cluster that often yields synergistic gains in catalytic activity[1], improved gas separation[2], and enhanced stability[3]. Developing reliable synthetic approaches for mixed-metal 2D MOFs is therefore an important step toward expanding their structural and functional diversity.

In this work, we investigated the incorporation of Co and Zn into the layered MOF DUT-158(Cu) ($[Cu_2(cdc)]_n$, cdc = carbazole-3,6-dicarboxylate)[4]. Two approaches were considered: post- synthetic metal exchange and one-pot synthesis. Post-synthetic attempts, using Zn did not yield an isostructural analogue of DUT-158 but instead produced a new compound. In contrast, in one-pot reactions, Co or Zn could be successfully incorporated into DUT-158 in varying ratios. SEM–EDS confirmed the formation of mixed-metal MOFs and the homogeneous distribution of metal ions within the crystals. These findings highlight the feasibility of incorporating secondary metals into DUT-158, establishing a versatile platform to further explore mixed-metal strategies in two- dimensional MOF systems.

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INFLUENCE OF POROSITY OF BIMODAL SILICA MONOLITHS ON THE PERFORMANCE OF DMAP IN HETEROGENEOUS CATALYSIS

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Keywords: *porous silica monolith, physisorption, organocatalysis, heterogeneous catalysis*

Heterogeneous catalysis by use of immobilized organocatalysts on a solid support show great advantages compared to its homogeneous analogue like simpler product workup, better recyclability of the catalyst and use in flow applications.[1] Important prerequisites of a porous solid support for flow applications are a high surface area and optimized mass transport through the system, which can be achieved by the introduction of well-defined meso- and macropores.[2] In this report we investigated the influence of meso- and macropores sizes in silica monoliths as solid support on the catalytic performance of immobilized DMAP, an organocatalyst, which is known for its high activity in acetylation reactions.[3] For that purpose, meso-macroporous silica monoliths with a mesopore size range of 12 nm to 19 nm and a macropore size range of 2.0 µm to 4.0 µm were synthesized by a modified Nakanishi process.[4] The monoliths were functionalized in two steps, first by imobilization of (3-azidopropyl)trimethoxy silane and subsequently by a Click-reaction of propargyl functionalized 4-methylaminopyridine.[5] The the monoliths were characterizided by Hg-porosimetry (MIP), nitrogen physisorption, DRIFT and elemental analysis measurements. To test the catalytic activity, flow catalysis experiments of the acetylation of 1-phenyl ethanol, (−)-menthol and α-tocopherol with acetic anhydride were performed. Overall, the acetylation of 1-phenyl ethanol (86% at 0.1 mL·min^{-1}) and α-tocopherol (89% at 0.1 mL·min^{-1}) showed similar conversions, while the conversions of (−)-menthol were lower (72% at 0.1 mL·min^{-1}). This shows that the molecular size difference of 1-phenyl ethanol and α-tocopherol does not influence the reaction, while the steric hinderance of the isopropyl group of (−)-menthol could be the reason for the decreased conversions. Turnover frequency (TOF) values showed a range up to 0.029 s^{-1}, 0.011 s^{-1} and 0.0026 s^{-1} for the acetylation of 1-pheny ethanol, (−)-menthol and α-tocopherol, respectively at 1 mL·min^{-1} for the monolith with the smallest meso- and macropore size. With increasing pore sizes, the TOF values decreased. This finding can be explained by improved mass transport through the macropores, as smaller macropores were accompanied by a higher macropore volume. The influence of the mesopores could be explained by the higher concentration of smaller mesopores as well by the increased surface area, which leads to less blocking of catalyst by other catalysts. In conclusion, we show that in a size range of 12 nm to 19 nm for mesopores and 2.0 µm to 4.0 µm for macropores, monoliths with smaller pore size display a superior catalytic performance.

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Single-Atom Water Model: Evaluating Accuracy for Adsorption in Metal–Organic Frameworks

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Atmospheric water harvesting and humidity-driven separation processes increasingly rely on metal–organic frameworks (MOFs) that adsorb water efficiently. Molecular simulation can guide materials discovery and atomistic understanding of studied processes. However, the conventional all-atom water models are often prohibitively expensive when applied to porous materials. In nanoconfinement, water tends to form strongly coordinated clusters that reorganize slowly, and simulating these processes requires long computational times and advanced simulation techniques [1]. This limits both systematic screening and the precise analysis of adsorption mechanisms.

Coarse-grained/single-atom water models, such as mW [2], offer a practical alternative route by representing water with a single interaction center. Such models have demonstrated the ability to reproduce thermodynamic properties and structural characteristics of the all-atom water model at a substantially reduced computational cost. However, to employ them reliably in MOFs, reparameterization of standard force fields is necessary, as conventional Lennard-Jones plus point charge approaches are incompatible.

A Python workflow was developed to optimize MOF-mW pairwise potentials by matching reference energetics and local structure from TIP4P-based calculations at representative adsorption sites. This procedure fits simple pairwise terms to reproduce the depth, position, and curvature of adsorption relevant energy profiles and further validate and optimize them via radial distribution function (RDF).

The developed multi-step optimization scheme produced reasonable initial LJ parameters between MOF sites and mW water model. RDF calculation demonstrated that the newly derived parameters are capable of reproducing the structure of adsorbed water. We will discuss the resulting flat-histogram Monte Carlo isotherms and accuracy-efficiency trade-offs. The workflow presented herein provides a practical foundation for developing robust, scalable, and mechanism-aware MOF-mW force fields for AWH and related applications.

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HYDROGEN STORAGE IN CARBON-BASED POROUS MATERIALS

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Keywords: *adsorption, hydrogen, clathrate, carbon*

Hydrogen has become a key energy carrier in the global shift toward sustainable and carbon-neutral energy systems. Developing cost-effective storage technologies with high capacity and fast operation is crucial for realizing a hydrogen economy, particularly in the transportation sector. A variety of technologies can be utilized to store hydrogen such as high-pressure gas tanks, cryo- compressed hydrogen storage, porous materials, metal hydrides, and hydrogen hydrates. One promising storage technology is the formation of hydrogen clathrates. Hydrogen molecules can be confined within cages formed by water through physical encapsulation, where van der Waals interactions stabilize the clathrate structure. To make the approach practicable, porous materials with tuned pore structure can be used as a nanoconfining medium lowering the thermodynamic requirements enabling clathrate formation under moderate conditions. In this context, carbon materials are promising candidates for hydrogen storage due to highly tailorable pore structure and surface chemistry.[1,2] The aim of the study is to investigate an approach that utilizes clathrate hydrate formation to physically confine hydrogen gas within porous carbons under moderate pressure and temperature conditions.

For this purpose, various porous carbons were synthesized and doped with nitrogen. The synthesis of porous carbons with doping and activation from organic waste products and the condensation of the nitrogen-containing precursor were carried out.[3,4] Firstly the porosity of produced carbons was examined. Nitrogen physisorption (77 K) reveals a microporous structure of the nitrogen-doped carbon and a mesoporous structure of the pristine carbon. Water vapor physisorption (298 K) was performed to investigate water-carbon interactions, allowing the estimation of both the material's water loading capacity and its inherent wettability. The correlation between nitrogen content, and the carbons' hydrophilicity was established. Furthermore, water- carbon interaction was investigated by inelastic neutron scattering. The data indicate that strongly bound water in the more hydrophilic carbons leads to non-freezable water, while ordered cluster- like arrangements of water are revealed for less hydrophilic carbons, which may potentially influence the kinetics of clathrate formation. Then, hydrogen-carbon interactions were studied. Hydrogen adsorption measurements were performed at 273 K up to 200 bar, showing that microporous materials with higher surface areas and pore volumes lead to higher hydrogen uptake.

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DISCRIMINATORY WATER-METHANOL SIEVING IN AN ADAPTIVE METAL-ORGANIC PEPTIDE-FRAMEWORK

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Keywords: *molecular sieves, methanol dehydration, structural adaptivity*

Methanol and ethanol are key platform chemicals used as fuels, solvents, and intermediates, playing a vital role in sustainable energy technologies. Dehydration of crude alcohol mixtures is crucial but energy-intensive via conventional techniques. Adsorption-based methods offer a more efficient alternative. An adaptive peptide-based ultramicroporous coordination polymer (DUT- 240, DUT = Dresden University of Technology) shows preferential water uptake but negligible alcohol adsorption enabling highly selective adsorptive separation of water/methanol mixtures, a merit unattained so far by any other porous material. Single-crystal X-ray structural analyses combined with theoretical calculations unveil the adaptive nature of host–guest interactions playing a key role in the mechanism of selective water uptake, highlighting the potential of peptide-based frameworks for competitive energy-efficient alcohol dehydration [1].

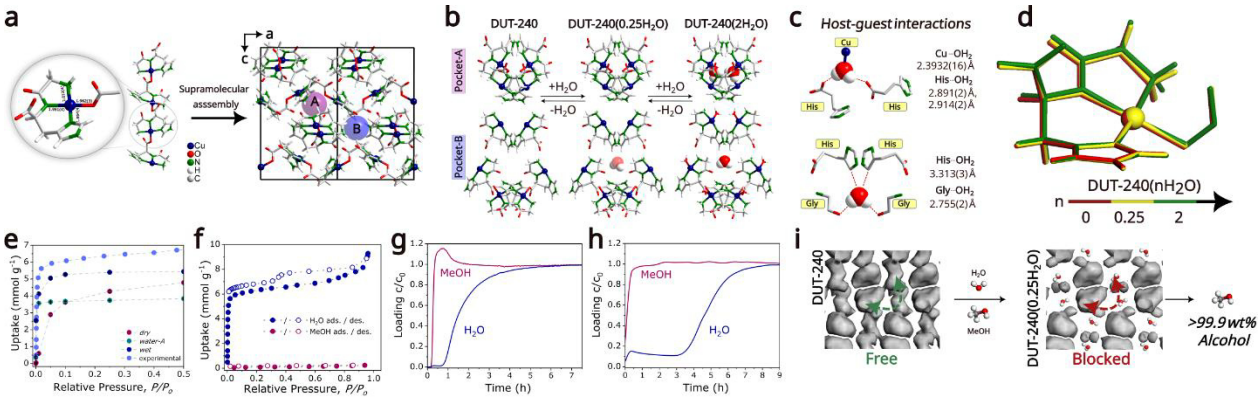

Figure 1 ***a,*** *Assembly of the 1D metal-peptide chains into an ultramicroporous supramolecular architecture.* ***b,*** *Crystal structures of DUT-240 with various water loadings.* ***c,*** *Atomically precise host-guest interactions.* ***d,*** *Subtle structural adaptivity around the peptide ligand depending on the water loading.* ***e,*** *GCMC isotherms calculated for structural variants with different water loadings.* ***f,*** *Experimental physisorption isotherms of H2O and MeOH recorded at 298K.* ***g, h,*** *MeOH/H2O breakthrough curves (ratios 50:50 and 95.5:4.5 respectively).* ***i,*** *Proposed mechanism of H2O over MeOH selectivity.*

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Click-enabled Grafting for Adaptive Chiral Recognition in Porous Crystals

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Keywords: *Chiral recognition, click chemistry, adaptive porosity, post-synthetic modification, metal–organic frameworks (MOFs).*

Reticular frameworks are ideal candidates for engineering chiral environments, [1] yet most strategies rely on the static incorporation of stereogenic units, often overlooking the role of adaptive host–guest interactions in enantioselective recognition. We report a modular post-synthetic click strategy to install amino acid–derived peptidic moieties into UiO-68 frameworks without compromising crystallinity. [2, 3] Only the histidine-functionalized material exhibits high enantioselectivity (~80% *ee*) for cetirizine. Simulations reveal the formation of conformationally adaptive interaction pockets, emphasizing the importance of local pore reorganization in chiral molecular recognition. [4]

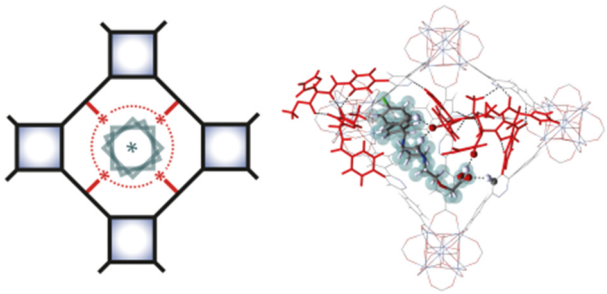

Figure 1. *Adaptive chiral pockets for enantioselective recognition.*

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Tuning gas separation performance in Mg-fumarate MOF (DUT-153) through controlled desolvation

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Metal–organic frameworks (MOFs) are highly promising materials for gas adsorption and separation applications because of their exceptionally high surface areas and structural tunability.[1] This allows adjustment of surface affinity toward specific adsorptives as well as tailoring the framework structure to enable size selective gas separation.[2]

$[Mg_3(DMF)_2(fum)_3]\cdot(DMF)$ (DUT-153), a novel Mg-fumarate (fum) MOF, demonstrates an interesting ability to adjust its adsorption behavior through the solvent molecules contained within the pores of the network. As illustrated in Fig. 1a, a key characteristic of this three-dimensional MOF is the presence of dimethylformamide (DMF) molecules, blocking the channel-like pores.

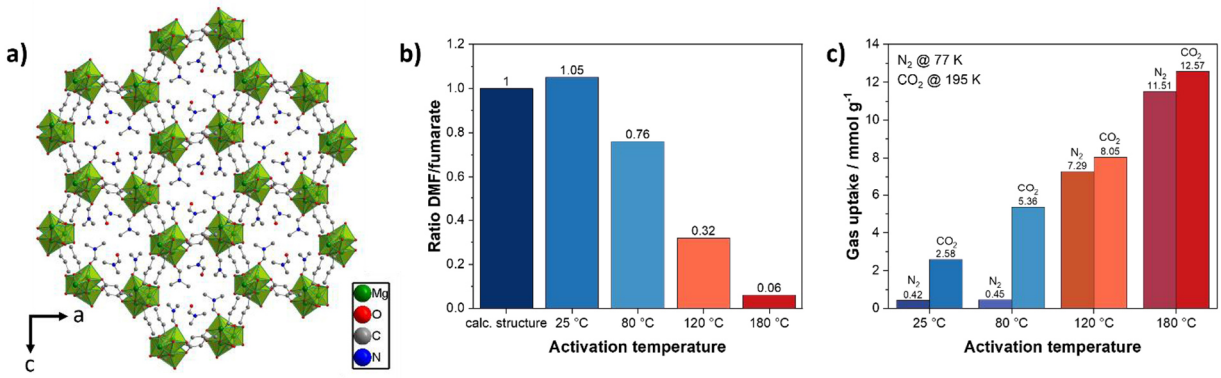

Figure 1: a) Crystal structure of DUT-153 along the b-axis. (Mg green, O red, N blue, C grey, H omitted). b) Ratio of DMF to fumarate based on 1H-NMR experiments. c) Compared N2 and CO2 uptake in DUT-153 after activation at different temperatures.

This structure containing coordinated and uncoordinated DMF enables controlled tuning of pore accessibility by selective removal of solvent molecules. During the desolvation process, DMF is removed stepwise, resulting in variable pore diameters. The correlation between solvent content and pore size was explored through theoretical calculations of pore accessibility, which were experimentally validated using 1H-NMR spectroscopy (Fig. 1b), as well as nitrogen and carbon dioxide physisorption measurements (Fig. 1c). Physisorption experiments revealed substantial differences in gas uptake, attributed to the varying kinetic diameters of the respective gases, and they are in line with the expectation from the given pore diameters. Thus, by regulating the solvent content in DUT-153, the pore accessibility can be finely tuned. This achieves gas separation through size exclusion, with selectivity that can be dynamically adjusted based on the degree of solvation.

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Atomic-Scale Detection of Surface Defects in $CuInS_2$ Quantum Dots Using Advanced (S)TEM Imaging and Multislice Simulation

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Keywords: *TEM, STEM, Surface defects, simulation, quantum dots,*

$CuInS_2$ (CIS) quantum dots (QDs) have attracted significant attention over the past two decades due to their synthesis-tunable photoluminescence, and reduced toxicity compared to Cd- and Pb- based QDs [1][2]. At the nanoscale the optical and catalytic behavior of CIS is strongly governed by its surface structure. Undercoordinated metal and chalcogen sites play a decisive role in charge recombination, carrier trapping, and catalytic activity, meaning that even subtle surface defects can substantially modify functionality [2][3]. Such defects may arise unintentionally during ligand stripping, chemical processing, shell growth, or even during the characterization procedure itself. CIS QDs share fundamental characteristics with high-surface-area hybrid systems, and understanding and detecting subtle surface modifications is therefore essential for correlating synthesis, structure, and function across a wide class of hybrid nanomaterials.

Here, we combine theoretical and experimental electron microscopy with complementary spectroscopy to assess the conditions under which surface modifications in CIS QDs become detectable. CIS QDs synthesized via a green aqueous colloidal route [4] were characterized by TEM to assess particle morphology and dispersion. A comparative analysis of pristine and ligand-stripped QDs was conducted using XRD to monitor average structural variations and XPS to probe surface chemistry and ligand loss. High-resolution TEM, HR-STEM, and EDS mapping were used to identify vacancy-like signatures, changes in surface ordering, facet rounding, and near-surface compositional variations. To rationalize these observations, CIS structures containing representative defect motifs were investigated using multislice simulations. These simulations provide fingerprints for distinct defect configurations and define imaging conditions under which surface disorder or missing atom contrast should be experimentally resolvable. Comparison between experiment and simulated image signatures enables discrimination between competing defect models and reveals the dominant structural motifs responsible for the observed reconstructions.

This multimodal approach establishes a robust framework for identifying surface defects in colloidal nanomaterials and demonstrates how electron-based imaging and spectroscopy can be correlated to reveal defect landscapes at the atomic scale.

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Phase selection of ZIF-8 in Aqueous: Directing ZIF-L to ZIF-8 via modulating ligand

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Keywords: Zeolitic imidazolate frameworks (ZIFs), Ligand modulation, Phase selection

Controlling the crystallization pathway of zeolitic imidazolate frameworks (ZIFs) is essential for enhancing porosity, stability, and surface chemistry for applications such as gas adsorption, catalysis, and host–guest systems[1]. Despite significant progress in the synthesis of ZIF-8, many methods still rely on co-solvent systems because pure aqueous media introduce additional complexities[2]. In this study, we investigate how introducing a modulating ligand affects the phase selection and structural development of ZIF nanocrystals in aqueous media.

By systematically adjusting the ratio between the primary linker and a modulating ligand, we observe a notable shift in the crystalline phases accompanied by significant differences in morphology of particles. A combination of X-ray diffraction, infrared spectroscopy, electron microscopy, and thermogravimetric analysis reveals that ligand modulation changes the phases from ZIF-L, a 2D layered structure to a 3D cubic stable ZIF-8 phase. These changes are further confirmed by N2 sorption analysis, highlighting differences in porosity and surface area.

Our findings suggest that the modulating ligand disrupts the hydrogen-bonding interactions that stabilize ZIF-L, thereby slowing both nucleation and growth and promoting the formation of larger ZIF-8 particles under mild and environmentally friendly synthesis conditions. The modulator avoids the need for high concentrations of the primary ligand in water-based synthesis and provides insight into how adjustments in precursors of MOFs can govern phase selection and the resulting structural features of ZIF materials. The ability to direct ZIF phase formation through simple ligand tuning opens new opportunities for environmentally friendly formation of porous crystalline materials with tailored properties.

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INVERSE OLEFIN/PARAFFIN GAS SEPARATION WITH FUNCTIONALIZED FLEXIBLE METAL-ORGANIC FRAMEWORKS

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Keywords: *metal-organic framework, gas separation, gas adsorption, reticular chemistry*

The industrial production of polyethylene (PET) and polypropylene (PP) requires a flow of the starting light olefin (ethylene, propylene) with a high purity (>99.5 %). To achieve this, olefin/paraffin mixture feeds are separated by the energy-intensive cryogenic distillation [1]. Efficient selective sorbents to be used in PSA and membrane schemes can substitute distillation. In addition, a paraffin-selective sorbent is highly desired as it simplifies the operational scheme [2]. Metal-organic frameworks (MOFs), porous crystalline materials with high tailorability, have potential as advanced sorbents, and their unique structural flexibility can be leveraged for olefin/paraffin inverse separation.[3]

Here, we present the MOF structure ZIF-7 containing Zn^{2+} ions and benzimidazole (bim) linkers. This MOF show gate opening/closing phenomena with increasing/de-creasing gas pressures transitioning from a close pore (cp) to an open pore (op) phase. (Fig. 1a) These transitions are gas dependent and can be used to efficiently separate gases. We explore structural modifications by introducing functionalized linkers *via* Solvent-Assisted Linker Exchange (SALE) (Fig. 1b). Some of our results have shown that the introduction of methyl groups separates propane and propylene gate transitions, potentially benefiting separation at low pressures (Fig. 1c). Overall we present a versatile strategy to tune advanced sorbents for challenging gas separations

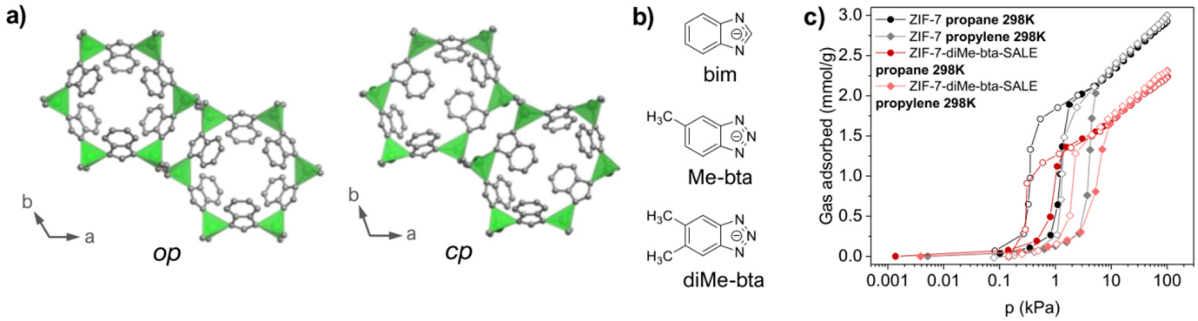

Figure 1. (a) Open- and closed-pore structures for ZIF-7. (b) Structural ligands explored in this work. (c) Propane and propylene adsorption/desoprtion isotherms (298 K) for ZIF-7 and ZIF-7- diMe-bta-SALE.

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From Pore to Defect Engineering: Cu_2 Triazolyl Isophthalate MOFs for Dihydrogen Adsorption and Isotopologue Separation

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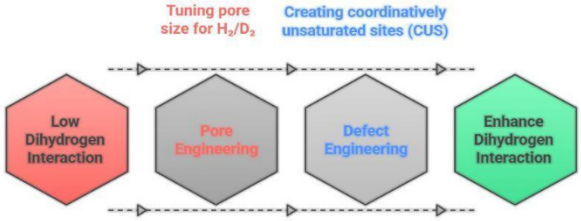
Keywords: *Isotopologue Separation, H2/D2 Sorption, EPR, XPS, Defect(Pore) Engineered MOFs*

This study explores the complementary roles of pore engineering and defect engineering in Cu_2paddle-wheel Metal–organic frameworks (MOFs) for dihydrogen adsorption and isotopologue separation. In the pore engineering approach, a series of [Cu-R-R'-trz-ia] (R=H, R' = –H, –Me, – Et, –^{n}Pr) frameworks were synthesized to investigate how linker substituents influence pore size distribution (3.2–5.0 Å), and their adsorption behavior. These ultramicroporous structures exhibited steep dihydrogen uptake below 10 kPa, with isosteric heats of adsorption between 8.9 (11.5)-12.2 (12.8) kJ mol^{-1} for H_2 (D_2).[1]

In parallel, defect engineering was achieved in [Cu_2(H-Me-trz-ia)$_2$] MOF by introducing mixed linkers approach to generate coordinatively unsaturated sites (CUSs). Spectroscopic analyses (FTIR/Raman, XPS, and EPR) confirmed that increasing defect concentration enhanced adsorption enthalpies, with Qads rising from 8.9 (11.52) to 14.4 (16.5) kJ mol^{-1} for H_2 (D_2).[1] Thermal desorption spectroscopy and pyGAPS[2] calculations further demonstrated that defects strengthen adsorbate interactions and improve hydrogen isotopologue separation efficiency. Together, these findings highlight how structural tuning through both pore and defect engineering provides a strategy for optimizing MOFs in dihydrogen adsorptions and separation applications.



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Porous Magnets and Organic 2D Frameworks

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Keywords: *Magnetism, Organic Frameworks, Theoretical Design, DFT, 2D Polymers*

Organic 2D frameworks with metal-free magnetism have garnered significant attention due to their potential applications in organic spintronics and quantum information technologies [1–3]. However, achieving stable spin polarization and precisely controlling magnetic interactions in these systems remains challenging, primarily because of strong electronic coupling and the closed- shell electronic configuration of most organic building blocks.

In this talk, I will present two distinct strategies to induce spin polarization and tailor magnetic interactions in organic 2D frameworks. The first approach exploits charge transfer to generate unpaired spins in otherwise diamagnetic 2D covalent organic frameworks (COFs) [4]. The second strategy employs nanographenes bearing stable radical centers as building blocks, with particular focus on triangulene — the smallest polybenzenoid hydrocarbon featuring a triplet ground state and intrinsic spin polarization [5]. By assembling triangulene monomers into dimers and extended 2D frameworks, we theoretically investigate methods to control magnetic interactions and electronic structures. Rational chemical design of triangulene dimers yields strong antiferromagnetic coupling with exchange constants (J) as large as –198 meV [5]. Furthermore, triangulene-based 2D frameworks display intriguing electronic properties, including a Dirac point flanked by twin flat bands. In triangulene-based 2D radical frameworks, Mott–Hubbard-type antiferromagnetic ordering is predicted with J = –32 meV. By tuning the Fermi level, we demonstrate the emergence of metal-free ferromagnetism with estimated Curie temperatures around 260 K and half-metallic behavior in nitrogen-centered triangulene 2D frameworks [6,7]. Moreover, we propose a mixed-topology design strategy that enables purely organic 2D ferromagnetic frameworks with exceptionally strong ferromagnetic coupling (J up to 127 meV) and Curie temperatures exceeding 500 K [8]. These findings pave the way for the development of 2D porous magnetic materials for future spintronic and nanoscale devices.

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Screening Open Metal Sites in Metal-Organic Frameworks for Catalysis and Isotope Separation

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Keywords: *metal-organic frameworks, quantum chemistry, statistical models, high-throughput screening, ^{3}He-^{4}He separation, CO oxidation*

Metal-organic frameworks (MOFs) offer an unprecedented diversity of structures, many of which can host active, under-coordinated open metal sites (OMSs) that enable catalysis and separation. The building-blocked based nature of MOF catalysts renders them amenable to precise tuning of these active sites as required to a target a specific chemical task. However, the vast combinatorial space of MOFs poses a significant challenge in identifying optimal candidates appropriate for a given application. Recent advances in computational modeling and machine learning offer the potential to explore and sort out this myriad of possibilities and prioritize synthetic planning. As such, computer-aided MOF discovery is highly desirable, yet the computational prediction of MOF activity remains an inherently difficult task. In this work, I will discuss our efforts for predicting the activity of open metal sites in MOFs, particularly relevant catalysis and separation.

We show that simplified models of open metal sites (OMSs) in MOFs capture activity trends with reasonable accuracy and can be leveraged to predict the performance of realistic material models. This approach is illustrated through two applications: (i)CO oxidation catalysis and (ii) helium isotope separation.

(i) We demonstrate how this approach identifies chemical descriptors for CO oxidation that enable prediction of catalytic performance and comparison of realistic active sites across diverse MOF families. Our results uncover the origins of exceptional catalytic activity and emphasize the role of cooperative neighboring metal centers in breaking conventional scaling limitations.[1]

(ii) By using simplified cluster models, we reveal that Cu(I) sites with suitable ligand environments bind helium strongly enough to permit ^{4}He/^{3}He separation at technologically relevant temperatures. Leveraging these findings, we construct a predictive model to screen synthesized MOFs with Cu(I) sites and identify the most promising candidates.[2]

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PHASE IDENTIFICATION AND REPRODUCIBLE SYNTHESIS OF Fe–TEREPHTHALATE METAL–ORGANIC FRAMEWORKS

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Keywords: *Fe–BDC MOFs, phase identification, reproducible synthesis, framework flexibility*

Iron–terephthalate metal–organic frameworks (Fe–BDC MOFs) display pronounced polymorphism, which often complicates reproducible synthesis and reliable phase identification due to their dynamic nature [1-4]. In this study, we explore how variations in precursor, solvent, temperature, and pH effcet the formation of the main Fe–BDC phases MIL-88B, MIL-53, MIL- 101, and MIL-68. Solvent-dependent powder X-ray diffraction is shown to capture distinct breathing-related responses, enabling fast and robust phase discrimination. These findings are supported by complementary characterization using FTIR, SEM, TGA, XPS, Mössbauer spectroscopy, and elemental analysis. Overall, this work provides practical reference data and clear guidelines for controlling phase formation and understanding flexibility in Fe–BDC MOFs.

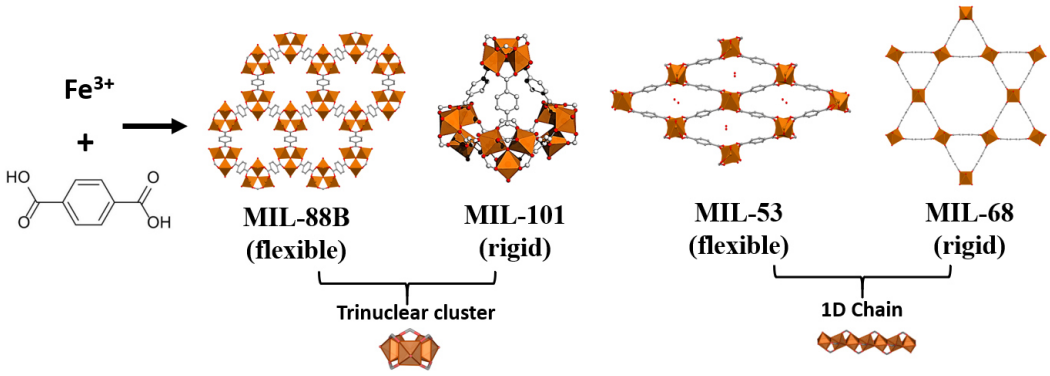

Figure 1. Schematic representation of Fe–BDC MOFs

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Sulfur Impregnation in Porous Materials for CO2 Adsorption

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Keywords: *Sulfur confinement, N2 adsorption, immersion calorimetry, Raman Spectroscopy*

Sulfur-doped porous materials are of great interest in the field of gas capture and storage. [1] The most common methods for doping materials are functionalization and liquid impregnation, described in detail in the literature. [2][3] Our research work focuses on a third route, which is confinement of elemental sulfur (S) by vapor impregnation that allows a better control of the filling of the porosity. In order to provide a complete picture of the confinement, we investigate the effects of different sulfur loadings, pore size, pore geometry and surface chemistry. Our work is twofold: (i) fundamental research to provide a better and deep understanding of the thermodynamic, structural and dynamic properties of sulfur confined in nanopores (ii) applied research to develop a generic methodology to prepare new sulfur nanocomposites for optimized CO_2 capture.

In this contribution we will first present a complete description of the porous matrices using standard techniques, such as thermal analysis, nitrogen adsorption at 77K, X-ray diffraction and Raman spectroscopy, but also less common method such as tomography by transmission electron microscopy. This method allows a 3D view of porous network and gives information on pore size and connectivity, enabling visualisation and better understanding of porous network.

In a second part, the energies of interaction between liquid sulfur and the various matrices (carbon and silicas) obtained by immersion calorimetry will be presented. We recently showed that this method, generally used at ambient temperature with standard organic solvents[4] can be extended to high temperature conditions and with liquid sulfur. [5] This technique also gives information about the kinetics of filling.

Finally, we will present the physico-chemical characterization of several nanocomposites and propose the required compositions for enhanced CO_2 adsorption.

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Synthesis and Characterization of COF-Metal Nanoparticle Hybrids for Catalytic Applications

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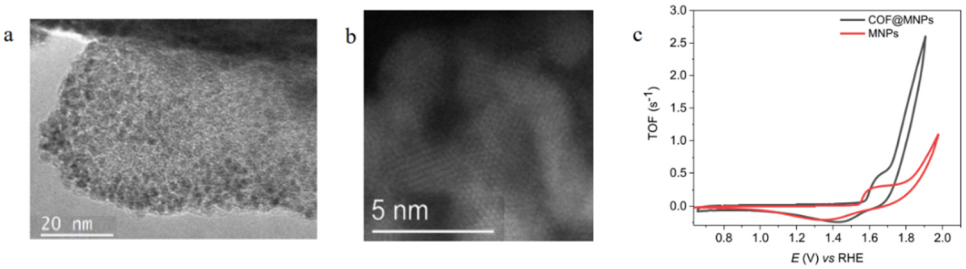
Keywords: *covalent organic frameworks, metal nanoparticles, hybrid materials, water splitting, electrocatalysis*

The European Union (EU) has set an ambitious goal: to achieve net-zero CO2 emissions by 2050, as outlined in the EU Green Deal approved in 2020.[1] A key component of this transition is the development of new, efficient, and robust materials capable of driving key electrochemical transformations such as the hydrogen evolution (HER) and oxygen evolution (OER) reactions.[2] Covalent Organic Frameworks (COFs) provide high crystallinity, ordered porosity, and well- defined organic linkages, enabling the precise control of chemical environments at the nanoscale. Their catalytic performance can be significantly enhanced through the incorporation of active metal nanoparticles (MNPs).[3] In this work, we develop COF@MNP hybrids using two complementary synthetic approaches. In the first route, MNPs are generated *in situ* within pre-formed COFs, and in the second strategy, pre-synthesized MNPs are used as nucleation centers for framework growth, leading to core-shell-like hybrid architectures. Together, these methods enable systematic control over metal dispersion and particle size. Characterization of the obtained porous hybrid materials confirms the effective integration of the MNPs while preserving the crystallinity and structural integrity of the COF. In particular, PXRD and IR demonstrate the crystallinity and the successful formation of the COF framework, while HRTEM (Figure 1a), SEM, and STEM-HAADF (Figure 1b) reveal the crystalline lattice planes of the MNPs, the framework morphology, and the dispersion of the incorporated nanoparticles. In addition, electrochemical studies (Figure 1c) demonstrate the successful application of these hybrid materials in water splitting reactions, both in alkaline and NaCl-containing electrolytes. Comparative benchmarking against MNPs in the absence of the COF support indicates that the hybrid materials improve catalytic activity and stability.

Figure 1. *(a) HRTEM image of the COF@MNPs; (b) STEM-HAADF image showing lattice fringes of the*



MNPs; (c) TOF- normalized cyclic voltammograms for OER (borate buffer, pH 9) comparing MNPs (in red) and the COF@MNP hybrid (in black).

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An Interesting Case Of Nanoporous Graphitic Carbon Nitride Films

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Two-dimensional nanoporous materials are highly attractive for separation applications because the flux scales inversely with the thickness of the selective layer. Over the past decade, significant progress has been made in developing porous graphene membranes for separations. However, pristine graphene is impermeable to gases, and size sieving pores need to be incorporated into the graphene lattice for separation applications. The pore incorporation in graphene inevitably leads to a pore size distribution which compromises the separation performance and is often considered to be the biggest bottleneck in translating graphene membranes for practical applications.1,2 In this context, inherently nanoporous materials like graphdiyne or graphitic carbon nitride (GCN), have emerged as particularly promising alternatives.

GCN is both an interesting and a controversial material. A large majority of published papers erroneously report the polymeric form of carbon nitride as crystalline, based on the misinterpretation of the XRD pattern. GCN exists in two structural variants: triazine-based GCN (t-GCN) and heptazine-based GCN (h-GCN). Although the actual pore size of t-GCN is suitable for separating light gases, its staggered stacking and the presence of ions in the pores make it unsuitable for membrane applications. In contrast, h-GCN features a larger pore size and is devoid of pore-blocking ions. The staggered stacking of h-GCN reduces the effective pore size, making it suitable for gas separation applications.

Our research group explores the synthesis of h-GCN by the chemical vapor deposition method.3 We observed that under specific CVD conditions, nanocrystalline domains of h-GCN are formed. This talk will focus on our research group's efforts to understand the structure and transport properties of the resulting h-GCN thin film by a combination of gas permeation and diffraction/spectroscopy-based techniques.

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NON-UNIFORM SITES ON ZEOLITES: STATIC FIELD HETEROGENEITY

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Keywords: *surface chemistry, numerical modelling, transient kinetics, catalysis*

Introduction: NH3-TPD is used to characterise zeolite acidity. Weakly bound ammonia is attributed to the low- temperature (LT) peak, while the high-temperature (HT) peak is ascribed to Brønsted acidity. From a kinetic perspective, three fundamental questions must be answered to understand the kinetics of the nature and behaviour of the acid site: (1) How many site ensembles are responsible for intrinsic transient kinetic behaviour? (2) what are the site-interdependence criteria for static (linear) and dynamic (nonlinear) sites? and (3) what is the relationship between site density and the source term for static, and dynamic sites? This work uses a combination of TPD and numerical modelling tools.

Methodology: Vacuum [1] and atmospheric-NH3-TPD [2] profiles are obtained from archived literature. Five site models (single-site (SS), multi-site (MS), subunit-cell (SC), crystal grain surface (CSM), and a probability density function model (PDF)) are used to simulate NH3-TPD profiles.

Results and Discussion: Vacuum NH3-TPD profile can be represented by a single site ensemble. Atmospheric-NH3-TPD profiles give six site ensembles for desorption over ZSM-5 catalysts using the MS and CSM models. The SC and PDF models use 4 site ensembles. The novel static field heterogeneity model bridges vacuum and atmospheric NH3-TPD profiles using one high temperature active centre consisting of three site ensembles and multiple sites (figure 1).

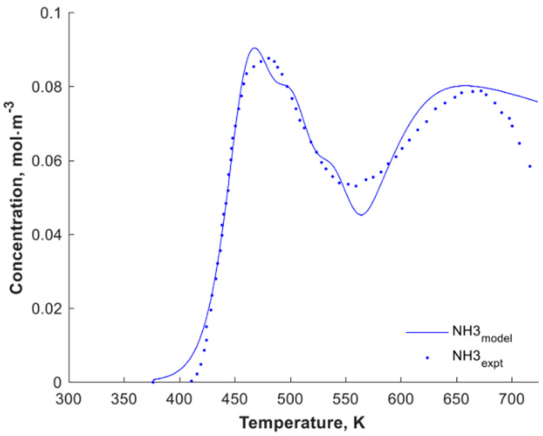

Figure 1: *Desorption of NH3-TPD over ZSM-5 (Si/Al=15) catalysts simulated by static field heterogeneity model*

Conclusion: The results of this work show that the nature of acid sites obtained from vacuum NH_3-TPD prorfiles can be bridged with atmospheric NH_3-TPD prorfiles using a static field heterogeneity model. The results are important for the characterisation of the dynamics of working catalysts.

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