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Wrocławski

Wydział Chemii

MOFebruary 2026

Polish *micro* symposium in celebration
of the 2025 Nobel Prize in Chemistry

10-12 February 2026

Faculty of Chemistry, University of Wrocław

e-Book of Abstracts



The **2025 Nobel Prize in chemistry** was officially presented in Stockholm on December 10, 2025, at a ceremony organized by the Royal Swedish Academy of Sciences. The Nobel Committee awarded the prize in chemistry for the development of metal-organic frameworks to Professor Susumu Kitagawa (University of Kyoto, Japan), Professor Richard Robson (University of Melbourne, Australia), and Professor Omar M. Yaghi (University of California, Berkeley).

This distinction has been a major source of inspiration for the MOF community worldwide. In that spirit, an initiative emerged at the end of last year to bring together the Polish MOF community. Therefore, on **10–12 February 2026**, we will host two distinguished scientists at the **Faculty of Chemistry, University of Wrocław**: Dr Stefano Canossa (ETH Zürich) and Dr Stefan Wuttke (AGH University of Kraków). We hope this will be an excellent opportunity for Poland-based MOF researchers to meet, exchange ideas, and discuss MOF-related topics. In addition, Dr Canossa will conduct a one-day workshop entitled *“Professional single-crystal diffraction analysis inside and outside the average box”*, open to all interested participants.

Due to the small and spontaneous nature of this event, participation is **free of charge**. The micro-symposium will include invited lectures by experienced researchers as well as a **poster session** for PhD and undergraduate students.

*Prof. Wojciech Bury
Dr Marzena Pander
Dr Min Ying Tsang*

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Organizing Committee

- dr hab. Wojciech Bury, prof. UWr
*Faculty of Chemistry
University of Wrocław*
- dr Marzena Pander
*Faculty of Chemistry
Jagiellonian University in Kraków*
- dr Min Ying Tsang
*Łukasiewicz Research Network – PORT
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Local Organizing Committee



Reticular Chemistry and Catalysis Group:

- dr hab. Izabela Czełuśniak
- mgr Magdalena Kozieł-Szymańska
- mgr Emilian Stachura
- mgr Oliwia Stani

Honorary Chair: prof. dr hab. Anna M. Trzeciak

Patronage

The Dean of the Faculty of Chemistry



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The event was organized in line with the objectives for improving quality of research and education at the University of Wrocław within the Excellence Initiative – Research University project (IDUB UWr).



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General Information

Symposium will take place in the **Faculty of Chemistry** of the University of Wrocław, which is part of the **Grunwaldzki Campus** and conveniently situated close to the historic part of the city ([map](#)). The lectures will take place in *Ignacy Z. Siemion Lecture Hall (IBB, Tuesday-Wednesday, 10-11.02.2026)* and *Józef J. Ziółkowski Lecture Hall (Room 145, Thursday, 12.02.2026)*.

Faculty of Chemistry
University of Wrocław
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Invited Speakers

Prof. Stefan Wuttke

*Head of the Department of Nanoscience
Academic Centre for Materials and Nanotechnology
AGH University of Krakow in Poland*

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

Dr. Stefano Canossa

*Senior Scientist at the Laboratory of Inorganic Chemistry
ETH Zürich in Switzerland*



Stefano Canossa is currently a senior scientist at ETH Zürich. His research activities focus on structural chemistry, with particular contributions to crystallography, defect structure determination, and metal-organic frameworks. He has been actively involved in initiatives such as MOFschool, workshops, and scientific associations aimed at delivering high-quality research data and materials. His work has been published in numerous international journals, including *Nature Communications*, *Nature Synthesis*, *Advanced Materials*, *Advanced Functional Materials*, *JACS*, and *Angewandte Chemie International Edition*. The visibility of his research has resulted in invitations to present at international conferences and universities in multiple countries, as well as chairing major scientific meetings. His academic activities also include participation as a PI and a co-PI in national and international research projects, supervision of graduate and postgraduate students, and engagement in peer review and educational initiatives.

Program of symposium

Day 1 – Tuesday (2026/02/10)

11:00-13:00	Registration	Students' Entry WCh-UWr
13:00-13:15	Opening Welcome	Prof. Wojciech Bury IBB
13:15-14:00	PL-01	Prof. Stefan Wuttke IBB
14:00-15:00	Group photo Lunch break	U1
15:00-16:30	1st session	Chair: Prof. Anna Trzeciak IBB
15:00-15:30	OL-01	Prof. Bogdan Kuchta
15:30-16:00	OL-02	Prof. Dariusz Matoga
16:00-16:30	OL-03	Prof. Justyna Łuczak
16:30-17:00	Coffee break	U1
17:00-18:40	2nd session	Chair: Prof. Dariusz Matoga IBB
17:00-17:30	OL-04	Prof. Szymon Chorąży
17:30-18:00	OL-05	Prof. Piotr Smoleński
18:00-18:20	OC-01	Dr. Kornel Roztocki
18:20-18:40	OC-02	Dr. Felix Hengersdorf
20:00	Dinner at Drevny Kocur (optional)	

Day 2 – Wednesday (2026/02/11)

9:00-10:40	3rd session	Chair: Prof. Bogdan Kuchta IBB
9:00-9:30	OL-06	Prof. Adriana Zaleska-Medynska
9:30-10:00	OL-07	Prof. Mihails Arhangeliskis
10:00-10:20	OC-03	Dr. Gabriela Jajko-Liberka
10:20-10:40	OC-04	Dr. Emilia Ganczar
10:40-11:00	Coffee break	U1
11:00-11:45	PL-02	Dr. Stefano Canossa IBB
12:00-13:00	Poster session	U1-IBB Hall
13:00-14:00	Lunch break	U1
14:00-17:10	4th session	Chair: Prof. Adriana Zaleska-Medynska IBB
14:00-14:30	OL-08	Prof. Barbara Gil
14:30-15:00	OL-09	Prof. Michał Chmielewski
15:00-15:30	OL-10	Prof. Łukasz Kuterasiński
15:30-15:50	OC-05	Dr. Chiranjib Gogoi
15:50-16:10	OC-06	Dr. Marzena Pander
16:10-16:30	OC-07	Dr. Jan Zaręba
16:30-16:50	OC-08	Dr. Rodrigo Gil-San-Millan
16:50-17:10	OC-09	Dr. Min Ying Tsang
17:10-17:30	Closing	Prof. Wojciech Bury IBB

Day 3 – Thursday (2026/02/12)

145 or U1

Workshop Day with Dr. Stefano Canossa

Professional single-crystal diffraction analysis inside and outside the average box	
10:00-12:00	Part I: Quality assessment of single crystal diffraction analysis
12:00-13:00	Lunch break
13:00-15:00	Part II: Real structure effects in reciprocal space: a primer to single crystal scattering

List of oral presentations

PL-01	Prof. Stefan Wuttke	AGH University of Kraków
PL-02	Dr. Stefano Canossa	ETH Zürich
OL-01	Prof. Bogdan Kuchta	Wrocław University of Science and Technology
OL-02	Prof. Dariusz Matoga	Jagiellonian University in Kraków
OL-03	Prof. Justyna Łuczak	Gdańsk University of Technology
OL-04	Prof. Szymon Chorąży	Jagiellonian University in Kraków
OL-05	Prof. Piotr Smoleński	University of Wrocław
OL-06	Prof. Adriana Zaleska-Medynska	University of Gdańsk
OL-07	Prof. Mihails Arhangeliskis	University of Warsaw
OL-08	Prof. Barbara Gil	Jagiellonian University in Kraków
OL-09	Prof. Michał Chmielewski	University of Warsaw
OL-10	Prof. Łukasz Kuterasiński	Jerzy Haber Institute of Catalysis and Surface Chemistry, PAS
OC-01	Dr. Kornel Roztocki	Adam Mickiewicz University in Poznań
OC-02	Dr. Felix Hengersdorf	Rigaku Europe SE
OC-03	Dr. Gabriela Jajko-Liberka	Jagiellonian University in Kraków
OC-04	Dr. Emilia Ganczar	University of Wrocław
OC-05	Dr. Chiranjib Gogoi	University of Cape Town
OC-06	Dr. Marzena Pander	Jagiellonian University in Kraków
OC-07	Dr. Jan Zaręba	Wrocław University of Science and Technology
OC-08	Dr. Rodrigo Gil-San-Millan	Technical University of Dresden
OC-09	Dr. Min Ying Tsang	Łukasiewicz Research Network – PORT

PL = Plenary Lecture (40 min lecture + 5 min Q&A)

OL = Oral Lecture (25 min lecture + 5 min Q&A)

OC = Oral Communication (15 min lecture + 5 min Q&A)

List of poster presentations

P-01	Paweł Adamczyk	University of Wrocław
P-02	Beata Barszcz	Trzebiatowski Institute of Low Temperature and Structure Research, PAS
P-03	Weronika Bodylska-Maj	Trzebiatowski Institute of Low Temperature and Structure Research, PAS
P-04	Dr. Joanna Drzeżdżon	University of Gdańsk
P-05	Hubert Dziełak	Jagiellonian University in Kraków
P-06	Aleksandra Gerszendorf	Łukasiewicz Research Network – PORT
P-07	Wiktoria Gromelska	Adam Mickiewicz University in Poznań
P-08	Dr. Sabina Jaros	University of Wrocław
P-09	Negin Khosroshahi	Max Planck Institute for Solid State Research
P-10	Amelia Kołomańska	Wrocław University of Science and Technology
P-11	Adrian Kowaliński	Wrocław University of Science and Technology
P-12	Magdalena Koziel-Szymańska	University of Wrocław
P-13	Alicja Król	University of Wrocław
P-14	Dawid Kruczek	Jagiellonian University in Kraków
P-15	Dr. Natalia Łukasik	Gdańsk University of Technology
P-16	Karolina Matuszak	Wrocław University of Science and Technology
P-17	Bartosz Mazur	Wrocław University of Science and Technology
P-18	Hesham Mousa	University of Wrocław
P-12	Mateusz Najman	University of Wrocław
P-19	Patryk Pakuła	Wrocław University of Science and Technology
P-20	Dr. Aleksandra Pieczyńska	University of Gdańsk
P-21	Julia Prus	University of Wrocław
P-06	Dr. Tappendu Samanta	Łukasiewicz Research Network – PORT
P-22	Szymon Sobczak	Adam Mickiewicz University in Poznań
P-13	Emilian Stachura	University of Wrocław
P-18	Oliwia Stani	University of Wrocław
P-23	Kinga Szczecińska	Jagiellonian University in Kraków
P-24	Gaja Wota	Jagiellonian University in Kraków
P-25	Dr. Mateusz Janeta	University of Wrocław

Abstracts – oral presentations

PL-01

Combining Reticular Pore Design with Green Promises to Sustainable Practices

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

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

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

References:

- [1] J. Zhe, M. Srijit, A. Jacopo, A. Sinelshchikova, F. Peccati, S. Wuttke, S. G. Boxer, *Nat. Chem.* **2025**, *17*, 1920.
- [2] A. Ghaffarkhah, M. Panahi-Sarmad, S. Rostami, O. Zaremba, L. Alexander Bauman, S. A. Hashemi, S. Dutta, P. Yang, T. Guo, F. Jiang, S. Wuttke, M. Arjmand, O. J Rojas, *Adv. Funct. Mater.* **2025**, *35*, 2506427.
- [3] S. Dutta, M. A. Aretxabaleta, M. M Shirolkar, S. Wuttke, E. Lizundia, *Chem. Eng. J.* **2025**, *526*, 170898.
- [4] S. Dutta, M. Walden, A. Sinelshchikova, R. Ettliger, E. Lizundia, S. Wuttke, *Adv. Funct. Mater.* **2025**, *34*, 2410751.
- [5] E. Chernova, S. Dutta, E. Lizundia, S. Wuttke, *ACS Sust. Chem. Eng.* **2025**, *13*, 18577-18589.

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PL-02

Defects, Distortions, Dynamics: Revealing 3D Complexity by Single-Crystal Total Scattering Methods

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“Periodicity” is a human-made concept — any crystalline material has some degree of structural non-periodicity in the form of defects, distortions, and dynamics. In metal–organic frameworks (MOFs), disorder is not only abundant, but potential gateway for a vast structural and functional diversity that can arise from even a single MOF type [1]. Nevertheless, this potential remains largely unexplored due to the rarity of techniques suited for determination of 3D non-periodicity in crystals, and the widespread overreliance on traditional crystallography and average crystal structures. In this context, single-crystal total scattering analysis offers the unique advantage of providing 3D-resolved information on the real atomic structures of crystals with essentially no limitation of type, composition, or size. In this lecture I describe how this still-rare crystallographic method delivers such information by presenting published and undisclosed results, which reveal how ordinary materials can be hiding extraordinary and unexpected complexity in the form of locally structured disorder [2, 3].

References:

- [1] Canossa, S. Yaghi, O. M. *et al.*, *Nature Reviews Materials* **2023**, *8*, 331–340.
- [2] Canossa, S., Lotsch, B. V. *et al.*, *Journal of the American Chemical Society*, **2023**, *145*, 10051–10060.
- [3] S. Griffin, S. Canossa, N. Champness *et al.*, *Nature Communications*, **2025**, *16*, 3209.

Adsorption Mechanism in Crystalline Micropores

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Understanding molecular adsorption in microporous materials is key to advancing gas separation, storage, and catalysis. Here, we study CO₂ and CH₄ adsorption in crystalline metal-organic frameworks (IRMOF-1, 8, 10, and 14), emphasizing the emergence of metastable states. Molecular simulations reveal that adsorption is governed by a fine balance between fluid–fluid and fluid–framework interactions, leading to transitions between low- and high-density pore-filling states [1,2]. These metastable features are highly sensitive to pore geometry and thermodynamic conditions, especially near the adsorbate's triple point. In contrast, water adsorption displays more complex behavior: strong hydrogen bonding induces stable clusters, multiple free energy minima, and exceptionally slow equilibration. Our results underscore the importance of metastability in accurately modeling and designing advanced nanoporous materials for practical applications [3,4].

Overall, our results provide fundamental insight into the molecular origins of adsorbate metastability and highlight its critical role in accurately modeling adsorption in ordered nanoporous materials. Although many microporous materials are conventionally classified as exhibiting IUPAC Type I isotherms, our simulations show that such a description oversimplifies the rich adsorption features of highly ordered MOFs. Near the triple point, adsorption proceeds via a low-density precursor followed by a sharp pore-filling transition; with increasing temperature, this behavior evolves toward a smoother, Type V–like profile [4].

Acknowledgements: supported by the National Science Centre (NCN), Poland (grant no. 2022/45/B/ST8/02028). Monte Carlo numerical simulation results are created using resources provided by Wrocław Centre for Networking and Supercomputing (<https://wcoss.pl>).

References:

- [1] Mazur, B.; Formalik, F.; Roztocki, K.; Bon, V.; Kaskel, S.; Neimark, A. V.; Firlej, L.; Kuchta, B. *J. Phys. Chem. Lett.* **2022**, 13, 6961–6965.
- [2] Kuchta, B.; Dunder, E.; Formalik, F.; Llewellyn, P.; Firlej, L. *Angew. Chem., Int. Ed.* **2017**, 56, 16461–16464
- [3] Dorhauer A.; Stankiewicz M.; Mazur B.; Kuchta B.; Wexler C. *ACS Omega* **2025**, 10, 51, 63044–63050
- [4] Stankiewicz M.; Dorhauer A.; Roztocki K.; Bon V.; Mazur B.; Wexler C.; Kaskel S.; Firlej L., Kuchta, B. *ACS Nano*, **2026**, DOI: 10.1021/acsnano.5c16606

Tailoring MOF Structures for Proton Conduction

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Metal-organic frameworks (MOFs) represent a broad class of materials characterized by modularity, crystallinity and porosity. These features enable the design and exploration of MOFs in a wide range of applications, such as catalysis, drug delivery, sensing, gas storage, mixture separations, and energy storage and conversion. Notably, proton-conductive MOFs (PC-MOFs) hold significant promise as solid electrolytes in proton-exchange membrane fuel cells. Several strategies have been developed for synthesizing PC-MOFs, with the most effective approaches involving the incorporation of Brønsted acid groups into the organic framework and the filling of cavities with acidic ions or molecules [1]. In this presentation, our original synthetic strategies for creating PC-MOFs will be presented [2].

One approach involves chlorosulfonation of selected organic building blocks, which, upon assembly into MOFs, results in the incorporation of terminal sulfonic groups into the MOF backbones. Another strategy involves the conversion of non-conductive MOFs with open metal sites into proton conductive MOFs (or hydrogen-bonded organic frameworks, HOFs) through a solvent-free mechanochemical process, utilizing thiocyanate salts with protic cations. Lastly, we employ an inverse electron-demand Diels-Alder reaction as a covalent post-synthetic modification of MOFs containing a tetrazine entity.

References:

- [1] D.-W. Lim, H. Kitagawa, *Chem. Soc. Rev.* 50 (2021) 6349-6368.
[2] Representative papers: M. Szufła, J.A.R. Navarro, K. Góra-Marek, D. Matoga, *ACS. Appl. Mater. Interfaces* 15 (2023) 28184-28192; M. Lupa-Myszkowska, M. Oszejca, D. Matoga, *Chem. Sci.* 14 (2023) 14176-14181; D. Jędrzejowski, M. Pander, E. Stachura, K. Matlak, W. Bury, D. Matoga, *J. Mater. Chem. A* 13 (2025) 23671-23679.

OL-03

Conductive HHTP Based MOF Thin Films as High Performance Electrocatalysts for Ammonia Oxidation

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Two-dimensional conductive metal-organic frameworks (cMOFs) have emerged as a promising class of functional materials for electrocatalytic applications. We present the fabrication of thin films of 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP)-based cMOFs grown on nickel foam *via* a layer by layer (LbL) deposition strategy. Ni, Cu, and Co were employed as metal nodes to synthesize mono- and bimetallic HHTP frameworks. Among the monometallic systems, Ni-HHTP showed the highest activity toward ammonia oxidation reaction (AOR). The bimetallic system consisting of a top layer of Ni-HHTP and a bottom layer of Cu-HHTP exhibited the highest AOR performance in terms of current density ($174 \text{ mA}\cdot\text{m}^{-2}$ at 1.55V vs. RHE), which was approximately 1.5 times higher than that of the monometallic Ni-HHTP system and the bimetallic system with the reversed layer sequence. The inclusion of Cu-based cMOF also resulted in an increase in turnover frequency (to 1.26 s^{-1}) and a reduced charge transfer resistance (to 0.38Ω). Furthermore, the catalyst exhibited 92% N_2 selectivity and 79% NH_3 oxidation efficiency over 24 h. DFT results showed that a higher oxidation state of the ligand leads to a larger interplanar distance and shifts the electronic structure towards metallic behavior. Another finding suggests that a higher protonation of the ligands also leads to a larger interplanar distance and causes deviations from the planarity that may result in an amorphous structure.

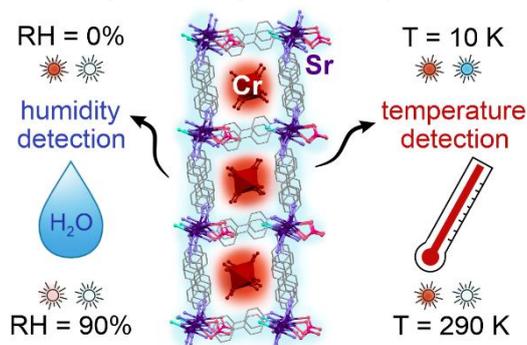
Luminescent Sensing of Humidity and Temperature by a Cationic MOF Encapsulating Hexacyanidochromate(III) Guest Ions

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Metal-organic frameworks (MOFs) revealing photoluminescence are good candidates for the application as optical sensors of various physical and chemical stimuli [1,2]. On the other hand, cyanido transition metal complexes were presented by us to be effective molecular building blocks for the construction of stimuli-responsive coordination polymers, including those undergoing reversible desolvation that governs their luminescence and magnetism, as well as those serving as luminescent molecular thermometers [3-6]. In this context, we decided to search for high-performance optical sensors through the combination of these two mentioned research lines, i.e., photoluminescent MOFs and polycyanidometallates. As the latter are usually anionic, our idea was to construct cationic MOFs that can incorporate cyanido metal complexes as guest ions. We achieved this challenge using neutral blue-emissive 4,4'-bipyridine-*N,N'*-dioxide (4,4'-bpdo) linkers combined with optically silent s-block metal ions (e.g., Sr²⁺) and anionic hexacyanidochromate(III) ions exhibiting a spin flip emission in the NIR range (see figure below). The resulting MOF material, described by the formula of $\{[Sr^{II}(4,4'-bpdo)_{2.5}(NO_3)][Sr^{II}(4,4'-bpdo)_{2.5}(H_2O)]\}[Cr^{III}(CN)_6] \cdot n(\text{solvent})$, exhibits dual photoluminescence from organic linker and cyanido complexes that was employed for ratiometric and lifetime-based detection of humidity and temperature. Its multifunctional character is additionally realized by humidity-variable proton conductivity [7].



References:

- [1] Huang, R.; Yu, Z.; Li, Z.; Lin, X.; Hou, J.; Hu, Z.; Zou, J. *Coord. Chem. Rev.* **2025**, *526*, 216358.
- [2] Cai, Y.; Dong, T.; Bian, Z.; Liu, H.; Liu, X.; Liu, A. *Coord. Chem. Rev.* **2025**, *529*, 216470.
- [3] Xin, Y.; Wang, J.; Zychowicz, M.; Zakrzewski, J. J.; Nakabayashi, K.; Sieklucka, B.; Chorazy, S.; Ohkoshi, S. *J. Am. Chem. Soc.* **2019**, *141*, 18211.
- [4] Wang, J.; Zakrzewski, J. J.; Zychowicz, M.; Xin, Y.; Tokoro, H.; Chorazy, S.; Ohkoshi, S. *Angew. Chem. Int. Ed.* **2023**, *62*, e202306372.
- [5] Zakrzewski, J. J.; Jankowski, R.; Romanowska, M.; Wang, J.; Pinkowicz, D.; Sieklucka, B.; Ohkoshi, S.; Chorazy, S. *Angew. Chem. Int. Ed.* **2025**, *64*, e202424651.
- [6] Zakrzewski, J. J.; Hoffman, A.; Wang, J.; Pander, M.; Matoga, D.; Tokoro, H.; Ohkoshi, S.; Chorazy, S. *Angew. Chem. Int. Ed.* **2025**, *64*, e202517109.
- [7] Niemiec, M.; Zakrzewski, J. J.; Reczyński, M.; Chorazy, S. *Adv. Optical Mater.* **2025**, *13*, 2403564.

OL-05

Coordination Engineering of 1,3,5-Triaza-7-phosphaadamantane as a Multidimensional Organic Linker in the Design of Copper(I/II) Coordination Polymers

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Research on transition metal coordination compounds containing the cage-like ligand PTA (1,3,5-triaza-7-phosphaadamantane) has been carried out continuously for over three decades. Based on the HSAB theory, which considers both the properties of transition metals and the phosphorus and nitrogen donor atoms of the PTA molecule, it is possible to design multimetallic systems as well as CPs featuring different metal oxidation states, with PTA acting as an organic linker. This presentation outlines the main research directions in the synthesis of coordination polymers involving PTA and discusses selected potential applications of these compounds. Special attention is given to systems containing the non-noble metal copper, which is inexpensive and readily available, yet exhibits interesting chemical properties, particularly in catalysis.

Application of MOFs in Heterogeneous Photocatalysis

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The global drive toward sustainable energy conversion has intensified interest in advanced photocatalytic materials capable of harnessing solar energy with high efficiency and selectivity. Among these materials, MOFs have attracted significant attention as versatile photocatalysts owing to their tunable crystalline structures, high surface areas, modular compositions, and well-defined active sites. This work highlights MOF-based photocatalysts for H₂ photogeneration and CO₂ photoconversion, and discusses the opportunities and limitations of employing MOFs in photocatalysis.

The effect of NH₂-MIL-125 modification by Cu, Co and Ni and thermal treating on the chemical nature of finally obtained photocatalyst was systematically investigated. Obtained materials have been explored for simultaneous photogeneration of H₂ and photodegradation of 5-Fluorouracil drugs (5-FU) from seawater under UV-Vis irradiation. We found that the most active MOF-based material achieved high H₂ generation (1079 μmolg_{cat}⁻¹ h⁻¹) and 5-FU removal (264 μmolg_{cat}⁻¹·h⁻¹) within the UV-Vis range.

To enhance stability of NH₂-MIL-125 during photocatalytic reaction, Cu-incorporated NH₂-MIL-125(Ti) was embedded inside of a PVDF porous matrix (membrane). The most effective performance of the composite material was achieved with a 10% wt/wt loading of MOF into the PVDF matrix. UV-vis -driven reaction revealed that increasing the MOF content from 1 to 10% led to an improvement in the H₂ production rate from 86.0 to 389.1 μmol h⁻¹ m⁻² and from 55.5 to 466.0 μmol h⁻¹ m⁻² for water-based and acetonitrile-based electrolytes, respectively.

To enhance photoactivity towards CO₂ conversion, PCN-222 was post synthetically modified by Cu²⁺ ions. Applied modification route resulted in both: combining of Cu²⁺ with porphyrins in MOF and formation of copper oxides at the MOF surface. the most active PCN-222 photocatalyst (Cu75) exhibited excellent performance in the photoreduction of CO₂ to HCOOH, achieving a conversion factor of 92.8 μmol g⁻¹ h⁻¹ and a quantum yield of 1.58% at 400 nm.

References:

- [1] M.A. Baluk, D.Makowski, Pieczyńska A., Nikiforow K., Łuczak J., Mikołajczyk A., Hoang K., Pinna N., Zaleska-Medynska A., Effects of copper, cobalt, or nickel modification of NH₂-MIL-125 oxide-derivatives on simultaneous photocatalytic pollutant degradation and hydrogen generation from natural seawater, *Journal of Hydrogen Energy* **197**, 152491 (2026).
- [2] E. Gontarek-Castro, A. Pancielejko, M. Baluk, M.Kroczevska, P. Gnatowski, K. Matus, J. Łuczak, A. Zaleska-Medynska, Photocatalytic membranes based on Cu-NH₂-MIL-125(Ti) protected by poly(vinylidene fluoride) for high and stable hydrogen production, *Materials Horizons* **12**, 1504-1515, (2025).

Ab initio Design of Functional Metal-Organic Frameworks through Crystal Structure Prediction and Machine Learning

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This presentation will demonstrate the opportunities brought by the computational design of MOFs as an alternative to experimental screening based on isorecticular node-and-linker approach. With the help of *ab initio* crystal structure prediction (CSP), structural landscapes of MOFs can be generated starting from a chemical diagram of individual nodes and linkers, without any restrictions for metal coordination geometry or network topology. It will be shown that this methodology can accurately reproduce the experimentally-observed structures from a variety of MOF classes, including zeolitic imidazolate frameworks (ZIFs), hexafluorosilicate (SIFSIX) and carboxylate MOFs [1].

Next, the first CSP-driven discovery of hypergolic MOF materials will be presented [2]. Hypergolicity, defined as a rapid ignitability upon contact with an oxidizer, is a key characteristic for solid rocket fuels. Thanks to the *ab initio* CSP calculations, the structural landscapes of several hypergolic copper(II)-based frameworks were studied prior to their synthesis, with the subsequently-synthesized materials matching the theoretical predictions.

Finally, the use of machine-learned interatomic potentials (MLIPs) for the purpose of accelerating the CSP calculations will be presented. This high-throughput CSP approach will be tested on the most polymorphic MOF system known to date, namely zinc imidazolate [3]. By sampling nearly 3 million trial structures via high-throughput MLIP-based simulations, we reproduce multiple existing polymorphs, as well as propose likely candidate structures for future experimental discovery.

References:

- [1] Darby, J. P.; Arhangel'skis, M.; Katsenis, A. D.; Marrett, J. M.; Frišćić, T.; Morris, A. J. *Chem. Mater.* **2020**, *32*, 5835–5844.
- [2] Xu, Y.; Marrett, J. M.; Titi, H. M.; Darby, J. P.; Morris, A. J.; Frišćić, T.; Arhangel'skis, M. *J. Am. Chem. Soc.* **2023**, *145*, 3515–3525.
- [3] Xu, Y.; Dorrell, J.; Lisac, K.; Brekalo, I.; Darby, J. P.; Morris, A. J.; Arhangel'skis, M. *arXiv* **2026**, DOI: 10.48550/arXiv.2601.05097.

Capture, Protect, Release: the Journey of MOFs (and Some Zeolites) in Drug Delivery

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Metal-organic frameworks (MOFs) are still looking for their place outside of labs, but they have already proven to be very promising materials for drug delivery applications owing to widely adjustable pore sizes, supremely high surface areas, and great capabilities for the design of chemical environment. By engineering framework composition and functional groups or stimuli-responsive linkers, MOFs can offer controlled, targeted, and on-demand release, making them attractive candidates for next-generation nanocarriers or theranostic agents in medicine [1].

Beyond biomedical use, MOFs also play a significant role in addressing environmental challenges, particularly the removal of pharmaceutical residues from wastewater. MOFs can remove or concentrate pharmaceuticals, which reduces the volume of the substances that needs to be treated. This offers an advanced alternative to conventional water-treatment technologies [2].

Similarly, zeolites have long been studied for drug delivery and water purification because their rigid aluminosilicate frameworks are highly durable, making them reliable hosts for small drug molecules and good adsorbents for certain pharmaceutical contaminants. However, unlike the highly tuneable MOFs, zeolites offer limited control over pore size and surface chemistry, restricting their capacity to accommodate bigger therapeutic molecules or to be tuned for specific molecular interactions.

Recent advances in layered zeolites expand the capabilities of traditional zeolitic materials [3]. By delaminating, swelling, or exfoliating zeolite layers, more accessible mesoporous pathways are created, which allows overcoming diffusion limitations typical for purely microporous structures. These structural modifications enable the loading of larger drug molecules, improves release kinetics, and enhances the adsorption of bulkier pharmaceuticals. All these enhancements make layered zeolites more responsive and selective, bringing their performance closer to that of MOFs while maintaining the inherent robustness and stability of their frameworks.

Acknowledgements

Financial support from NCN, grant no 2020/37/B/ST5/01258 is acknowledged.

References:

- [1] Wang, A.; Walden, M.; Ettliger, R.; Kiessling, F.; Gassensmith, J. J.; Lammers, T.; Wuttke, S.; Peña, Q. *Adv. Funct. Mater.* **2023**, 2308589.
- [2] Rincon, I.; Salles, F.; Jimenez-Duro, M.; Svensson Grape, E.; Willhammar, T.; Inge A. K.; Hidalgo, T.; Horcajada, P. *Applied Water Science*, **2025**, 15, 315.
- [3] Roth, W. J.; Opanasenko, M.; Mazur, M.; Gil, B.; Čejka, J.; Sasaki, T. *Adv. Mater.* **2024**, 36, 2307341.

The Inner Life of a MOF: Templated Self-Organization of Linkers in a Pillared-Layer MOF

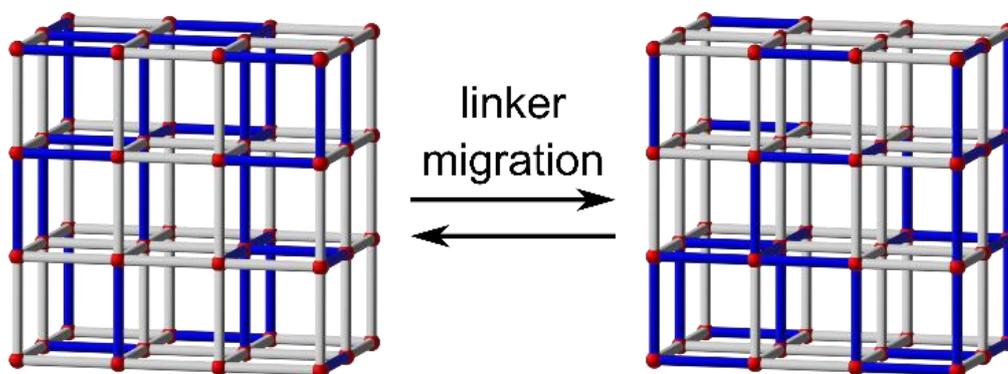
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Metal-organic frameworks (MOFs) are well-known to undergo post-synthetic linker exchange and reorganization [1]. Surprisingly, however, structural reorganizations in which linkers simply reshuffle their positions in a metal-organic framework, without changing the overall composition and topology of the MOF (Scheme 1), have not been investigated thus far.

Here we show that linker migration in MOFs may indeed take place, and that the kinetics of this process may be easily controlled by changing temperature, solvent, and catalysts. More importantly, we show also that linker reshuffling allows templated self-organization of the MOF structure, giving unprecedented control over spatial distribution of linkers in the crystalline lattice.



Scheme 1. Schematic representation of random linker place exchange in a MOF.

References:

[1] P. Deria, J.E. Mondloch, O. Karagiari, W. Bury, J.T. Hupp, O.K. Farha, *Chem. Soc. Rev.* **2014**, *43*, 5896.

Medical Applications of Zr-MOFs for Detoxification in Living Organisms

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Drug addiction is a mental disorder involving an overwhelming urge to use substances despite known risks. Rising cases of psychoactive substance abuse necessitate new detox methods. This study evaluates zirconium metal-organic frameworks (Zr-MOFs)—NU-1000, MOF-808, UiO-66, and UiO-67—for their ability to adsorb common drugs like amphetamine, methamphetamine, cocaine, mephedrone, and MDMA. Zr-MOFs, especially NU-1000, showed high drug removal efficiency, with notable results for both individual and mixed drug systems in various solutions. Adsorption performance varied by MOF structure, and modified synthesis improved efficiency for some drugs. The Zr-MOFs exhibited low cytotoxicity and were found to be safe in biological models. Zebrafish tests showed that while all substances increased activity, MOFs neutralized stimulant effects and reduced toxicity, supporting normal development and demonstrating cardioprotective benefits.

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References:

[1] Liu, L.F.; Li, J. X. *Acta Pharmacol. Sin.*, **2018**, 39, 1823.

The Impact of a Single Atom on MOF Flexibility

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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 dicarboxylate group [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 time-resolved in situ powder X-ray diffraction dataset was collected under varying CO₂ 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.

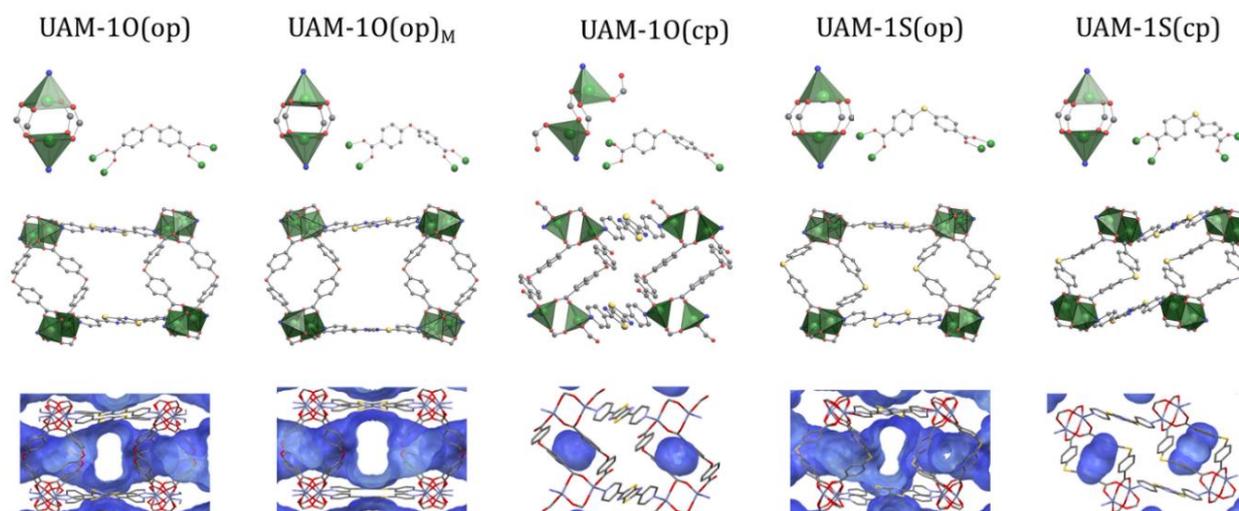


Figure 1 Comparison of single crystal structures of open pore phases and desolvated phases.

References:

- [1] Small 2024, 2402486.
- [2] J. Mater. Chem. A 2023, 11, 18646–18650.
- [3] J. Am. Chem. Soc. 2025, 147, 25, 21575–21585.

Overcoming Size Limitations in MOF Research: Structural Elucidation by Electron Diffraction

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Since its launch in 2021, the XtaLAB Synergy-ED [1] has been used to solve over 600 unique structures in Rigaku laboratories alone. While most measurements were initially performed at ambient temperature, recent low-temperature studies, particularly using cryo-transfer, have demonstrated significant advantages for preserving samples sensitive to vacuum and electron-beam damage.

Owing to its compatibility with the established ecosystem of TEM specimen holders, the XtaLAB Synergy-ED enables structural scientists to access a variety of experimental approaches commonly used in X-ray crystallography. Cryo-transfer holders facilitate protection of samples prior to vacuum exposure, enabling investigation of solvates and other vacuum-sensitive materials [2], as well as exploration of phase behaviour. Selected case studies are presented where cryo-transfer was essential.

In addition, the MEMS biasing and heating holder allows in situ heating, enabling phase-behaviour studies of materials such as porous frameworks. Recent single-crystal 3D ED/microED measurements of the MOF Cu(ta)₂ (Hta = 1H-1,2,3-triazole) collected at room temperature and 200 °C are compared with earlier SC-XRD and PXRD results reported by Grzywa et al. in 2012 [3].

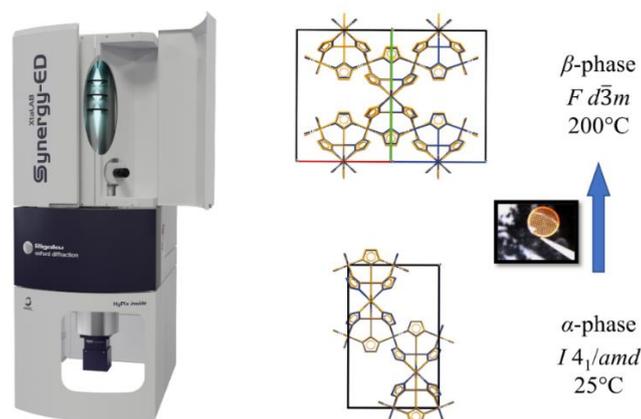


Figure 1 Overlays of the ambient and high temperature phases of Cu(ta)₂ from the XtaLAB Synergy-ED (blue) and the X-ray structures by Grzywa *et al.* (orange).

References:

- [1] S. Ito, F.J. White, et al. *CrystEngComm* **2021**, 23, 8622–8630.
 [2] K.-N. Truong, S. Ito, et al. *Symmetry* **2023**, 15(8), 1555.
 [3] M. Grzywa, D. Denysenko, et al. *Dalton Trans.* **2012**, 41, 4239–4248.

Mechanistic Insights into Multicomponent Adsorption in MOFs from Monte Carlo Modeling

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Monte Carlo (MC) simulations, particularly in the grand canonical ensemble, are widely employed to study adsorption phenomena in metal–organic frameworks (MOFs), as they capture equilibrium host–guest behavior at the molecular level. For single-component adsorption, MC modeling is relatively well established: despite challenges in force-field development, especially for polar molecules or frameworks with open metal sites [1], simulations often reproduce experimental isotherms with reasonable accuracy. In contrast, multicomponent adsorption poses a greater challenge, as force fields must consistently describe framework–guest and guest–guest interactions for chemically distinct adsorbates under confinement, severely limiting transferability and agreement with experiment.

This challenge is well illustrated by the competitive adsorption of CO₂, water, and methanol in MOFs with heterogeneous adsorption sites [2]. While CO₂ preferentially occupies high-energy sites at low loadings, strongly hydrogen-bonding species can dramatically alter the adsorption landscape. Water may block primary sites and mediate others, while methanol can outcompete both CO₂ and water due to a subtle balance of dispersive and hydrogen-bonding interactions, highlighting the sensitivity of mixture adsorption to force-field parametrization. Similar effects are observed for immiscible or weakly interacting mixtures, such as toluene–water systems [3]. MC simulations reveal confinement-induced nanoscale phase separation, with aromatic molecules occupying pore interiors and water being excluded or localized at defect sites. These effects depend critically on the accurate description of dispersive interactions and framework polarity. Contrarily, for nonpolar hydrocarbons, selectivity is predominantly entropic, arising from steric constraints and pore topology rather than adsorption energetics [4]. In this context, mixture simulations are essential, as single-component calculations fail to capture competitive exclusion and cooperative packing mechanisms that govern separation performance. Moreover, structural defects further complicate multicomponent adsorption [5], as missing-linker or missing-node vacancies can generate high-affinity sites that strongly affect mixture behavior, and may even reverse selectivity trends predicted for idealized frameworks.

Overall, multicomponent MC simulations are essential for elucidating competitive adsorption mechanisms in MOFs. Despite persistent limitations in force-field transferability, carefully validated mixture simulations provide critical molecular-level insight for interpreting experiments and guiding the design of MOFs for complex separations.

References:

- [1] Jajko, G.; Gutiérrez-Sevillano, J. J.; Sławek, A. *et al. Micropor. Mesopor. Mat.* **2022**, 330, 111555.
- [2] Jajko, G.; Kozyra, P.; Gutiérrez-Sevillano, J. J.; Makowski, W.; Calero, S. *Chem. Eur. J.* **2021**, 27, 14653.
- [3] Jajko, G., Gutiérrez-Sevillano, J. J., Calero, S. *et al. J. Phys. Chem. Lett.* **2023**, 14(24), 5618–5623.
- [4] Sławek, A.; Jajko, G.; Ogorzały, K.; Dubbeldam, D. *et al. Chem. Eur. J.* **2022**, 28, e202200030.
- [5] Jajko, G., Calero, S., Kozyra, P. *et al. Commun Chem* **2022**, 5, 120.

Mechanochemical Synthesis and MicroED Structure Determination of Coordination Compounds

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Coordination compounds attract sustained attention for their unique structural properties, which can be easily tailored by modifying the organic linker or metal core. These materials are highly versatile, finding applications in catalysis, selective molecular separation, gas storage, or chemical sensors [1]. Mechanochemical synthesis is emerging as a promising strategy for the preparation of these materials from a green chemistry perspective, as it reduces the consumption of organic solvents, minimizes energy consumption and chemical waste while delivering high yields [2]. On the other hand, characterizing new materials requires a thorough examination of their crystal structure. Since mechanochemical products typically form nanocrystalline powders, they are usually unsuitable for Single-Crystal X-ray diffraction (SCXRD). 3D Electron Diffraction is an excellent technique that complements mechanosynthesis [3-4]. Copper(I) and silver(I) coordination compounds with triazole Schiff bases tend to form diverse structural motifs, frequently resulting in flexible frameworks capable of sorption of various organic molecules. Appropriate ligand modifications allow the formation of a variety of motifs, from binuclear, flexible frameworks to one- or multidimensional coordination polymers defined by a rigid host framework and channel structures [5-6]. This presentation will discuss copper(I) and silver(I) coordination compounds, as well as a greener approach to their synthesis. The results obtained demonstrate that 3D ED is an indispensable tool for the precise structural characterization of such nanocrystalline products, where conventional diffraction methods reach their limits.

References:

- [1] Kitagawa, S.; Kitaura, R.; Noro, S.-I. *Angew. Chemie - Int. Ed.* **2004**, 43, 2334.
- [2] Desai, A. V.; Lizundia, E.; Laybourn, A.; Rainer, D. N.; Armstrong, A. R.; Morris, R. R.; Wuttke, S., Ettliger, R. *Advanced Functional Materials*, **2023**, 34, 2304660.
- [3] Lorenzo, F.; Katsavou, C.; Rolán, K., P.; Dias, S.; Fernández Cortés H.; Collado, J.; Chichón, F. J.; Arranz, R.; Santiago, C.; Sañudo, C. *Inorganic Chemistry*, **2025**, 64, 13824.
- [4] Celik, E.; Le Magueres, P.; Reinheimer, E. W.; Carter, K. P.; Forbes, T. Z. *CrystEngComm*, **2026**, 28, 255.
- [5] Ganczar, E.; Bialońska, A. *Acta Cryst.*, **2023**, B79, 392.
- [6] Ganczar, E.; Bury, W.; Gawryszewska, P.; Kinzhybalov, V.; Bialońska, A. *Cryst. Growth Des.* **2025**, 25, 9702.

Superhydrophobic Self-Cleaning Composite of a Metal-Organic Framework with Polypropylene Fabric for Efficient Removal of Oils from Oil-Water Mixtures

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As well-established porous materials, metal-organic frameworks (MOFs) are a class of inorganic and organic hybrid materials formed by metal ions and organic ligands, offering near unlimited tunability with respect to component diversity and structural hierarchy. In this work, a MOF $[\text{Hf}_6\text{O}_4(\text{OH})_4(\text{TFNDC})_6] \cdot 6\text{H}_2\text{O} \cdot 2\text{DMF}$ [**1**, where TFNDC = 1-(2,2,2-trifluoroacetamido)naphthalene-3,7-dicarboxylate] synthesized under solvothermal conditions, which possesses excellent chemical and thermal stability along with remarkable hydrophobic characteristics. The hydrophobic **1** was used for in situ coating on the polypropylene (PP) fabric to make a superhydrophobic **1@PP** fabric composite. The immobilization of nanocrystalline particles of **1** creates a nanoscale hierarchy that enhances the hydrophobicity of the material. The superhydrophobic **1@PP** composite showed a water contact angle of 160° . The successful integration of the MOF compound with PP fabric was confirmed using field-emission scanning electron microscopy, X-ray powder diffraction spectroscopy, Fourier transform infrared spectroscopy, and energy-dispersive X-ray analysis experiments. Superhydrophobic **1@PP** composite displayed a high separation efficiency (93–99%) for separating light, heavy, and crude oils from oil–water mixtures. The flux for oil–water separation was found to be $13\text{--}18\text{ k L m}^{-2}\text{ h}^{-1}$. Importantly, the **1@PP** composite can be used repetitively up to a minimum of 20 times for oil–water separation. The recyclability was also maintained in high acidic and alkaline media. Moreover, superhydrophobic **1@PP** composite showed excellent oil absorption capacity (29–39 g/g) for heavy and light oils at ambient temperature. A gravity-driven active-filtration process and separation against the gravity process were also performed to examine the flexibility of the composite for separation. We demonstrate that the **1@PP** composite has the merit of very high separation efficiency, absorption capacity, good recyclability, and exceptional robustness, showing high potential for versatile oil–water separation.

References:

- [1] Gogoi, C.; Rana, A.; Ghosh, S.; Fopase, R.; Pandey, L. M.; Biswas, S. *ACS Appl. Nano Mater.* **2022**, *5*, 10003-10014.
- [2] Dalapti, R.; Nandi, S.; Gogoi, C.; Shome, Arpita.; Biswas, S. *ACS Appl. Mater. Interfaces.* **2021**, *13*, 8563-8573.

When MOFs met SALI: Solvent-Assisted Ligand Incorporation in Metal-Organic Frameworks

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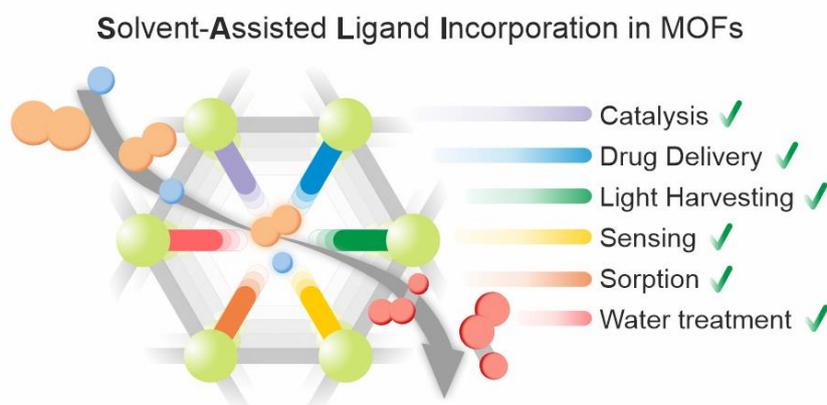
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Post-synthetic modification (PSM) offers an effective strategy to expand the functionality of metal-organic frameworks (MOFs) beyond the limitations of conventional solvothermal synthesis. Many PSM reactions proceed under mild conditions which enable targeted functionalization of well-established MOF platforms and allow the incorporation of sensitive building units without the need to develop new synthetic routes. Among these approaches, solvent-assisted ligand incorporation (SALI) is based on post-synthetic coordination of nonstructural organic ligands to metal nodes and has emerged as a particularly versatile PSM method.[1]

In this contribution, we highlight our recent applications of the SALI strategy, including the design of MOF-based drug delivery systems with prolonged release profiles,[2] enhancement of catalytic activity of Zr- and Hf-based MOFs in the cyclic addition of CO₂ to epoxides,[3] and the development of novel MOF/polymer hybrid materials for detoxification of warfare agents.[4]



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References:

- [1] Pander, M.; Stachura, E.; Kozieł-Szymańska, M.; Bury, W., *Chem. Commun.* **2025**, 61, 17715-17734.
- [2] Pander, M.; Żelichowska, A.; Bury, W., *Polyhedron* **2018**, 156, 131–137.
- [3] Pander, M.; Janeta, M.; Bury, W., *ACS Appl. Mater. Interfaces* **2021**, 13 (7), 8344–8352.
- [4] Pander, M.; Gil-San-Millan, R.; Delgado, P.; Perona-Bermejo, C.; Kostrzewa, U.; Kaczkowski, K.; Kubicki, D. J.; Navarro, J. A. R.; Bury, W., *Mater. Horiz.* **2023**, 10 (4), 1301–1308.

First Steps Toward Using Nonlinear Optics for Postsynthetic Modification of MOFs

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Over the last decade, MOFs have been recognized as strong two-photon absorbers due to, e.g., push–pull structures, rigidification effects, and also aggregation effects.[1,2] The bulk of research has focused on studies of 2PA properties as such, mostly emphasizing structure–property relationships. Others have employed exceptionally high nonlinear absorption to enable useful phenomena such as multiphoton lasing.[1, 3] However, one of unexplored consequences of two- and multi-photon absorption in MOFs is a photochemical reaction, provided that framework itself permits such a pathway.

This presentation explores how 2PA could be used to trigger solid-state reactions such as [2+2] photocycloaddition. This transformation is usually driven by one-photon excitation (UV–Vis) and is well known as a route to post-synthetic MOF modification,[4] including photopolymerization in a single-crystal-to-single-crystal manner.[5] The key point, however, is that 2PA is not simply “the same excitation at a different wavelength.” Compared with one-photon excitation, which often activates all accessible reactive sites and can be limited by surface penetration, 2PA follows different selection rules and enables bulk, long-wavelength excitation. That combination creates a real opportunity for site-selective chemistry: if we build crystals that contain multiple photoactive components with different 2PA cross-sections, we may be able to preferentially activate and transform selected molecular fragments within the lattice. At the same time, long-wavelength excitation in NIR allows to achieve more homogeneous conversion across the whole crystal and reduce damage, improving the chances of retaining crystal integrity. Indeed, our initial results indicate that realization of [2+2] photocycloaddition through two-photon absorption can alleviate or completely suppress strain-formation phenomena which otherwise sometimes cumulate to give a so-called photosolvent effect, or „exploding crystals”. Finally, we will see that two-photon realization of postsynthetic [2+2] photocycloaddition reaction in MOF can be very conveniently monitored by observation of spectral changes of two-photon excited luminescence and can be used to guess the photoreaction conversion rate.

Acknowledgements

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References:

- [1] Zaręba, J.K.; Nyk, M.; Samoć, M. *Adv. Optical Materials*, **2021**, 9, 2100216.
- [2] Mayer, D. C.; Zaręba, J. K.; Raudaschl-Sieber, G.; Pöthig, A.; Chotuj, M.; Zaleśny, R.; Samoć, M.; Fischer, R. A. *Chem. Mater.*, **2020**, 32, 5682.
- [3] He, H.; Ma, E.; Cui, Y.; Yu, J.; Yang, Y.; Song, T.; Wu, C.-D.; Chen, X.; Chen, B.; Qian, G. *Nat. Commun.*, **2016**, 7, 11087.
- [4] Kole, G. K.; Medishetty, R.; Mir, M. H.; Zaręba, J. K.; Hasegawa, M.; MacGillivray, L. R.; Konar, S.; Steed, J. W. *Cryst. Growth Des.* **2025**, 25, 1949.
- [5] R. Medishetty, I.H. Park, S.S. Lee, J.J. Vittal, *Chem. Commun.* **2016**, 52, 3989-4001.

Inverse Olefin/Paraffin Gas Separation with Functionalized Flexible Metal-Organic Frameworks

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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 Zn²⁺ ions and benzimidazole (bim) linkers. This MOF shows gate opening/closing phenomena with increasing/decreasing 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.

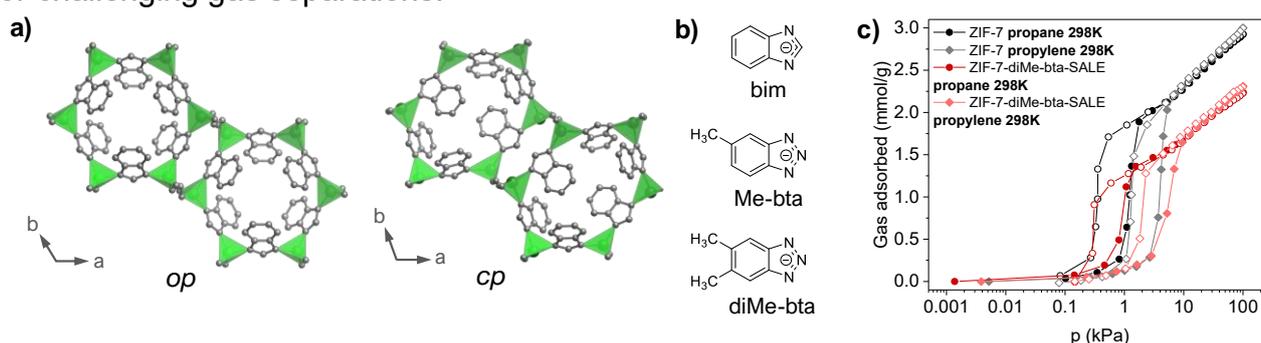


Figure 1. (a) Open- and closed-pore structures for ZIF-7. (b) Structural ligands explored in this work. (c) Propane and propylene adsorption/desorption isotherms (298 K) for ZIF-7 and ZIF-7-diMe-bta-SALE.

References:

- [1] (a) A. van Miltenburg, W. Zhu, F. Kapteijn, J. A. Moulijn, *Chemical Engineering Research and Design*, 2006, 84 (5), 350–354. (b) Y. Wang, S. Bo Peh, D. Zhao, Y. Wang, S. B. Peh, D. Zhao, *Small*, **2019**, 15 (25), 1900058.
 [2] C. Gücüyener, J. van den Bergh, J. Gascon, F. Kapteijn. *J Am Chem Soc*, **2010**, 132 (50), 17704–17706.
 [3] I. Senkowska, V. Bon, A. Mosberger, Y. Wang, S. Kaskel. *Advanced Materials*, **2025**, 2414724.

A Strategy to Enhance Photon Upconversion Emission in Lanthanide Metal-Organic Frameworks

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Lanthanides are known to have specific photoluminescence properties that are attributed to their shielded 4*f* valence electrons [1]. These unique features allow manipulation of band gaps and thus result in predictable and stable emission bands. One particularly intriguing property is the photon upconversion (UC) process, enabling the conversion of low to high energy wavelengths via sequential two or multi-photon absorption steps. These characteristics make Ln-based materials promising candidates for optical applications. In particular, the UC emission of conventional inorganic phosphors has been utilized in multiple domains, including imaging, optoelectronics, and catalysis [2]. Introduction of Ln into the MOF (LnOFs) system has already been reported for outperforming conventional phosphors [3]. However, the translation of the UC properties from conventional Ln-based phosphors to LnOFs remains largely unexplored. Since lanthanide UC efficiency is significantly reduced in materials containing organic ligands, due to competitive nonradiative decay pathways that arise from vibrational coupling mechanisms. Therefore, the proximity of lanthanide centers to organic ligands in MOF structures exacerbates these quenching effects, as the energy transfer efficiency scales with the inverse sixth power of the donor-acceptor separation distance. While conventional strategies rely on short linkers to partially address this, the development of efficient UC-active LnOFs remains challenging. Here we show that engineering multinuclear metal clusters within LnOFs, specifically $\{Y_6(OH)_6(COO)_8\}$ nodes co-doped with Yb^{3+} and Er^{3+} , dramatically enhances UC emission and efficient intracluster energy transfer. This cluster-based strategy circumvents fundamental limitations imposed by organic linkers, establishing a new approach for designing LnOFs with improved UC activity.

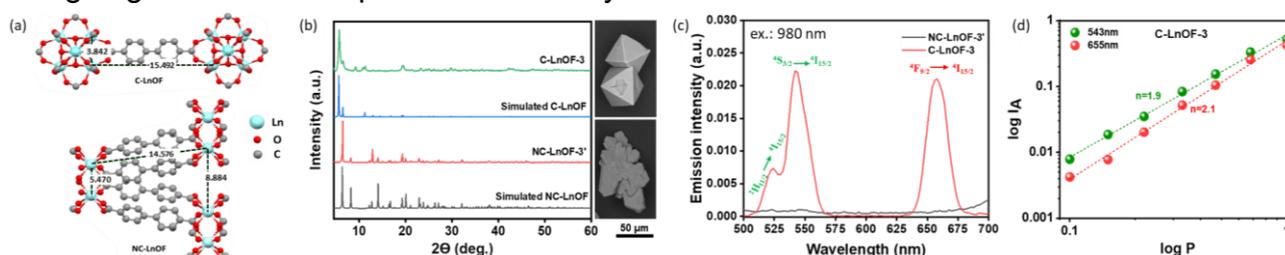


Figure 1: Preliminary data of a) structures of LC-MOF (C-LnOF-3) vs conventional LnOF (NC-LnOF-3); b) PXRD; c) NIR-to-visible UC emission and b) power dependence.

References:

- [1] De Bettencourt-Dias A., *Modern Applications of Lanthanide Luminescence*, Springer, Cham, **2023**, vol.19
- [2] Malhotra K., Hrovat D., Kumar B., Qu G., Houten J. V., Ahmed R., Pionno P. A. E., Gunning P. T. and Krull U. J., *ACS Appl. Mater. Interfaces*, **2023**, 15, 2499–2528
- [3] Sun S., Zhao Y., Wang J. and Pei R., *J. Mater. Chem. B*, 2022, 10, 9535–9564; Wang X., Jiang Y., Tissot A. and Serre C., *Coordination Chemistry Reviews*, **2023**, 497, 215454.

Abstracts – posters

P-01

Synthesis and Structure of Original Zirconium Metal-Organic-Clusters

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Metal-organic polyhedra (MOPs) are constructed from secondary building units (SBUs), which can be metal ions or clusters linked by multifunctional organic ligands (linkers). In the last decade, zirconium-based MOPs (ZrMOPs) have been the subject of intense research due to their interesting structural properties, high stability and durable porosity. By selecting the building units, it is possible to control the size and nature of the cavity in the MOP (size, shape, and chemical function), which is important for potential applications in gas sorption and separation, catalysis, water purification, biomedicine, and energy storage [1]. It can be assumed that MOPs are molecular (0-periodic) and soluble counterparts of MOFs [2]. However, the use of zirconium-based metal-organic polyhedra may be limited due to their poor solubility [3], which is why new derivatives are being sought.

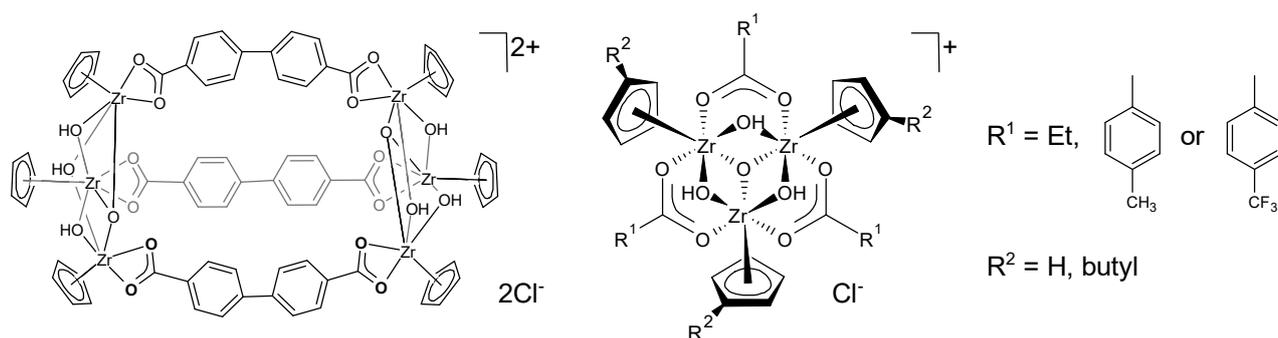


Figure 1. Schematic representation of the structure of the MOP cage (left) and the zirconium trimer cluster (center).

In my presentation, I will present the original zirconium trinuclear clusters obtained in our team, which can be used as substrates in the synthesis of MOP cages. Furthermore, I will analyze the weak intermolecular interactions in the the crystal.

Secondary building units, and MOP cages, offer potential solutions due to their unique and still insufficiently studied nature, the full understanding of which may open new possibilities in designing and synthesizing metal-organic structures.

References:

- [1] M. G. Sullivan, H. K. Welgama, M. R. Crawley, A. E. Friedman, T. R. Cook, *Chem. Mater.*, **2024**, *36*, 567.
- [2] J. J. Perry IV, J. A. Perman, M. J. Zaworotko, *Chem. Soc. Rev.*, **2009**, *38*, 1400.
- [3] M. G. Sullivan, G. E. Sokolow, E. T. Jensen, M. R. Crawley, S. N. MacMillan, T. R. Cook, *Dalton Trans.*, **2023**, *52*, 338.

P-02

First Example of COF/Bioactive Glass Hybrid Material for Biomedical Application

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Bacterial infections remain one of the leading causes of medical implant failure, highlighting the need for biomaterials that combine therapeutic and regenerative functions. Covalent organic frameworks (COFs) have recently attracted increasing attention due to their antibacterial activity, structural stability, permanent porosity, high surface area, and metal-free frameworks, making them promising candidates for biomedical applications [1]. However, COF-based systems have so far been primarily explored for antibacterial purposes, and their integration with regenerative biomaterials remains unexplored.

From a regenerative perspective, bioactive glass (BG), with Bioglass® 45S5 as its most representative composition, has been extensively studied and widely applied due to its ability to form a direct bond with bone tissue. Nevertheless, BG does not inherently address implant-associated infections. Recently, we demonstrated that sol-gel-derived BGs offer enhanced bioactivity and improved control over composition and textural properties, enabling their integration with functional components [2].

Considering the complementary capabilities and inherent limitations of both components, we present a proof of concept for a novel COF@BG hybrid system, developed by integrating a boron-based COF-1 with BG in a binary SiO₂-CaO system. The physicochemical properties of COF-1 and the COF-1@BG hybrid were systematically investigated using PXRD, FTIR spectroscopy, TEM and SEM imaging, thermogravimetric analysis, and N₂ sorption isotherms at 77 K. The biological performance of the obtained materials was evaluated through *in vitro* biocompatibility and antibacterial activity assays, complemented by reactive oxygen species (ROS) generation studies.

Acknowledgements

Financial support of the National Science Center (NCN, Poland) with grant no. 2023/50/E/ST11/00196 is gratefully acknowledged.

References:

- [1] Shi, Y.; Yang, J.; Gao, F.; Zhang, Q. *ACS Nano*, **2023**, *17*, 1879.
[2] Fandzloch, M.; Bodylska, W.; Roszek, K.; Szymański, D.; Jaromin, A.; Łukowiak, A. *Part. Part. Syst. Charact.*, **2023**, *40*, 2200184.

P-03

Coordination Polymer@Hydroxyapatite Composites: Design and Application Potential

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Chemically synthesized hydroxyapatite (HA) is widely used in bone treatments, controlled drug delivery, and as a coating material for orthopedic and dental implants due to its excellent biocompatibility and favorable mechanical properties. However, bacterial infections associated with medical implants, often leading to osteomyelitis, remain one of the most common causes of implant failure. To address this challenge and overcome the limitations of conventional biomaterials, the combination of HA with other functional materials to form antibacterial composites has emerged as a promising strategy.

In this context, new composite materials of the MOF@HA type have been developed by integrating HA with metal–organic frameworks based on Ti(IV) [1] or Ag(I). In these systems, HA may be additionally modified with –NH₂ groups to improve interfacial interactions, while the antibacterial activity is achieved through the controlled release of encapsulated antibacterial agents or metal ions from the MOF component.

On the other hand, owing to its high thermal and chemical stability, HA can also serve as a robust host material for luminescent coordination polymers. A new composite formed by combining HA with EuBTC (where H₃BTC = 1,3,5-benzenetricarboxylic acid) exhibits characteristic luminescent responses that enable chemical sensing, including the detection of iron(III) ions as a model analyte and the antibiotic ofloxacin (OFX) [2]. Taken together, these examples demonstrate the versatility of coordination polymer@HA composites exhibiting tailored antibacterial and sensing properties.

Acknowledgements

This work was supported by the National Science Centre within project 2024/53/N/ST11/00880.

References:

- [1] Bodylska, W.; Junka, A.; Brożyna, M.; Bartmański, M.; Gadzała-Kopciuch, R.; Jaromin, A.; Navarro, J. A. R.; Lukowiak, A.; Fandzloch M. *ACS Biomater. Sci. Eng.*, **2024**, *10*, 755.
[2] Bodylska, W.; Augustyniak, A. W.; Bieńko, D. C.; Fandzloch, M. *Dalton Trans.*, **2025**, *54*, 9376.

36



Heterogenization of Metal Complexes in MOFs for Catalysis

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Homogeneous catalytic systems, characterized by high activity and selectivity arising from well-defined active sites, are nonetheless constrained by inherent limitations, including thermal instability, susceptibility to aggregation, and challenges associated with recyclability. This presentation reviews the strategy of heterogenizing molecular catalysts within Metal-Organic Frameworks (MOFs) to bridge the gap between homogeneous and heterogeneous systems [1]. MOFs are indicated as ideal supports due to their high specific surface area, structural regularity, and chemical tunability, which allow for the precise confinement of active guest species. The review discusses primary synthesis strategies for creating "Cat@MOF" composites, including synthetic encapsulation, impregnation, and the "ship-in-a-bottle" approach (Figure 1).

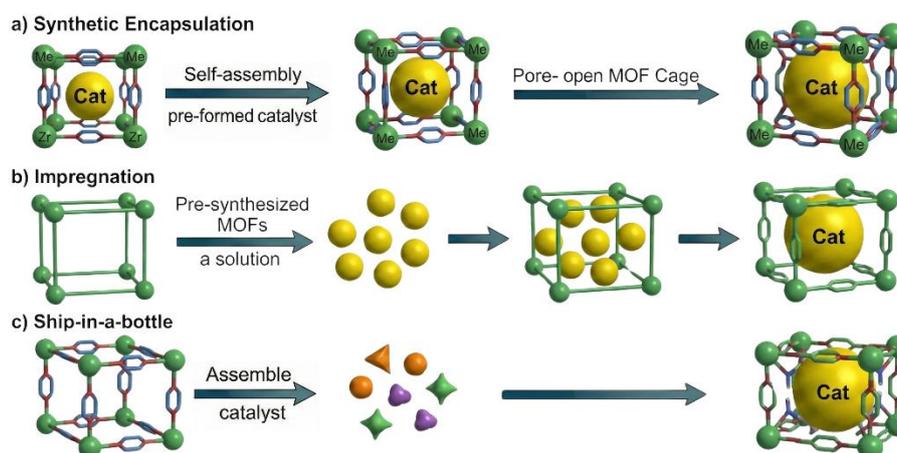


Figure 1. Synthetic strategies for the preparation of pore-functionalized Cat@MOFs (based on [2]).

The presentation elucidates the stabilization mechanisms, such as the aperture-opening process in Zr-based MOFs (UiO-66) and the restriction of substrate access to induce shape selectivity [3]. Moreover, this work shows a broad spectrum of encapsulated guests, ranging from metalloporphyrins and phthalocyanines to sensitive organometallic complexes like ruthenium and rhodium species. The versatility of these composites is demonstrated through applications in oxidation reactions, C-C cross-coupling, hydrogenation, and visible-light photocatalysis.

References:

- [1] Gascon, J.; Corma, A.; Kapteijn, F.; Llabrés i Xamena, F. X. *ACS Catal.*, **2014**, *4*, 361-378.
 [2] Mialane, P.; Mellot-Draznieks, C.; Gairola, P.; Duguet, M.; Benseghir, Y.; Oms, O.; Dolbecq, A. *Chem. Soc. Rev.*, **2021**, *50*, 6152-6220.
 [3] Li, Z.; Rayder, T. M.; Luo, L.; Byers, J. A.; Tsung, C. K. *J. Am. Chem. Soc.*, **2018**, *140*, 8082-8085.

Crystalline Solvent-Responsive Lanthanide(III)– Pentacyanidoazidocobaltate(III) Coordination Assemblies

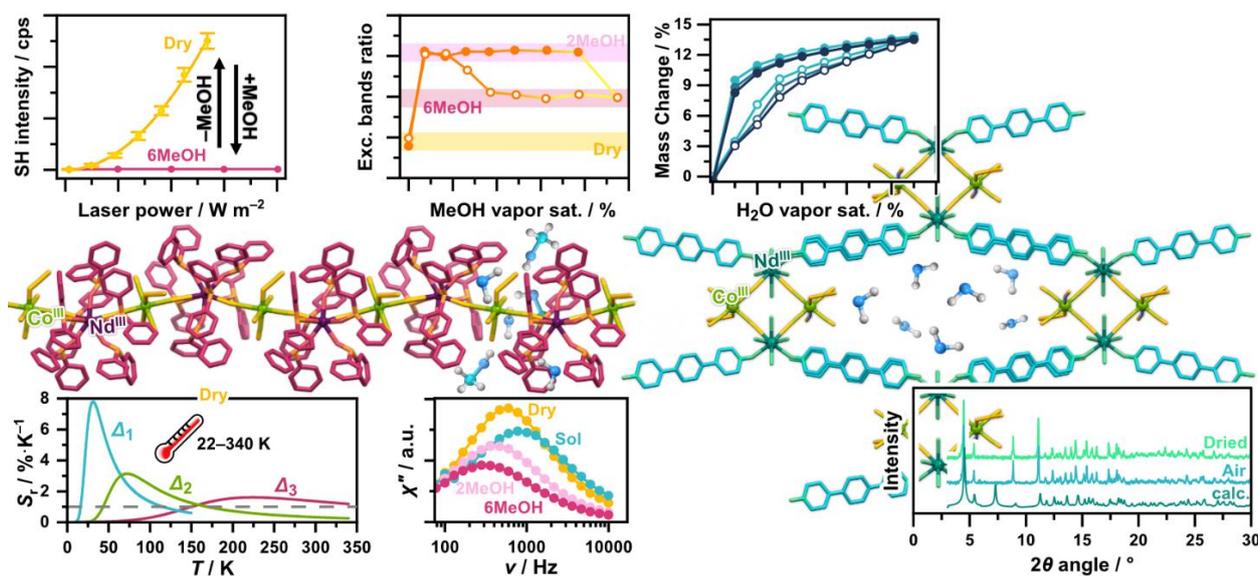
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Cyanido bridges are excellent linkers for the combination of soft and hard basic metal cations. They can work in synergy with organic ligands, which resulted in the materials, including coordination polymers, revealing the broad scope of physical functionalities [1,2]. Although successful, homoleptic octahedral hexacyanidometallates are usually limited to smaller, highly polar ligands. To expand this family of materials and take advantage of larger, pore-inducing ligands, heteroleptic $[\text{Co}^{\text{III}}(\text{CN})_5(\text{N}_3)]^{3-}$ ions were employed. Longer azide anions can interact with π -systems [3] or form specific hydrogen bonds [4], stabilizing a wider array of coordination assemblies. Two highly porous molecular assemblies resulting from this strategy are described in this contribution. The first material, besides pentacyanidoazidocobaltate(III), includes neodymium(III) complex with six diphenylphosphine oxide ligands (Figure below, left). The second material explores elongated 1,4-di(pyridine *N*-oxide)benzene linkers and the same lanthanide (Figure below, right). These materials show opposite sorption characteristics: the first one shows breathing behavior with large structural changes influencing all of its physical functionalities (e.g., magnetic and optical), while the second remains structurally almost unchanged upon removal of solvents from its pores.



References:

- [1] Zakrzewski, J. J.; Liberka, M.; Zychowicz, M.; Chorazy, S. *Inorg. Chem. Front.*, **2021**, 8, 452.
- [2] Zakrzewski, J.; Hoffman, A.; Wang, J.; Pander, M.; Matoga, D.; Tokoro, H.; Ohkoshi, S.; Chorazy, S. *Angew. Chem. Int. Ed.*, **2025**, 64, e202517109.
- [3] Bera, S.; Frontera, A.; Chattopadhyay, S. *Polyhedron*, **2025**, 269, 117422.
- [4] Zychowicz, M.; Dzielak, H.; Rzepiela, J.; Chorazy, S. *Inorg. Chem.*, **2024**, 63, 19213.

P-06

A Strategy to Enhance Photon Upconversion Emission in Lanthanide Metal-Organic Frameworks

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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 ensures 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 H₂BPDC linker, with Yb³⁺ as a sensitizer and Er³⁺ as an emitter. UC emission measurement showed Er³⁺ 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, we got the trend of increased UC intensity upon increasing conjugation, which can be excellent for tuning the UC efficiency for optical applications.

References:

- [1] J.-C. G. Bünzli, *Journal of Coordination Chemistry*, 2014, **67**, 3706–3733.
- [2] K. Malhotra, D. Hrovat, B. Kumar, G. Qu, J. V. Houten, R. Ahmed, P. A. E. Piuanno, P. T. Gunning and U. J. Krull, *ACS Appl. Mater. Interfaces*, 2023, **15**, 2499–2528.
- [3] K. Du, J. Feng, X. Gao and H. Zhang, *Light Sci Appl*, 2022, **11**, 222.
- [4] J. Wang, R. Deng, M. A. MacDonald, B. Chen, J. Yuan, F. Wang, D. Chi, T. S. Andy Hor, P. Zhang, G. Liu, Y. Han, *Nature Mater.*, 2014, **13**, 157–162.

P-07

Two-Dimensional Metal-Organic Frameworks Based on Halogen-Substituted Isophthalic Acids

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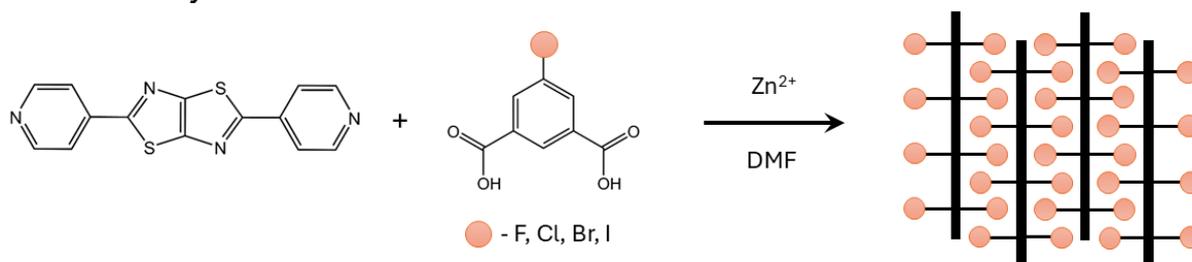
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Metal-organic frameworks (MOFs) are porous coordination polymers composed of metal ions or clusters and organic linkers, forming one- to multidimensional polymeric networks. Two-dimensional (2D) MOFs have attracted significant attention across various research fields owing to their exceptional physical and chemical properties, including ultrathin morphology, high surface area, a large number of exposed unsaturated metal sites, and tunable surface characteristics [1].

In this study, we report the synthesis of four novel 2D MOFs: $[\text{Zn}_2(\text{iso-F})_2(\text{BPTzTz})_2]_n$, $[\text{Zn}_2(\text{iso-Cl})_2(\text{BPTzTz})_2]_n$, $[\text{Zn}_2(\text{iso-Br})_2(\text{BPTzTz})_2]_n$ and $[\text{Zn}_2(\text{iso-I})_2(\text{BPTzTz})_2]_n$. These frameworks were prepared from zinc nitrate, 5-bis(4-pyridyl)thiazolo[5,4-d]thiazole (BPTzTz), and halogen-substituted derivatives of isophthalic acid ($\text{H}_2\text{iso-X}$, where X = F, Cl, Br, or I) using N,N-dimethylformamide (DMF) as the solvent.

All compounds were obtained in crystalline form, and their structures were elucidated by single-crystal X-ray diffraction. The materials exhibit two-dimensional architectures in which adjacent layers are laterally displaced relative to one another. The magnitude and nature of this interlayer shift depend on the halogen substituent and are governed by distinct halogen-bonding interactions. These interactions significantly influence stability, structural dynamics and adsorption properties towards CO_2 (195 K), N_2 (77K) and H_2O (298 K).

Scheme 1. Synthesis scheme.



References:

[1] G. Chakraborty, I. Park, et al. Chem. Rev. 2021, 121, 7, 3751–3891.

P-08

Multifunctional Composites with Silver(I) Metal-Organic Architectures

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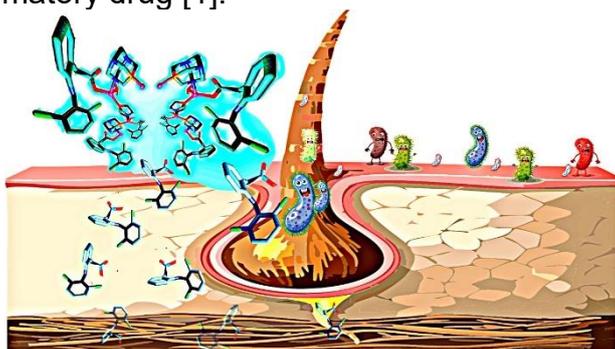
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The treatment and prevention of infections, as well as effective pain management strategies, are crucial elements of the Sustainable Development Goals, which greatly influence global health and well-being. Recent initiatives have emphasized creating advanced therapeutic materials for wound care, particularly through innovative methods involving metal-organic frameworks (MOFs) and coordination polymers (CPs).

Here we present multifunctional antimicrobial composite materials based on chia seed mucilage (CSM) and its modified form CSM/ST (starch), doped with a therapeutic silver(I) coordination polymers (designated as Ag@CSM or Ag@CSM/ST). The resulting composite demonstrate exceptional water absorption capacity and natable activity against a broad spectrum of pathogens, including Gram-positive and Gram-negative bacteria as well as yeast.

Furthermore, an *in vitro* study using human cadaver skin demonstrated the strong potential of the tested compounds for topical delivery to the upper epidermis, especially the stratum corneum, and also promoted transdermal delivery of diclofenac sodium, a common nonsteroidal anti-inflammatory drug [1].



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References:

[1] Jaros, S. W.; Markieton, J.; Florek, M.; Król, J.; Rath, S.; Talluri, S. R.; Albayati, N.; Michniak-Kohn, B. *Dalton. Trans.* **2026**, DOI <https://doi.org/10.1039/D5DT02494C>

P-09

Rational Design of Co-Doped Fe₂O₃/Fe₃O₄/Ce-UiO-66 Composites: Effect of Metal Oxide to MOF Ratio on Nitrogen Reduction Performance

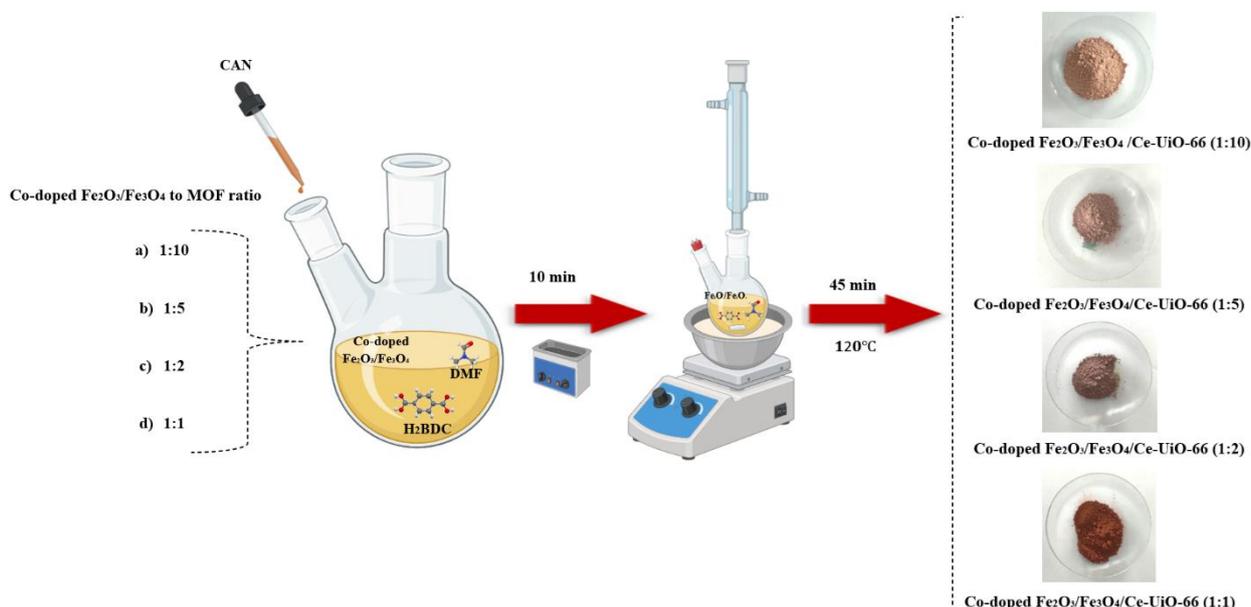
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Photocatalytic nitrogen reduction reaction (NRR) represents a sustainable pathway for ammonia production under mild conditions; however, its efficiency is still limited by insufficient N₂ activation and rapid charge recombination [1, 2]. In this study, a series of Co-doped Fe₂O₃/Fe₃O₄/Ce-UiO-66 composites was synthesized by systematically tuning the metal oxide-to-MOF ratio to enhance interfacial synergy (Scheme 1). The optimized Fe₂O₃/Fe₃O₄/Ce-UiO-66(1:2) composite exhibits significantly improved photocatalytic NRR performance compared to other ratios. The enhanced activity is attributed to efficient charge separation, increased density of active sites, and synergistic interactions between Co-doped iron oxides and Ce-based MOF. This work highlights the critical role of compositional balance in hybrid metal oxide/MOF photocatalysts and provides insights into rational design strategies for efficient photocatalytic nitrogen reduction.



Scheme 1. Synthesis method of Co-doped Fe₂O₃/Fe₃O₄/Ce-UiO-66 composites.

References:

- [1] Huang, R., Li, X., Gao, W., Zhang, X., Liang, S., & Luo, M. (2021). *RSC advances*, 11(24), 14844-14861.
[2] Zhu, Y., Ji, H., Huang, T., Sun, Y., & Pang, H. (2024). *Advanced Sustainable Systems*, 8(10), 2400225.

P-10

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.

This work was supported by the Polish National Science Centre (NCN) (grant no.2022/45/B/ST8/02028).

References:

[1] B. Mazur, L. Firlej, B. Kuchta, ACS Appl. Mater. Interfaces, 16, 19, 25559–25567 (2024)

[2] Molinero, Valeria & Moore, Bree. (2008). The journal of physical chemistry. B. 113. 4008-16. (2008).

Rare-Earth MCAs for Surrogate Studies in Actinide Immobilization

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Lanthanide MCAs (molecular cluster aggregates), composed of multinuclear metal cores encapsulated by organic ligands, have attracted considerable attention in the past few decades due to their diverse applications and interesting solid-state structures. They can be used as single molecular magnets [1], in luminescent sensing/probing [2], magnetic refrigeration [3], or catalysis [4]. By combining the best properties of lanthanide nanoparticles and molecular complexes, MCAs have recently established themselves as a highly efficient, next-generation solution for optical applications.

In our work [5], rare-earth cluster aggregates with the formula $[\text{RE}_9(\mu_4\text{-OH})_2(\mu_3\text{-OH})_8(\text{sal-R})_{16}]\text{X}$ ($\text{RE}^{\text{III}} = \text{Y}$ (1), Eu (2), Dy (3), Tm (4), Yb (5), Lu (6); $\text{X}^- = \text{Cl}^-$ (1–2, 4–6), or DyCl_4^- (3); Hsal-R = alkyl salicylate with R = Me (2, 4–6), Et (3), or a mixture of Me and Et (1)) were synthesized via direct reaction of trivalent rare-earth chlorides (RECl_3 , where $\text{RE}^{\text{III}} = \text{Y}$, Eu, Dy, Tm, Yb, Lu) with in situ generated lithium/zinc-methyl salicylate complexes in a ROH/THF solution (ROH = MeOH, EtOH) in the presence of trace amounts of water. In 1–6, the nine RE^{III} ions are bridged by two $\mu_4\text{-OH}$ and eight $\mu_3\text{-OH}$ groups, forming a central sandglass-shaped motif, $\{\text{RE}_9(\mu_4\text{-OH})_2(\mu_3\text{-OH})_8\}^{17+}$. This core is encapsulated by 16 chelating sal-R ligands that stabilize the structure and inhibit further aggregation.

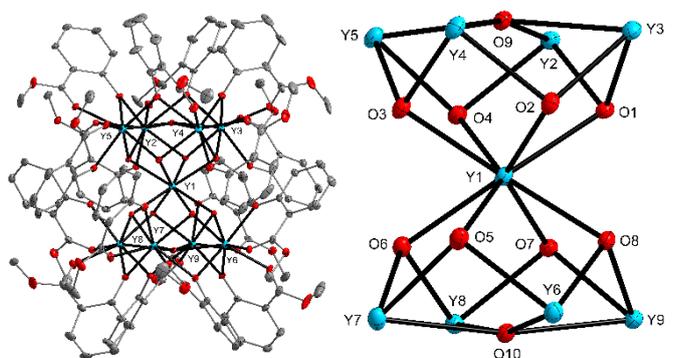


Figure 1. Molecular structure of $[\text{Y}_9(\mu_4\text{-OH})_2(\mu_3\text{-OH})_8(\text{sal-R})_{16}]\text{Cl}$ (R = Me (0.7), Et (0.3)).

Compounds 1–6 were used as a RE^{III} source (2 or 10 mol% of RE^{III}) for simulating minor actinides in high-level molecular waste (HLW), subsequently immobilized in alkaline earth manganites formed by thermal decomposition of $[\text{Ca}(\text{sal-Et})_2]_n$ or $[\text{Ba}(\text{sal-Et})_2(\text{THF})]_n$ with $[\text{Mn}_2(\mu\text{-OMe})_2(\text{sal-Me})_4]$ at 850 or 1100 °C. The resulting heterometallic oxide phases, $\text{CaMnO}_3/\text{CaMn}_2\text{O}_4$ and BaMnO_3 , effectively incorporated RE^{III} ions at the sites of $\text{Ca}^{\text{II}}/\text{Ba}^{\text{II}}$, highlighting their potential as host matrices for HLW.

Acknowledgements: The authors thank for the financial support from the Polish National Science Center under Grant Numbers 2017/26/D/ST5/01123 and 2023/49/B/ST4/04068.

References:

- [1] Sharples, J.W.; Zheng, J.; Tuna, F.; McInnes, E.J.L.; Collinson, D. *Chem. Commun.*, **2011**, 47, 7650.
- [2] Li, Y.; Wang, H.; Zhu, Z.; Li, J.; Zou, H.; Liang, F. *Inorg. Chem.*, **2021**, 60, 16794.
- [3] Yao, M.; Cai, L.; Deng, X.; Zhang, W.; Liu, S.; Cai, X. *New J. Chem.*, **2018**, 42, 17652.
- [4] Kowaliński, A.; Petrus, R.; Chomiak, K.; Lis, T. *Appl. Organomet. Chem.*, **2025**, 39, e70017.
- [5] Petrus, R.; Kowaliński, A.; Lis, T.; Siczek, M.; Sobota, P. *Inorg. Chem.*, **2025**, 64, 16020.

P-12

MOF/Polymer Hybrids with Tunable Hydrophilicity for Water Sorption

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Water is essential for life, yet by 2050, nearly half the world may face a water crisis. As a result, researchers are increasingly exploring materials that can efficiently capture water from the environment. One promising class of materials are Metal-Organic Frameworks (MOFs), known for their high surface area, tunable porosity, and chemical versatility, making them strong candidates for water harvesting, despite that classical MOFs exposed to humidity lose their crystallinity and porosity. Recently, Yaghi and co-workers demonstrated that MOFs can trap water even at 10% humidity with efficient uptake and release [1].

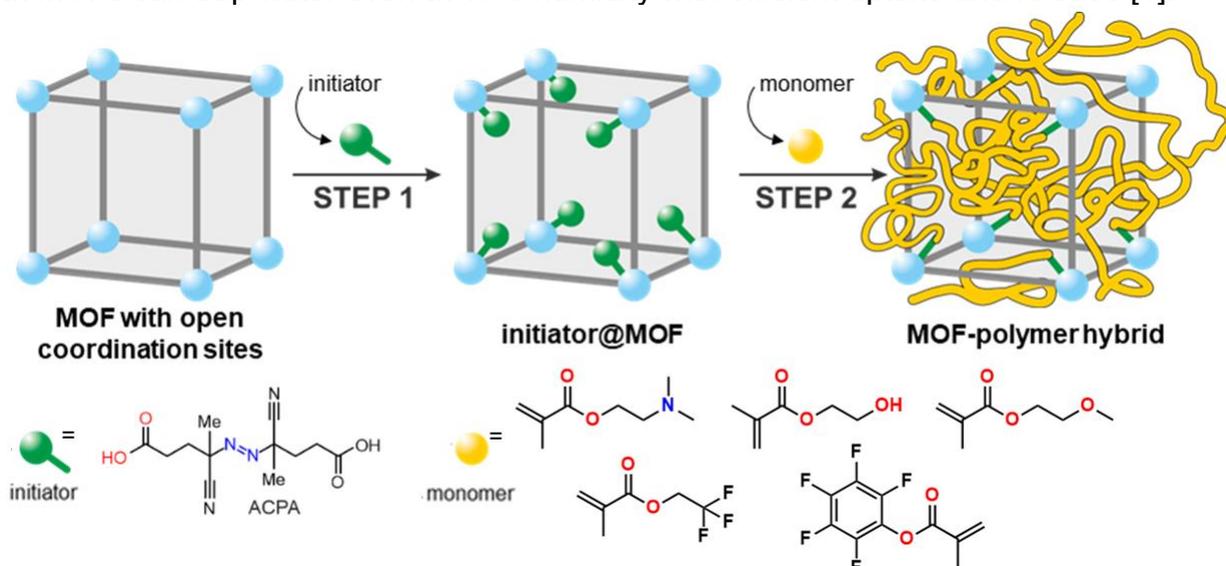


Figure 1. Scheme of the designed strategy of preparing MOF/polymer composites with selected initiator and monomers [2].

The aim of presented work was to design, synthesize and characterize new series of multifunctional MOF/polymer hybrid materials using simple and functionalized monomers as substrates. The research project was based on our original post-synthetic modification method - Free Radical Polymerization in Metal-Organic Framework (*FRaP-in-MOF*). In this method initiator is coordinated to the open metal sites of zirconium-based MOF (ZrMOF). The obtained polymer@ZrMOF hybrid materials exhibit varying level of water sorption depending on the attached polymer and retains constant porosity in contrast to the pristine NU-1000 when exposed to humid conditions.

References:

- [1] Xu, W.; Yaghi O.M. *ACS Cent. Sci.*, **2020**, 6, 8, 1348-1354.
 [2] Pander, M.; Perona-Bermejo, C.; Gil-San-Millan, R.; Delgado, P.; Kostrzewa, U.; Kaczkowski, K.; Kubicki, D. J.; Navarro, J. A. R.; Bury, W. *Mater. Horiz.*, **2023**, 10, 1301.

Synthesis and Photocatalytic Properties of Novel ZrMOPs

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Zirconium-based Metal-Organic Polyhedra (ZrMOPs) are molecular systems with well-defined structures. In contrast to metal organic frameworks, MOPs are soluble, which increases access to active sites, making them attractive systems for applications in catalysis.[1] Due to the diverse geometry of the linkers used in their synthesis, several molecular topologies can be identified (**Fig. 1**). So far, only ZrMOPs containing linkers with same spatial structure have been described, giving them unique properties and a specific symmetry. Recently, Bloch and co-workers have demonstrated the possibility of synthesizing cages that incorporate different ligands.[2]

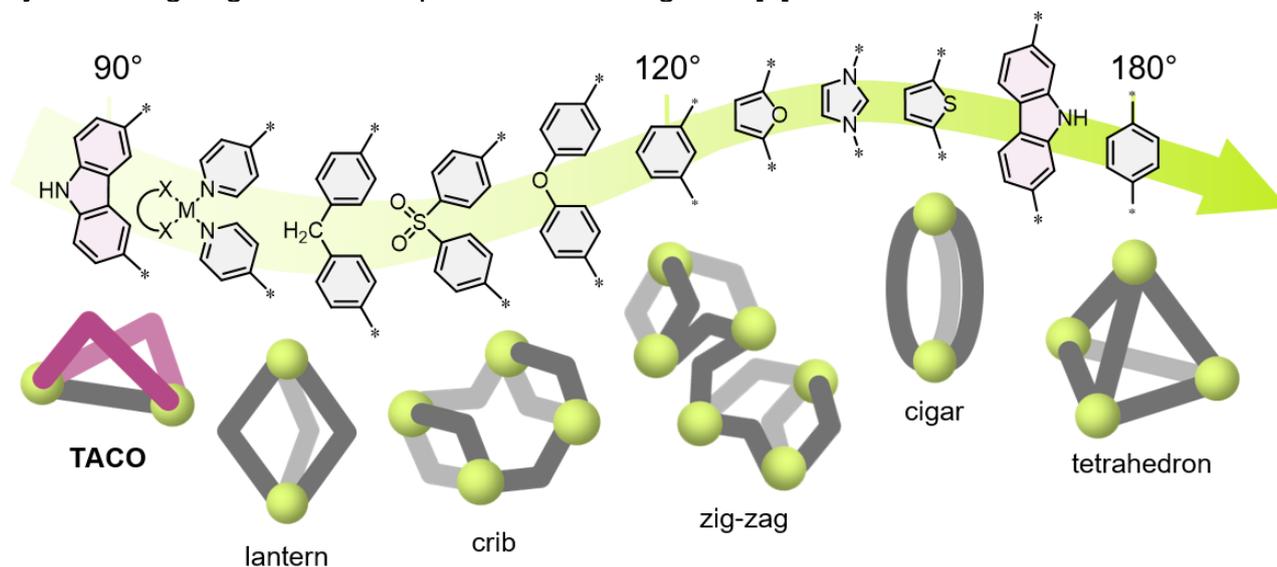


Figure 1. Schematic representation of Zr-MOP topologies depending on linker angularity.

The aim of this study was to design and synthesize a zirconium-based cage with a novel topology, incorporating two carboxylate ligands of different geometries. Based on the spatial structure of the $Zr_3(\mu_3-O)(\mu_2-OH)_3Cp_3$ nodes, two types of linkers were designed – linear and angular – with their geometries carefully selected to ensure optimal fit within the cage structure. We obtained a series of cages with an original topology resembling the shape of a "taco" sandwich, which were determined using crystallographic methods. These compounds represent the first example of Zr-MOPs in which the simultaneous presence of two types of ligands with distinct geometries has been unequivocally confirmed. The resulting cages exhibit high activity in the photocatalytic oxidation of sulfides.

References:

- [1] Delgado, P.; Martín-Romera, J. D.; Perona, C.; Vismara, R.; Galli, S.; Maldonado, C. R.; Carmona, F. J.; Padiál, N. M.; Navarro, J. A. R. *ACS Appl. Mater. Interfaces*, **2022**, *14*, 23, 26501.
 [2] Morey, M. N.; Montone, M. C.; Dworzak, M.; Yap, G. P. A.; Bloch, E. D. *Chem. Sci.*, **2025**, *2*, 16, 816.

Solvent-Vapor-Responsive Ce(III)-Pt(II) Magneto-Luminescent Coordination Polymer

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Luminescent coordination compounds based on lanthanide(3+) ions combined with polycyanidometallate complexes have been the subject of extensive research in recent years, due to their outstanding physicochemical properties, including multi-colored emission highly sensitive to external stimuli, such as relative humidity, organic solvent vapors, or temperature. The incorporation of lanthanide(3+) ions not only enhances the optical luminescent properties but also introduces the potential Single-Molecule-Magnet (SMM) behavior, originating from the strong magnetic anisotropy of the rare-earth metal ions^[1]. Systems linking the stimuli-responsive optical properties with magnetic ones, including *d-f* cyanido-bridged frameworks, are ideal candidates for future development and application in various fields of technology^[2-5]. In this regard, we present two coordination polymers, i.e., a 3-D coordination network of $\{[\text{Ce}^{\text{III}}(\text{MeOH})_2]_2[\text{Pt}^{\text{II}}(\text{CN})_4]_3\} \cdot 4\text{MeCN}$ (**1^{MS}**) and a 2-D layered framework $\{[\text{Ce}^{\text{III}}(\text{H}_2\text{O})_6]_2[\text{Pt}^{\text{II}}(\text{CN})_4]_3\} \cdot 4\text{H}_2\text{O}$ (**1^{air}**) linking guest-molecule variable emission with solvent-switchable SMM characteristics (Figure 1).

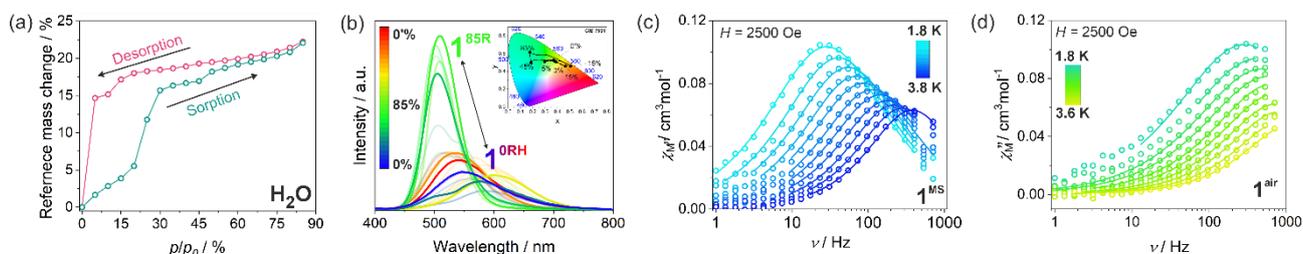


Figure 1. Water vapor sorption isotherm of **1^{air}** (a); emission spectra of **1^{air}** in the 0–85% RH range with the related changes shown on the CIE 1931 chromaticity diagram (b); ac magnetic characteristics of **1^{MS}** (c) and **1^{air}** (d).

References:

- [1] Woodruff, D. N.; Winpenny, R. E. P.; Layfield, R. A. *Chem. Rev.* **2013**, *113*, 5110–5148.
- [2] Zakrzewski, J. J.; Jędrzejowski, D.; Wang, J.; Tokoro, H.; Ohkoshi, S.; Matoga, D.; Chorazy, S. *Adv. Optical Mater.* **2025**, *13*, 2403168.
- [3] M. Wyczęsany, R. Jankowski, S. Chorazy, *Chem. Commun.* **2023**, *59*, 5961–5986.
- [4] J. Rocha, C. D. S. Brites, L. D. Carlos, *Chem. Eur. J.* **2016**, *22*, 14782–14795.
- [5] Wyczęsany, M.; Heczko, M.; Reczyński, M.; Sieklucka, B.; Chorazy, S. *J. Mater. Chem. C* **2024**, *13*, 2732–2744.

P-15

Metal-Organic Frameworks as Tunable Precursors for Copper-Containing Oxide Catalysts in Methanol Steam Reforming

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Hydrogen is a key energy carrier for the transition toward a low-carbon energy system, with significant potential for decarbonization of industry and transportation [1]. Among hydrogen production routes, methanol steam reforming (MSR) is an attractive technology due to its high hydrogen yield, relatively low operating temperature, and compatibility with renewable methanol as a liquid hydrogen carrier [2]. However, the development of efficient and stable catalysts remains essential for practical implementation of MSR-based hydrogen technologies.

Metal-organic frameworks (MOFs) offer a versatile platform for the design of advanced catalytic materials owing to their high surface area, tunable porosity, and well-defined structures [3]. In this work, selected MOFs were used as precursors for the preparation of oxide-based catalysts for methanol steam reforming. The MOF materials were subjected to controlled thermal treatment to obtain porous MOF-derived oxide phases, followed by modification with copper to generate catalytically active systems. The obtained materials were characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA) to investigate phase evolution, structural changes, and thermal stability during the MOF-to-oxide transformation and subsequent copper incorporation.

The catalytic performance of the copper-modified MOF-derived oxides was evaluated in the methanol steam reforming reaction. The materials exhibited activity toward hydrogen production, demonstrating the potential of MOF-derived oxides as tunable catalysts for MSR. The results indicate that both the precursor MOF structure and thermal treatment conditions significantly influence the properties and performance of the resulting catalysts.

Acknowledgements: The authors are grateful for financial support from the Gdańsk University of Technology by the DEC-9/1/2023/IDUB/I3b/Ag grant under the Argentum Triggering Research Grants – ‘Excellence Initiative – Research University’.

References:

- [1] Rosen, M.A., Koochi-Fayegh, S. *Energy Ecol Environ*, **2016**, 1, 10.
[2] Abbas, A.H.M., Cheralathan, K.K., Porpatham, E., Arumugam, S.K. *Renew. Sustain. Energy Rev.*, **2024**, 191, 114147.
[3] Chughtai, A.H, Ahmad, N., Younus, H.A., Laypkov, A., Verpoort, F. *Chem. Soc. Rev.*, **2015**, 44, 6804.

Heterometallic Alkali Metal-Magnesium/Zinc/Calcium Aggregates

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The aim of this work is a structural analysis of heterometallic zinc/magnesium/calcium aryloxides with alkali metal ions. The dominant group of heterometallic aggregates are centrosymmetric tetranuclear compounds based on a double-opened dicubane core structure with two missing vertices $[M_2M'_2(\text{sal-Me})_6(X)_x]$ (where $M^{2+} = \text{Mg}^{2+}$ and $M'^+ = \text{Li}^+$ (**1**), Na^+ (**2**), K^+ (**3**); $M^{2+} = \text{Zn}^{2+}$ and $M'^+ = \text{Li}^+$ (**4**), Na^+ (**5**), K^+ (**6**); or $M^{2+} = \text{Ca}^{2+}$ and $M'^+ = \text{Li}^+$ (**7**), Na^+ (**8**), K^+ (**9**) with $X = \text{THF}$ or MeOH and $x = 0, 2, 4$). In these structures, the metal atoms are held together by two $\mu_3\text{-O}$ and four $\mu\text{-O}$ aryloxo oxygen atoms. The vertices of the common face of the defective dicubane units in **1**, **4**, and **7** are occupied by M^{2+} ions, and the external vertices are Li^+ ions. The same structural motif, with external Na^+/K^+ ions and internal Ca^{2+} ions, was observed in **8** and **9**. However, reverse arrangements of the metal atoms in the central cores of **2** and **3**, or **5** and **6**, are observed with peripheral Mg^{2+} or Zn^{2+} centers, and alkali-metal ions Na^+/K^+ occupy the vertices of the common face. Heterometallic aryloxides $[\text{Mg}_4\text{Na}_2(\text{sal-Me})_6(\text{sal})_2(\text{THF})_4]$ (**10**) or $[\text{Ca}_4\text{M}'(\mu_5\text{-OH})(\text{sal-Et})_8(\text{EtOH})]$ ($M'^+ = \text{Na}^+$ (**11**), K^+ (**12**)) are examples of structurally uncommon compounds synthesized by exposure of reagents to atmospheric moisture or the deliberate addition of water.

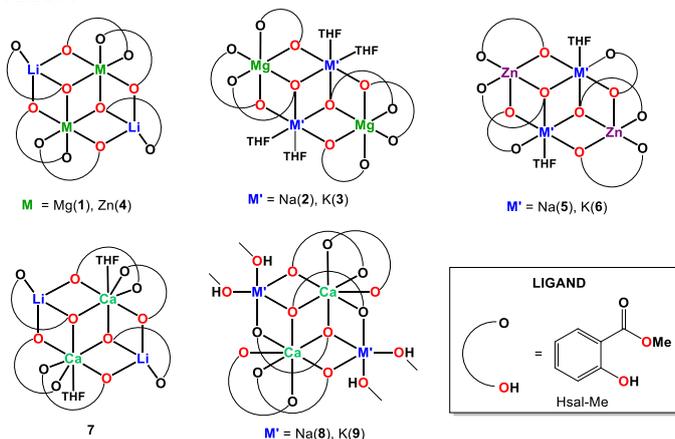


Figure 1. The structures of 1-9.

Within the series of heterometallic compounds, $[\text{Mg}_2\text{M}'_2(\text{sal-Me})_6(\text{THF})_x]$ (**1-3**) showed remarkable catalytic activity in the chemical recycling of high-consistency silicone rubber waste by alcoholysis to low-molecular-weight alkoxy silane derivatives. Binary metal catalysts $[\text{Zn}_2\text{M}'_2(\text{sal-Me})_6(\text{THF})_x]$ (**4-6**), and $[\text{CaLi}_6(\text{sal-Me})_8]$ (**13**) exhibited the highest catalytic activity in the methanolysis of nylon-6 at 220 °C.

References:

- [1] Petrus, R.; Matuszak, K.; Kowaliński, A.; Lis, T.; *Inorganic Chemistry Frontiers*, **2025**, 12, 7083-7106.
 [2] Petrus, R.; Utko, J.; Gniłka, R.; Fleszar, M.G.; Lis, T.; Sobota, P.; *Macromol*, **2021**, 54, 2449-2465.
 [3] Petrus, R.; Matuszak, K.; Kinzhybalov, V.; *Chem. Asian J.*, **2024**, 19, e202400526.

P-17

From Hydrophilic to Hydrophobic – A Systematic Study of Water Adsorption in the QMOF Database with Flat-Histogram Monte Carlo

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Water can be either a working fluid or a poison for metal-organic frameworks (MOFs). Strong, cooperative uptake is imperative for atmospheric water harvesting and humidity control, while hydrophobicity is mandatory in applications such as CO₂ capture. However, a systematic examination of the structural and chemical factors that determine a framework's propensity towards hydrophilicity or hydrophobicity remain underrepresented in existing studies. A systematic computational analysis of large MOF databases for the adsorption of CO₂, CH₄, and other small molecules has become quite common in recent years. However, a similar study for water has long been missing, due to the well-known challenges of simulating water adsorption [1].

In this study, we performed a high-throughput screening of 8,565 structures from the QMOF database [2-3] using flat-histogram Monte Carlo method to obtain the full macrostate probability distribution (density of states) for water in each framework. This approach yields water isotherms with effectively “infinite” resolution and enables thermodynamic extrapolation across temperatures, providing access to the pressure-temperature landscape of water adsorption from a single simulation set [1,4]. From the resulting data, we quantify adsorption mechanisms (continuous filling or adsorption through phase transition, with metastable gas-like and liquid-like states and barrier height) and identify properties that are significant from an application point of view, such as condensation pressure or hysteresis propensity. By correlating these with geometric and chemical features we identify structure-property relationships that govern hydrophilicity versus hydrophobicity in MOFs. The utilization of these relationships is twofold: first, they serve to identify promising AWH candidates, and second, they can be employed to deliberately design hydrophobic MOFs suitable for CO₂ capture and other applications influenced by the presence of water.

This work was supported by the Polish National Agency for Academic Exchange (decision no. BPN/BEK/2024/1/00218/DEC/1), and the National Science Centre (NCN), Poland (grant no. 2022/45/B/ST8/02028).

References:

- [1] B. Mazur, L. Firlej, B. Kuchta, *ACS Appl. Mater. Interfaces*, **16**, 19, 25559–25567 (2024)
- [2] A.S. Rosen, S.M. Iyer, D. Ray, Z. Yao, A. Aspuru-Guzik, L. Gagliardi, J.M. Notestein, R.Q. Snurr, *Matter*, **4**, 1578-1597 (2021)
- [3] A.S. Rosen, V. Fung, P. Huck, C.T. O'Donnell, M.K. Horton, D.G. Truhlar, K.A. Persson, J.M. Notestein, R.Q. Snurr, *npj Comput. Mat.*, **8**, 112 (2022)
- [4] N. A. Mahynski, H. W. Hatch, M. Witman, D. A. Sheen, J. R. Errington, V. K. Shen, *Molecular Simulation*, **47(5)**, 395–407 (2020)

Synthesis and Characterization of UiO-68-type core-shell MOFs with Tetrazine Linkers

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Porous materials, particularly Metal-Organic Frameworks (MOFs), represent promising platforms for pollutant removal or gas storage [1] due to their high porosity and tunable structures. Tetrazine-based linkers e.g. 4,4'-(1,2,4,5-tetrazine-3,6-diyl)dibenzoic acid (H_2TZDC) are highly attractive building units due to their high reactivity, which is a key factor in designing MOF functionalization strategies, including click reactions [2]. Their stability under humid conditions can be further improved through structural modifications, such as an incorporation of linkers functionalized with specific moieties. As was shown recently by Jędrzejowski et al., the solvent-assisted linker exchange (SALE) method enables core-shell swapping, control over the degree of linker ratio, and enhancement of stability of the material [3].

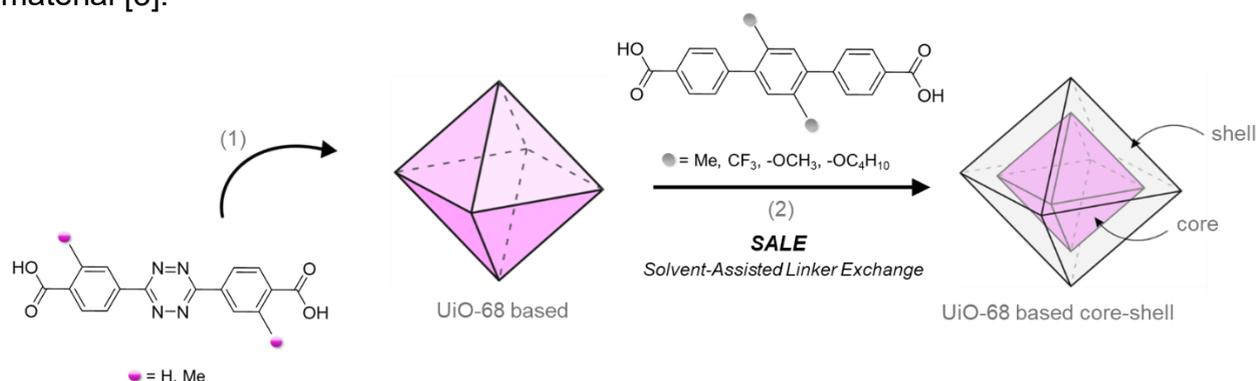


Figure 1. Schematic representation of the proposed strategy for MOF synthesis, involving (1) the use of selected tetrazine-based linkers and (2) the formation of core-shell structures employing linkers functionalized with specific moieties.

The aim of the presented work was to investigate this original approach for the modification of zirconium-based MOF materials presenting UiO-68-type structure towards dual-linker core-shell MOFs. In our work new combinations of dicarboxylate linkers were tested using SALE method for the preparation of UiO-68-type core-shell materials and the obtained materials were structurally characterized. Correlations between their sorption properties and the employed organic linkers were then established.

References:

- [1] Chen, Z.; Li, Y.; Cai, Y.; Wang, S.; Hu, B.; Li, B.; Ding, X.; Zhuang, L.; Wang, X. *Carbon Res.* **2023**, *2*, 8.
- [2] Gómez-Tenés, G.; Gimeno-Fonquernie, P.; Misturini, A.; Chinchilla-Garzón, C.; Carratalá, V.; Cisneros, L.; Martí-Gastaldo, C. *Chem. Commun* **2024**, *60*, 12977–12985.
- [3] Jędrzejowski, D.; Pander, M.; Stachura, E.; Matlak, K.; Bury, W.; Matoga, D. *J. Mater. Chem. A* **2025**, *13*, 23671–23679.

P-19

Comparative Adsorption Study of MOFs Synthesized from Various PET Waste Sources: Experimental Isotherms vs. GCMC Simulations

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Metal-Organic Frameworks (MOFs) are recognized for their exceptional porosity and potential in gas storage and catalysis [1]; however, the high cost of organic linkers limits their industrial scalability. This study evaluates the feasibility of upcycling polyethylene terephthalate (PET) waste into recovered terephthalic acid (TPA) linkers for MOF synthesis, comparing pure and contaminated waste streams.

Three representative MOFs - MIL-53(Al), UiO-66(Zr), and MIL-101(Cr) - were synthesized using linkers recovered via alkaline hydrolysis from four varied sources: (i) commercial TPA (reference), (ii) transparent PET, (iii) blue-dyed bottles, (iv) and a mixed "dirty" waste stream. The textural properties of the obtained materials were characterized by nitrogen (N₂) adsorption-desorption isotherms at 77 K. Finally, the experimental data are compared with theoretical isotherms generated through Grand Canonical Monte Carlo (GCMC) simulations to evaluate adsorption parameters of the waste-derived materials against ideal models.

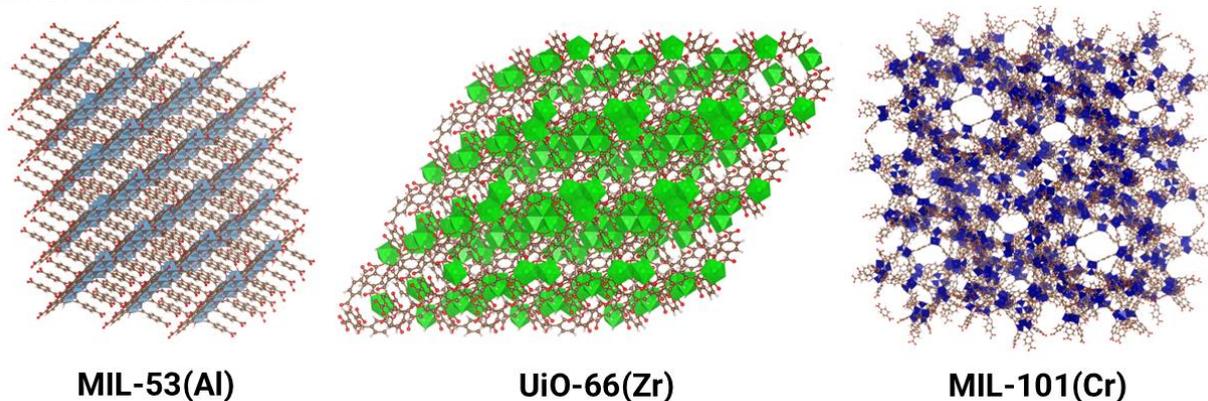


Figure 1. Crystal models of MIL-53(Al), UiO-66(Zr), and MIL-101(Cr) used for GCMC simulations.

Acknowledgements We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: WCSS) for providing computer facilities and support within computational grant no. PLG/2026/019117.

References:

[1] Furukawa, H.; Cordova, K. E.; O'Keeffe, M.; Yaghi, O. M. *Science*, 2013, 341, 1230444.

P-20

PCN-222 Thin Film on Ceramic Foam for Removal of Disinfection By-products

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MOFs cover a wide spectrum of applications including environmental remediation technologies for the removal of pollutants from water through both photocatalytic degradation and adsorption [1]. One of the subclass are porphyrin-based MOFs (PMOF) where porphyrin derivatives such as 5,10,15,20-tetrakis(4-arboxyphenyl)porphyrin (TCPP) are applied as a linker. PMOFs are characterized by broad visible light absorption, long-lived excited states and uncovered metal centers, creating the possibility of potential use as a photocatalyst [2]. A key challenge in scaling up MOFs' use for photocatalytic water and wastewater treatment lies in separating powdered materials from the treated aqueous phase. Herein, we address work addresses this issue by synthesizing a PCN-222 (Figure 1) thin film on porous Al₂O₃ ceramic foam to remove chlorophenols, representative disinfection by-products (DBPs), via combined adsorption and visible-light photocatalysis. PCN-222 thin film was fabricated through a solvothermal method, with thickness controlled by the number of deposition cycles. Owing to its large surface area and accessible porphyrinic sites, the supported film exhibited high adsorption efficiency. Under visible light, PCN-222 generated reactive oxygen species and effectively degraded chlorophenols. The ceramic foam enabled easy separation and reuse; the film retained structural integrity and activity over multiple regeneration cycles. The dual sorption–photocatalysis approach offers a sustainable, effective alternative for DBP removal and highlights PCN-222's strong visible-light activity and structural advantages.

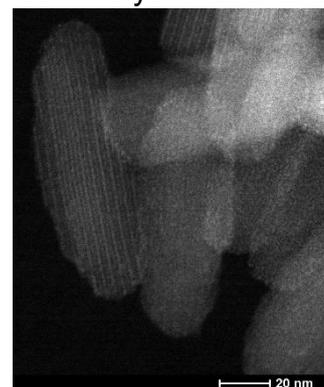


Figure 2. TEM image of PCN

Acknowledgements

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References:

- [1] A. Betard, R.A. Fischer, Metal - Organic Framework Thin Films : From Fundamentals to Applications, *Chem. Rev.*, **2012**, 112, 1055–1083
- [2] X. Zhang, Z. Liu, B. Shao, Q. Liang, T. Wu, Y. Pan, Porphyrin-based Metal-Organic Framework Photocatalysts: Structure, Mechanism and Applications, *Small Methods*, **2025**, 2402096, 1–25

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P-21

Design, Synthesis and Properties of Original Porous Polymer@MOF Gel Hybrids

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The majority of MOFs are obtained in form of microcrystalline powders. These may face inherent issues, including poor handling characteristics, mass transfer limitations, and mechanical instability [1]. In answer to that, in the past few years we can see a growing interest in different physical morphologies of this class of materials. One of them is **gel-state metal-organic frameworks**. The ability of metal-organic frameworks to gelate under specific synthetic conditions creates new possibilities for designing and shaping hierarchically porous MOF monoliths. This makes them directly applicable for catalytic and adsorptive purposes [2].

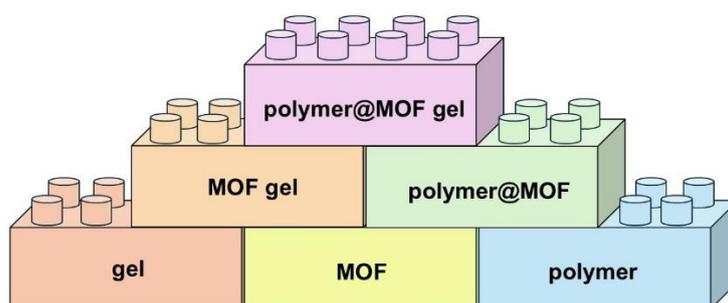


Figure 1. Schematic representation of polymer@MOF gel origin.

The aim of presented work was to design, synthesize and characterize new series of multifunctional **polymer@MOF hybrid gel materials** with various monomers. The original post-synthetic modification method - *Free Radical Polymerization in Metal-Organic Framework (FRaP-in-MOF)* was adapted to gel MOFs to perform series of polymerization reactions [3]. I obtained and characterized **polymer@NU-901 gel hybrid materials** that exhibit stable porosity. Depending on the polymer used, the obtained materials showed different properties and sorption, opening new possibilities in the use of MOF materials.

References:

- [1] B. Bueken *et al.*, *Chem. Sci.*, **2017**, 8, 3939.
[2] J. Hou *et al.*, *Chem. Sci.*, **2020**, 11, 310.

Flexible MOFs for *n*-Butane Storage

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UAM-1O and UAM-1S are isostructural flexible zinc-based MOFs that differ by a single atom (O or S) in the dicarboxylate linker, yet exhibit distinct structural responses: a gating transition in UAM-1O and a continuous transformation in UAM-1S.[1-2] These materials address key limitations of conventional high-pressure gas storage by enabling adsorption under near-ambient conditions. Both frameworks show quite high *n*-butane uptake, reaching 80 cm³/g for UAM-1O and 65 cm³/g for UAM-1S. Notably, a substantial fraction of the adsorbed gas remains trapped after desorption. Adsorption-induced phase transitions were monitored using in situ PXRD and Raman spectroscopy. Long-term gas retention was further confirmed by ex situ spectroscopic and diffraction analyses.[3]

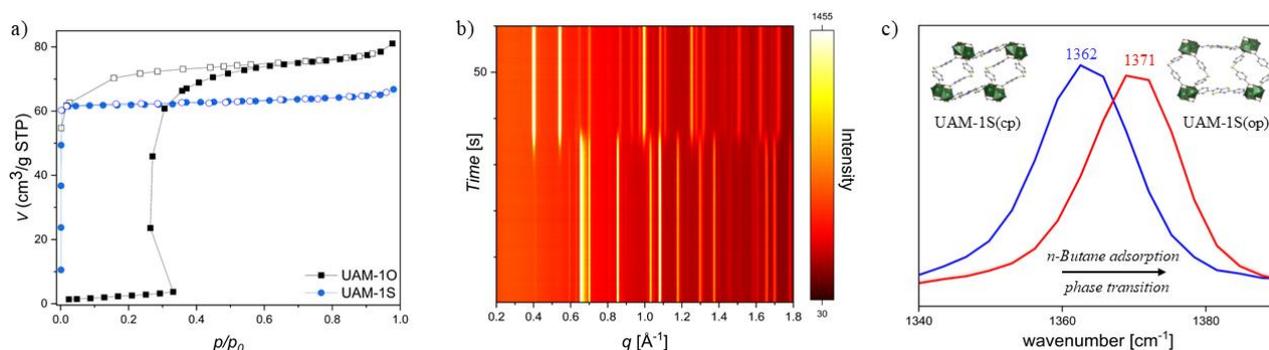


Figure 1 a) *n*-Butane adsorption isotherms (closed symbols adsorption; open symbols desorption; 273 K). b) Time-resolved PXRD during *n*-butane adsorption and c) corresponding in situ Raman spectra during *n*-butane adsorption.

References:

- [1] K. Roztocki, et al. *J. Mater. Chem. A* **2023**, *11*, 18646
 [2] S. K Sobczak et al. *J. Am. Chem. Soc.* **2025**, *147*, 25, 21575–21585
 [3] S. K Sobczak et al. Manuscript in preparation

Luminescent and Sorption Properties in a Cadmium(II)-Iridium(III) Coordination Polymer for Organic Solvents Sensing

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In recent years, significant effort in the field of molecular science has been devoted towards materials designed for sensing purposes. The constant need of miniaturization and the search for multifunctionality gave rise to molecular materials sensitive towards various external stimuli, with Metal-Organic Frameworks (MOFs) at the forefront of such research.[1] Molecular materials based on polycyanidometallates have also been shown to fulfill their role as high-performance multifunctional sensors, serving, e.g., as luminescent molecular thermometers, actuators, and sensors of guest molecules and solvent vapors.[2,3]

We present ferroelectric cyanido-bridged coordination chains of $\{[\text{Cd}^{\text{II}}(\text{S-mpm})_2][\text{Ir}^{\text{III}}(\text{ppy})_2(\text{CN})_2]_4\} \cdot \text{MeOH} \cdot 0.7\text{MeCN}$ (S-mpm = (S)- α -methyl-4-pyridinemethanol; ppy = carbanion of 2-phenylpyridine) (**1**). Here, the sorption of solvent molecules causes a single-crystal-to-single-crystal structural transformation, accompanied by significant changes in the charge-transfer-based luminescence. Such solvent-dependent behavior makes them suitable as sensors for ratiometric photoluminescent detection of organic solvents (**Figure 1**).

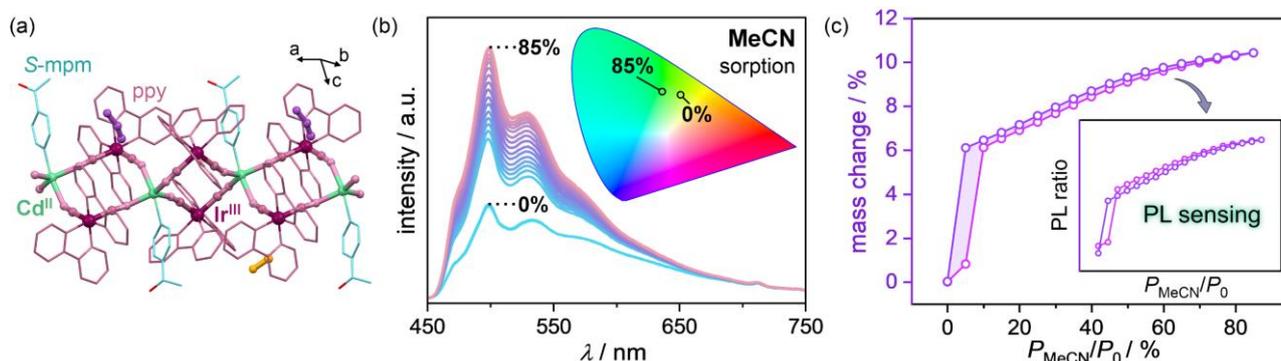


Figure 1. Representative view on the coordination chains in **1** (a); sorption-driven changes in luminescence of **1** in 0%–85% MeCN partial pressure range (b); MeCN sorption isotherm for **1** measured in 0%–85% partial pressure range, along with the sensing parameter (c).

References:

- [1] Kreno, L.; Leong, K.; Farha, O.; Allendorf, M.; Van Duyne, R.; Hupp, J.; *Chem. Rev.* **2011**, *112*, 1105.
[2] Niemiec, M.; Zakrzewski, J.J.; Reczyński, M.; Chorazy, S.; *Adv. Optical Mater.*, **2025**, *13*, 2404564.
[3] Zakrzewski, J.J.; Hoffman, A.; Wang, J.; Pander, M.; Matoga, D.; Tokoro, H.; Ohkoshi, S.; Chorazy, S.; *Angew. Chem. Int. Ed.*, **2025**, *64*, e202517109.

Switchable Coordination Network and Organic Polymer at Work

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New composite material of multi-switchable thermochromic and vapochromic properties has been produced by incorporation of a coordination chain $\{\text{NH}_4[\text{Ni}(\text{cyclam})][\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}\}_n$ (cyclam = 1,4,7,11-tetraazacyclotetradecane) [1] into poly(ϵ -caprolactone) (PCL) polymer matrix. The embedded coordination compound is characterized by reversible metal-to-metal charge-transfer, which can be triggered by changes in temperature, humidity or pressure, and at ambient conditions can exist in three phases of distinctly different colors. Unfortunately, the compound is easily damaged by contact with liquid water, and its crystals are easily breakable. The composite foils combine the switchability of the coordination chain with favorable mechanical properties of the organic polymer matrix. Most importantly, the use of hydrophobic PCL polymer renders full protection from water damage. The composite foils can be used as temperature and humidity sensors or for removable pressure writing, as shown in Figure 1.

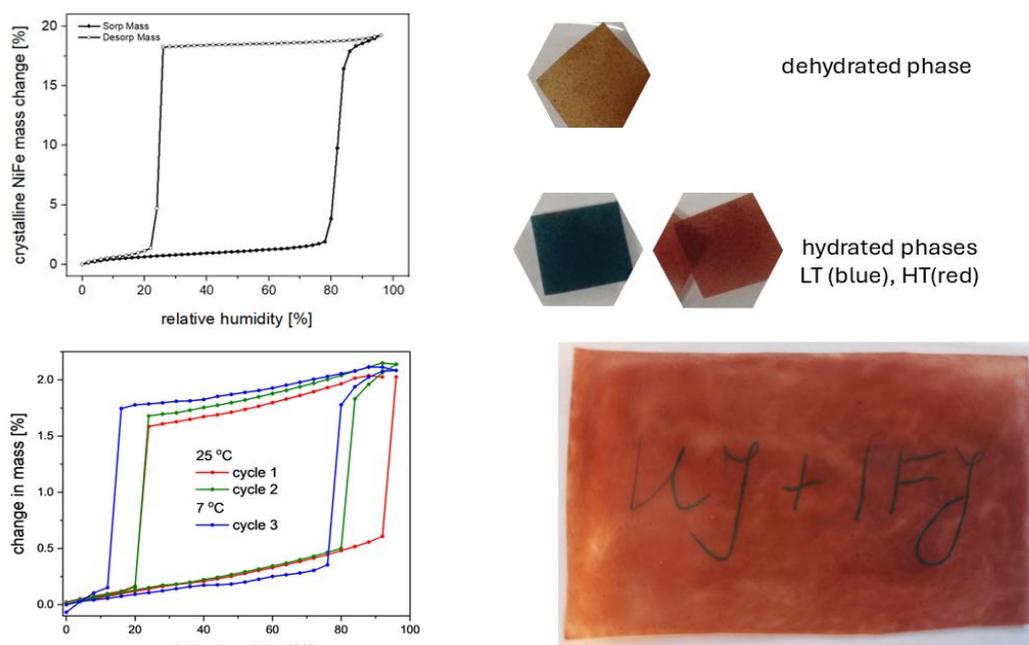


Figure 1. Sorption isotherms of crystalline $\{(\text{NH}_4)[\text{Ni}(\text{cyclam})][\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}\}_n$, and composite foils (left), composite foils in different phases (top right), and sample of pressure writing (bottom right).

References:

- [1] M. Reczyński, D. Pinkowicz, K. Nakabayashi, C. Näther, J. Stanek, M. Kozieł, J. Kalinowska-Tłuścik, B. Sieklucka, S. Ohkoshi, B. Nowicka, *Angew. Chem. Int. Ed.* 60, 2021, 2330

Porous Silsesquioxane Imine Frameworks as Highly Efficient Adsorbents for Cooperative Iodine Capture

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Radioactive iodine (^{129}I and ^{131}I) is a key fission product in the nuclear fuel cycle due to its volatility, long half-life, and accumulation in the thyroid, where it can cause severe health effects. Its release in off-gas streams during fuel reprocessing and waste handling must be controlled to meet strict regulations and limit the radiological footprint of nuclear energy. Solid sorbents with high capacity, selectivity, and recyclability offer a compact alternative to wet scrubbing, reducing secondary waste and improving long-term containment. In this context, robust, permanently porous hybrid materials such as PSIF aerogels address the need for efficient iodine management at elevated temperatures.

Porous silsesquioxane–imine frameworks (PSIFs) are hybrid aerogels for efficient capture and reversible storage of gaseous iodine. These three-dimensional networks, formed by imine condensation of octa(3-aminopropyl)silsesquioxane with multitopic aromatic aldehydes, combine micro-, meso-, and macroporosity, with surface areas up to $574\text{ m}^2/\text{g}$ and high thermal stability. Spectroscopic and sorption studies confirm intact POSS cages, quantitative imine (or enamine) formation, tunable pore architectures, and cooperative interactions between imine groups and the silsesquioxane core.

Under I_2 vapor at $75\text{ }^\circ\text{C}$, PSIF aerogels show very high iodine uptakes, up to 4.85 g/g (485 wt %) for PSIF-1a, among the highest reported for porous adsorbents, corresponding to about 20 I_2 molecules per POSS cage. Kinetic and desorption studies indicate pseudo-first- or pseudo-second-order sorption and two main binding environments with activation energies of 77.0 and 89.0 kJ/mol , exceeding the enthalpy of I_2 sublimation and evidencing strong host–guest interactions. PSIF-1a can be regenerated thermally or by solvent and reused for at least four cycles with $>90\%$ capacity retention, highlighting its promise for nuclear off-gas iodine management.[1]

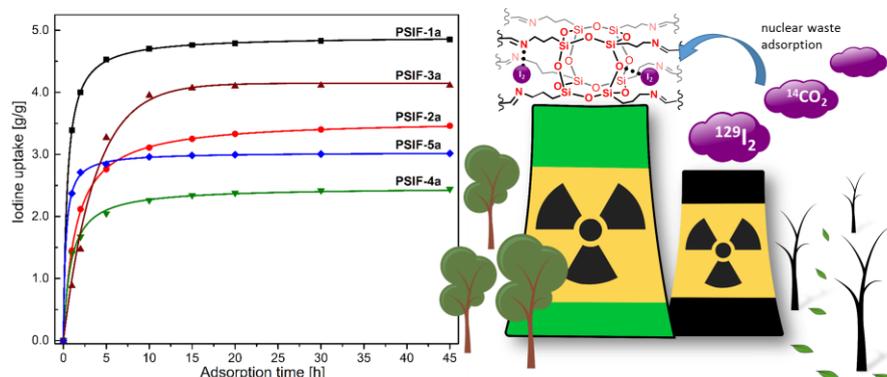


Figure 1. Gravimetric I_2 uptake of PSIFs as a function of time at $75\text{ }^\circ\text{C}$.

References:

[1] Janeta, M.; Bury, W.; Szafert, S. *ACS Appl. Mater. Interfaces* **2018**, *10* (23), 19964–19973.

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The year 2025 brought two significant milestones for the Wrocław and Polish chemical community.

First of all, it marked the 30th anniversary of the establishment of the Faculty of Chemistry at the University of Wrocław in 1995, which emerged from the former Faculty of Mathematics, Physics, and Chemistry. However, the story of our school of chemistry begins in 1969, when the Institute of Chemistry was established at the University of Wrocław. Nowadays, our faculty provides the framework for chemistry research and student teaching in different specialties.

Secondly, the year 2025 brought much inspiration and satisfaction to the MOF community, culminating in the 2025 Nobel Prize in Chemistry awarded to Robson, Yaghi, and Kitagawa.

We believe that the MOFebruary symposium idea, initiated by the Polish MOF community, will continue and expand in the future.

With best wishes,
Wojciech Bury
Marzena Pander
Min Ying Tsang



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