Institute for Functional Materials and Catalysis
Institut für Funktionelle Materialien und Katalyse

Mini-Symposium

May 28, 2 – 5 pm
Kleiner Hörsaal 3 (HS3), Boltzmanngasse 1, HP

Host: Assoz. Prof. Jia Min Chin, PhD

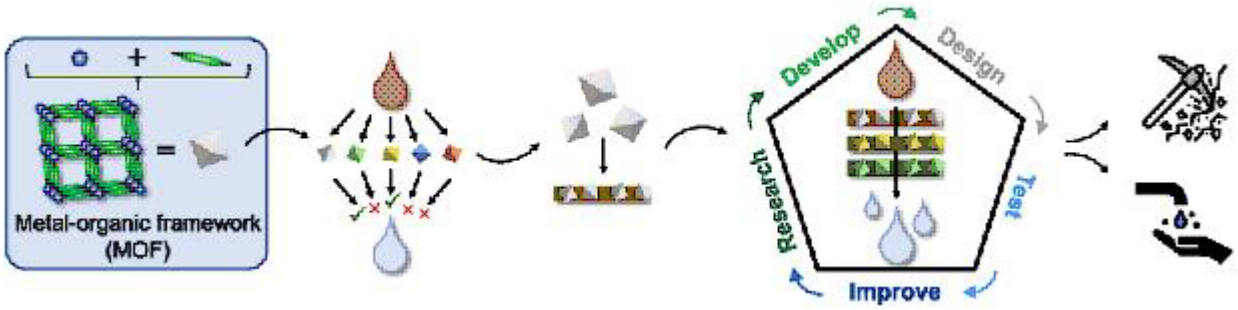
1. **Dr. Bettina Baumgartner**, Assistant Professor, Van 't Hoff Institute for Molecular Sciences, University of Amsterdam:
   Bringing Molecules Together: Reaction Monitoring in Nanometer-Sized Pores

Unravelling reactions in the confinement of porous materials like zeolites and metal-organic frameworks (MOFs) with pore sizes of a few nanometer and their response to changing conditions is challenging. Infrared spectroscopy is an indispensable tool for gaining both quantitative and qualitative insights into the guest molecules within the pores as well as the structural integrity of the host materials.
This presentation, will showcase two reactions in two microporous materials: The first example will explore the consequences of CO_2 and H_2O adsorption into photoactive MOFs, focusing on the sorption sites of the guest molecules and the structural and photophysical changes in the framework, and their impact on the photoreduction of CO_2. For the second example will discuss the implications of framework flexibility in zeolites – a material traditionally considered very ridged– on the industrially relevant methanol-to-olefine reaction.

2. **Dr. Romy Lena Ettlinger,** Liebig Fellow, TU Munich:
   Resource Recovery and Treatment of Water using Porous Composite Materials

In an era of crisis, overpopulation and industrial-related release of hazardous waste into our waterbodies, innovative technologies are much-needed. Covering almost 71% of the surface of our 'blue planet', water is the most important resource for all living beings – nonetheless only 0.5% of it is freshwater and can be used as drinking water.[1,2] Today, the growing threat of water scarcity due to pollution is increasingly problematic. To ensure access to clean water, among other things, the United Nations has set the 17 Sustainable Development Goals,[3] and porous materials, metal-organic frameworks (MOFs) in particular, may play a crucial role in achieving these goals and revolutionize the current water treatment. Self-assembling into diverse 3D frameworks of metal ions/oxoclusters and organic linkers with unprecedented ultra-high porosity (≥ 90% is free volume) and remarkable internal surface areas (≥ 7800 m^2/g), MOFs represent an ideal material

platform for various applications.[4] Their rich reticular chemistry allows for structurally precise fine-tuning of their adsorption properties for high selectivity to specific molecules and substances – thereby simultaneously recovering resources and purifying water. To promote the transformation of these research ideas into real-world applications, our work focuses on *i)* screening different MOFs in terms of their physico-chemical properties;
ii) investigating their suitability to selectively enrich specific impurities and raw materials from different water sources; *iii)* processing MOF powders into efficient MOF composites and *iv)* researching the efficiency of these innovative filtration system. Exploiting the good chemical and mechanical stability of the materials, their re-use, re-generation, or re-cycling will ultimately multiply their value. Establishing such MOF composites for water treatment could be a solution to combat the shortage of clean water.



Scheme 1: Overview of the MOF making, characterization, processing and utilization.

[1] Bureau of Reclamation, *Water Facts - Worldwide Water Supply*.
[2] M. A. Shannon, P. W. Bohn, M. Elimelech, J. G. Georgiadis, B. J. Mariñas, A. M. Mayes, *Nature* **2008**, *452*, 301.
[3] United Nations, *The 17 goals*.
[4] R. Freund, S. Canossa, S. M. Cohen, W. Yan, H. Deng, V. Guillerm, M. Eddaoudi, D. G. Madden, D. Fairen-Jimenez, H. Lyu, L. K. Macreadie, Z. Ji, Y. Zhang, B. Wang, F. Haase, C. Wöll, O. Zaremba, J. Andreo, S. Wuttke, C. S. Diercks, *Angewandte Chemie International Edition* **2021**, *60*, 23946.

3. **Dr. Sophie R. Thomas**, Schroedinger Fellow, University of Vienna:
   Gold at the Nanoscale: A Tale of Particles, Clusters, and Carbenes

N-heterocyclic carbenes (NHCs) have emerged as powerful ligands for stabilizing gold nanoparticles (AuNPs) and nanoclusters (NCs), offering significant advantages over traditional thiol-based systems. The strong σ-donating character and resistance to oxidation of NHCs result in exceptional ligand–metal bond strength, translating to enhanced thermal and chemical stability of the resulting nanomaterials. This superior robustness opens new avenues for practical applications

where conventional thiol-stabilized particles fail. In this talk, I will explore the synthesis, structural features, and functional properties of NHC-stabilized gold nanoparticles and nanoclusters. I will highlight their unique surface chemistry and tunable properties, which make them highly attractive for catalysis - particularly in selective oxidation and hydrogenation reactions - and for emerging applications in biomedicine, including imaging and catalysis in cells. By leveraging NHCs, we unlock new potential in gold nanomaterials with improved performance and stability under demanding conditions.