universität wien
Department of Functional Materials and Catalysis
Institut für Funktionelle Materialien und Katalyse

Workshop

When: **June 11, 2 – 5 pm**
Where: **Kleiner Hörsaal 3 / HS3, Halbstock, Boltzmanngasse 1**
Host: Univ.-Prof. Dr. Freddy Kleitz

1) Different Mobility Regimes in MOF Catalysis

Dr. Constanze N. Neumann
Max-Planck-Institut für Kohlenforschung

Our group aims to create ordered extended materials in which we can leverage varying degrees of active site mobility for catalytic applications. We make use of the lack of mobility in solid materials to enable catalytic reactions that are not possible in solution,[1-4] but we also design mobile heterogeneous ligand sets to heterogenize transformations that work well in solution.[5]

Open-shell reaction intermediates are crucial to a wealth of enabling transformations in modern synthetic chemistry, but radical generation requires large amounts of energy, usually in the form of light (63 kcal·mol–1 for blue light photons). MOF-heterogenization makes it possible to access a tri-component transition state for radical transfer, the assembly of which would not be possible in solution.[1-4] Instead of relying on free silyl radicals (activation energy for formation > 35 kcal·mol–1), the MOF makes it possible to transfer silyl radicals to ethylene in a concerted fashion (ΔG‡exp = 20 kcal·mol–1). The interaction between MOF-based Rh(II) centers and a silane leads to the formation of a novel 3-center-3-electron σ-adduct, which we characterized spectroscopically.

The attachment of high-performance molecular catalysts to a well-defined support is thus a desirable strategic approach, which in practice has generally been confounded by leaching, decreased activity and/or altered selectivity, and multiple additional synthetic steps being required for catalyst preparation. To replicate the performance of a molecular catalyst we reasoned that the heterogeneous active sites need to be i) easily accessible, ii) structurally uniform and iii) capable of sufficient mobility to accommodate all transition states and

intermediates. We developed a one-step click heterogenization in which sulfonated phosphine ligands are charge-tethered to the insides of the spacious supercages of MIL-101.[5] The non-directional nature of the ionic tethering enables substantial phosphine mobility (which was confirmed via 31P NMR spectroscopy), while the strength of the ionic interaction prevents the catalyst from leaving the pore spaces (no phosphine leaching in MeOH containing 50 equiv LiCl at 80 °C).

References

[1] Z. Qiu, P. Cleto Bruzzese, Z. Wang, H. Deng, M. Leutzsch, C. Farès, S. Chabbra, F. Neese, A. Schnegg, C. N. Neumann J. Am. Chem. Soc., 147, 12024–12039 (2025).
[2] M. Bengsch, C. N. Neumann ChemCatChem, e202402102 (2025).
[3] N. Gupta, H. Deng, H. Ding, Z. Qiu, C. N. Neumann Synthesis, 57, 2320-2330 (2025).
[4] Z. Qiu, H. Deng, C. N. Neumann Angew. Chem. Int. Ed., e202401375 (2024).
[5] J. Chen, C. Farès, A. Abbas, C. N. Neumann J. Am. Chem. Soc., 147, 48, 44087–44100 (2025).

Short Bio

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Connie was born in Germany, grew up in Austria, and received her chemistry training in the UK and the US. While completing her Masters at the University of Oxford, she worked on the synthesis of Inthomycin A under the supervision of Timothy Donohoe. For her PhD, she joined the group of Tobias Ritter at Harvard, where she studied concerted nucleophilic aromatic substitution reactions and the development of ^{18}F-labeled PET tracers.

Connie then joined the lab of Mircea Dincă at MIT where she developed MOF- and alloy nanoparticle-based catalysts for alcohol upgrading. In 2020, she started her independent career

as a Lise-Meitner group leader at the Max-Planck-Institut für Kohlenforschung. Her lab is interested in the precision synthesis of heterogeneous catalysts, with a focus on metal-organic frameworks and supported transition metal phosphide catalysts. The focus of her group's work lies on the optimization of the extended environment of active sites as well as the arrangement and mobility of active sites in heterogeneous catalysts.

2) Circular CO_2 Chemistry: From Pollutants to Fuels

Assist. Prof. Dr. Dogukan H. Apaydin
Institute of Materials Chemistry, Technische Universität Wien

Carbon dioxide sits at the nexus of pollution, energy storage, and chemical feedstocks, and can link environmental remediation with the production of valuable molecules in a circular way. In this lecture, a simple reaction scheme—from organic pollutants to CO_2 and H_2, to syngas or formic acid, and back again—is used as a backbone to explore a concept of circular CO_2 chemistry. The oxidative degradation of organic contaminants to CO_2 and H_2 by photoelectrocatalysis is first introduced, followed by the basic electrochemistry underlying CO_2 reduction and the conversion of CO_2 to CO/H_2 (syngas) or to formic acid using electrocatalytic approaches. Subsequently, the photoelectrocatalytic reforming of formic acid to CO_2 and H_2 is discussed, illustrating how a local carbon loop can be closed that connects waste treatment, energy carriers, and chemical feedstocks. Throughout the lecture, fundamental concepts in electrochemistry and photoelectrochemistry, the relevant materials and interfaces, and the opportunities and limitations of such circular CO_2 conversion schemes for future sustainable chemistry are highlighted.

Short Bio

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Dogukan H. Apaydın is an assistant professor and area leader at the Institute of Materials Chemistry at TU Wien. His research focuses on electrochemical and photoelectrochemical conversion processes, with a particular emphasis on CO_2 reduction, solar-driven fuel production,

and environmentally relevant oxidation reactions. He and his group work at the interface of semiconductor materials, electrocatalysis, and interfacial chemistry, developing hybrid electrodes and architectures for sustainable energy and circular carbon concepts.