

# Metal-Organic Frameworks (MOFs) as Next-Generation Photocatalysts

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## **Abstract**

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

In this talk, I will present a promising strategy to overcome this challenge. It involves the synthesis of mixed-ligand MOFs, followed by selective ligand removal (SELIRE) upon thermal stimulus to design microporous-mesoporous MOFs<sup>[1]</sup>. As an example, we synthesized photoactive MOFs of the MIL-125-Ti family with two distinct hierarchical pore architectures resembling either large cavities or branching fractures, both of which significantly improved the photocatalytic hydrogen evolution (HER) rates of the MOFs by up to 500%. In another study, we showed that these pores also greatly enhanced the potential of these MOFs to adsorb large molecules, such as glyphosate, from waste water<sup>[3]</sup>. The enhancements induced by the SELIRE process originate from 1) the formation of new under-coordinated adsorption sites and 2) a better access to catalytic sites by facilitating reactant diffusion through the pores.

I will also discuss reaction mechanisms for various MOFs (e.g. MIL-125<sup>[2]</sup>) towards photocatalytic HER and OER for different light irradiation, sacrificial agents and process conditions. The results show that methanol follows a direct charge transfer pathway, while TEOA prefers oxidation via radicals. The presence of amino-groups in the organic linker enables light absorption in the visible range, however it is detrimental to the catalytic conversion. In the last part, I will explore the benefits of photoactive MOFs with 2D-arranged Ti-SBUs (i.e. COK-47 as an example) on facilitating charge separation, transport and extraction to adsorbed reactants<sup>[4]</sup>.

## **References:**

- [1] Naghdi et al., **Nat. Commun.** 2022, 13, 282.
- [2] Naghdi et al., **Adv. Funct. Mater.** 2023, 2213862.
- [3] Wang et al., **Appl. Catal. B: Environ.** 2021, 283, 119626.
- [4] Ayala et al., **Adv. Ener. Mater.**, 2023, 2370133

### ***Biography***

Prof. Dr. Dominik Eder received his Ph.D. in Physical Chemistry in 2003 from the University of Innsbruck, Austria. After prolonged research stays at the University of Cambridge, UK, and the University of Münster, Germany, he became Chair Professor for Materials Chemistry in the Institute of Materials Chemistry (IMC) at TU Wien in 2015. He was awarded an Erwin Schrödinger Fellowship (2005), an APART Advanced Research fellowship from the Austrian Academy of Science (2008), was elected Fellow of the Royal Society of Chemistry (FRSC) and was recently awarded the Changjiang Chair Professor Scholarship (2023).