Metal-Organic Frameworks as Functional Catalyst Platform

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Molecular framework materials such as metal-organic frameworks (MOFs) allow to immobilize molecular catalysts into ordered extended materials and make their active sites accessible for chemical transformations via intrinsic porosity. Depending on the size of the pores and the substrate the porous host system itself can play an active role in the selectivity and activity of the catalytic system via confinement effects. From a holistic point of view, the catalytic activity will also depend on the ability of the substrates to enter and leave the pore space. Confinement effects in nanoporous systems can alter the product selectivity and allow for cooperative processes, e.g. when an active organic site is located in close proximity to the inorganic node. However, confinement can also impede the catalytic activity by active site inhibition or hindered substrate diffusion. In my presentation I want to show how molecular transport properties can be impacted by incorporation of active sites into nanoporous framework materials by a series of functionalized metal-organic frameworks. I will demonstrate how reagents such as acidic modulators that are used in the synthesis of Zr-based MOFs can impact the catalytic process beyond defect sites. I will furthermore detail the establishment of multivariate MOFs as an interesting catalysis platform that allows to optimize pore-space, activity and transport properties by mixing different components. I will finally provide an outlook on the ability to utilize and probe local dynamics in these framework materials with low-frequency Raman spectroscopy. This aspect of functional dynamics may allow to overcome transport limitations and result in a new approach towards catalysis in dynamic confinement. [1,2]

[1] S. Krause, J.V. Milić, Commun Chem 2023, 6, 151, [2] S. Krause, N. Hosono, S. Kitagawa, Angew. Chem. Int. Ed. 2020, 59, 15325-15341