Translating Insights from Gas Phase Catalysts into Solid State Materials for Sustainable Future

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Development of new catalytic materials plays an important role in the transition to sustainable energy. Systems with metal centers ranging from single atoms to well-defined size-selected clusters show promising catalytic performance. Theoretical and experimental gas phase studies provide information on their structural and electronic properties while allowing investigation of the influence of the size and composition on reactivity.

Transferring these insights into solid state materials facilitates the design of new catalysts with tailored activity and selectivity. In this context, metal-organic frameworks (MOFs) are a promising class of materials with three distinct catalytic sites available for reaction. Specifically, the gas phase system of {CuH} coordinated with bipyridine ligand serves as a model for incorporating catalytic center within the MOF linker. The goal is to propose a catalyst for hydrogen production from formic acid [1]. Similarly, ligated ruthenium clusters provide a basis for the design of zeolite-based catalysts using the "*ship-in-a-bottle"* principle for CO conversion into methane [2]. Another material design approach includes deposition of size-selected copper clusters on metal-oxide supports with the goal of CO_2 mitigation and production of valuable chemicals [3]. By combining DFT theoretical modeling with experiments, the goal is to predict and develop new catalysts with improved properties while gaining a deeper understanding of their structure-function relationships.

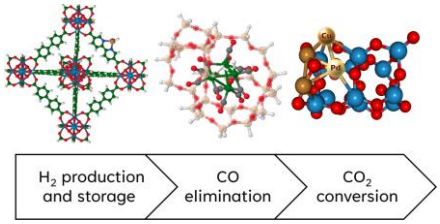

Figure 1. Overview of the designed catalysts.

References:

[1] R. A. J. O'Hair, A. Mravak, M. Krstić, V. Bonačić-Koutecký, *ChemCatChem* **11** (2019) 2443-2448.

[2] A. Mravak, M. Krstić, S. M. Lang, T. M. Bernhardt, V. Bonačić-Koutecký, *ChemCatChem* **12** (2020) 3857-3862.

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