CatLab Lecture Series hosted by FHI and HZB

Friday, January 19th 2024, 10:30-12:00

BESSY II, Seminar Room at the Entrance, Albert-Einstein-Straße 15, Berlin Adlershof

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Catalysis at Interfaces: Atom-Efficient Metal Catalysts based on Single Atoms, Clusters and Nanoparticles

Efficient utilization of transition metals is one of the most important requirements for heterogenous catalysts. Design rules for nanoparticle catalysts are well established and often imply that sub-optimal metal dispersion is desired for high activity. Metal-support interactions can have a strong impact on the catalytic performance of metal nanoparticles. Specific sites at the metal-support interface can give rise to unusual high reactivity. In this contribution, I will review structure sensitivity for monometallic and bimetallic catalysts and demonstrate the possibility to tune metal-support interfaces towards high CO_2 hydrogenation and CO oxidation activity. The approach entails experimental work involving synthesis of uniform active phases, operando characterization, transient kinetic analysis augmented with density functional theory calculations of mechanism and microkinetics simulations.

The first example deals with approaches to break structure sensitivity. For this, we use cobalt dispersed on ceria-zirconia support materials. We first establish how the size of the support crystallites can stabilize cobalt nanoparticles. Then, we investigate how incomplete reduction of cobalt oxide can lead to cobalt-cobalt oxide interfaces with a much higher CO_2 methanation activity than conventional cobalt nanoparticle catalysts. This work shows the promise of very small metal clusters stabilized on an oxide for achieving high CO_2 methanation activity.

Second, I will show how tuning the size of CeO_2 crystallites can strongly affect the stability and reactivity of single metal atoms. The improved reducibility displayed by CeO_2 particles of a few nanometer as contrasted to bulk CeO_2 with a size of tens of nanometers translates in retention of single Pd atoms with improved kinetics for low-temperature CO oxidation.

Key references:

- Parastaev, E.J.M. Hensen et al. *Nat. Catal.* 2020, **3**, 526-533
- V. Muravev, E.J.M. Hensen et al. *Nat. Catal.* 2021, **4**, 469-478
- V. Muravev, E.J.M. Hensen et al. *Angew. Chem. Int. Ed.* 2022, e202200434
- Parastaev, E.J.M. Hensen et al. *Nat. Catal.* 2022, **5**, 1051-1060
- V. Muravev, E.J.M. Hensen et al. *Science* 2023, **380**, 1174-1178