

Heterogenized catalysts – at the interface of molecular and solid-state chemistry

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Extensive research has been directed towards heterogenizing molecular catalysts, effectively erasing the distinctions between homogeneous and heterogeneous catalysis.[1] One approach in this context involves the anchoring of molecular metal complexes onto solid supports to obtain highly dispersed metal catalysts. We have therefore utilized gold phosphine complexes as precursors for the *in-situ* generation of CO oxidation catalysts. We found that the type and number of ligands significantly affect the catalyst activity and stability. By employing a variety of *ex-situ* and *operando* characterization techniques, we witnessed the formation of P-containing binding pockets for the stabilization of small Au particle (Fig. 1).[2]

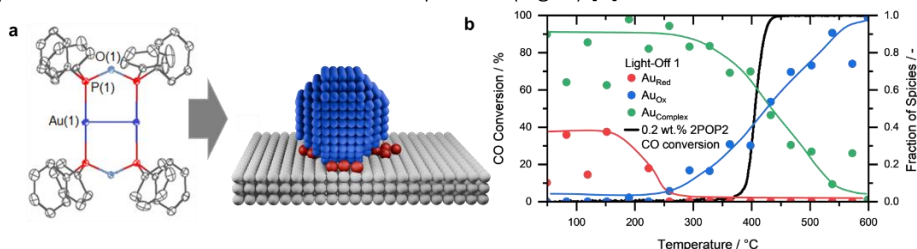


Figure 1: a) Schematic representation of the formation of Au particles stabilized by a P-containing binding pocket starting from $[\text{Au}_2(\mu_2\text{-Ph}_2\text{POPPh}_2)_2]\text{OTf}$ [3] and b) the respective *operando* X-ray absorption spectroscopy measurement of the different species of gold present during the first catalytic cycle (1000 ppm CO, 10 % O₂, balanced in N₂, 60 000 L gAu⁻¹ h⁻¹).

We have also extended our work in the field of heterogenized catalysts towards the combination of a d-metal with a p-block element to afford a main group stabilized metal phase, such as a metal phosphide or sulphide. Through the incorporation of a p-block element into the metal matrix, highly defined and uniformly distributed active sites can be formed, which are highly active catalysts in C–C bond formation reactions.[4]

[1] S. Hanf, Nachr. Chem., 2021, **69**, 75. [2] F. Rang, T. Delrieux, F. Flecken, F. Maurer, J. Grunwaldt, S. Hanf, ChemRxiv 2024, DOI: 10.26434/chemrxiv-2024-0vzrw. [3] F. Flecken, T. Grell, S. Hanf, Dalton Trans, 2022, **51**, 8975. [4] A. Neyyathala, E. Fako, S. De, D. Gashnikova, F. Maurer, J.-D. Grunwaldt, S. A. Schunk, S. Hanf, ChemRxiv 2024, DOI: 10.26434/chemrxiv-2024-8cxlz-v2, and under review.