Session of Focus Materialchemie – Wednesday, **26.06.2024** 16:00 – @ Seminarraum Lehar 01 (TU-Wien, Getreidemarkt 9, BC, OG. 01, room A46) – join us on ZOOM (ID: 983 0066 2349)

Gold Nanoclusters as Homogeneous and Heterogeneous Catalysts for Selective Hydrogenation

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Selective hydrogenation is an important process in the oil industry used, for example, to reduce alkyne impurities to alkenes that can be used for further processing. The catalysts used must have exceptional activity to selectively hydrogenate the impurities to the desired product. While significant improvements have been made in the design of these catalysts, the common Pd-based catalysts still lack selectivity and composition control.

Ligand-protected gold nanoclusters offer remarkable potential for optimizing their properties through metal doping and the composition of their ligand shells. In our previous work exploring the application of supported metal nanoclusters as nanocatalysts, it was shown that not only the ligands, but also the support and pretreatment of the catalysts play a crucial role in their performance. In this study, we examined the interplay between clusters' ligands and supports, and its impact on catalytic activity in the selective hydrogenation of alkynes. We used phosphine-protected Au11 and thiolate-protected Au25 nanoclusters supported on MgO, Al2O3 and hydrotalcite (MgAlO), chosen for their different properties, such as acid-base, porosity and structure, directly affecting their interaction with the nanoclusters.

We studied their catalytic activity in the hydrogenation of phenylacetylene in liquid phase, observing clear correlations between the ligands, support and pretreatment applied and reaching high conversion and selectivity. In order to understand the different catalytic behaviour and the influence of each parameter, X-Ray Absorption Fine Structure (XAFS) spectroscopic studies on the Au L3-edge and S -K edge were performed. A distinct interaction of the ligand shell with the support was observed, which varies depending on the oxide and affects the cluster structure and subsequently their catalytic performance. These results indicate the importance of careful selection of each variable in the design of heterogeneous catalysts based on monolayer protected metal nanoclusters.