FOXSI
Functional Oxide Surfaces and Interfaces

EINLADUNG

zum Vortrag
von

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Catalytic activity of metal clusters and substitutional ions at reducible oxide surfaces

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Abstract:

The catalytic activity of metal nanoparticles supported by highly reducible oxides in controlled by several factors, such as the size of the metal cluster, the ability of the support to supply oxygen during the reaction, and charge transfers across the metal/oxide interface
These factors will be described by focusing on the paradigmatic case of CO oxidation catalyzed by Au nanoclusters supported by cerium oxide (CeO2) surfaces and by substitutional Au, Pd, Cu and Pt ions dispersed into the ceria lattice. I will discuss successes and failures of the DFT and DFT+U approaches in capturing the surface chemistry of these systems. In particular, I will identify the interplay between the reaction mechanisms and the cluster size, charge, morphology as well as the reduction of the surface oxide. These results reveal the important role played by the structural flexibility and cohesion of the supported clusters for preserving their catalytic activity.

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