

Modelling for understanding the complexities originating from the interaction between oxide catalysts and the support

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Inhalt As the material and pressure gaps between real catalysis and traditional surface science are narrowing, experiments and modelling that straddle both sides of the gap appear essential for the understanding of heterogeneous catalysis and the rational design of catalysts. Producing well defined model systems that reproduce practical supported oxide catalysts, such as vanadia, is challenging because of the complexity of the real systems (e.g., possible multiple oxidation states, variable local coordination, etc.). Moreover, the catalytic performance in oxidation catalysis that is related to the surface reducibility (Mars-van Krevelen), depends on the specific support. Yet, the nature of the active surface and the role of the supporting oxide are far from being understood. Experimentally, vanadia catalysts have been emulated by the evaporation of vanadium in the presence of gas phase oxygen on well defined supports (e.g., alumina) and the structure characterized by STM, IR and XPS.

To this end, I discuss how by combining quantum mechanical calculations with statistical thermodynamics one is able to establish structure-reducibility/reactivity relationships for the stable model catalysts under relevant conditions, and provide a contribution to unveil support effects. The simulation of core-level shifts, vibrational spectra and scanning tunneling spectroscopy images allow the interpretation of experimental data, and the validation of the 'in-situ' theoretical modelling.

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