Metal-sulfides and oxides on Au(111): From catalysis on nanoparticles to electronic structure of epitaxial 2D materials

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Abstract: We pursue the goal of providing fundamental atomistic understanding of metal oxide and metal sulfide nanostructures supported on metal substrates. Such systems are important as model systems for heterogeneous catalysts and allow better understanding of epitaxial 2D materials, such as MoS_2 in contact with a metal. By focusing on what happens on the atomic-level we can for example evaluate the role of structure and surface defects on catalytic processes on nanoparticles. Scanning Probe Microscopies (SPMs) are particularly strong techniques in this regard, since they allow us to resolve surfaces and nanoparticles atomically and sometimes directly inspect the intermediate stages of a chemical reaction. We have used the scanning tunneling microscope (STM) to investigate models of several important catalyst systems, where nanostructures of the active phase could be synthesized on a Au(111) surface. The so-called hydrodesulfurization catalyst is a crucial catalyst used in oil refineries worldwide for upgrading crude oil and removing sulfur impurities to prevent pollution (acid rain). The catalyst mainly consists of so-called single-layer MoS_2 nanoparticles, and we can reveal in atom-resolved STM images how S-containing molecules representative of the oil interact and react on the surface of the MoS_2 nanoparticles [1]. In extension of these studies we have also synthesized single-layer MoS_2 flakes covering the the Au(111), which can be used to investigate the interesting geometrical and electronic properties of two-dimensional MoS_2 using STM and Angle-resolved Photoemission Spectroscopy (ARPES). In will also address studies of novel metal-oxide nanostructures [2] from earth-abundant transition metals (Co, Ni), which are promising replacements of typical expensive noble metals for catalytic water splitting for hydrogen production. In particular, I will show how we can follow the first steps of this reaction in STM movies, by in-situ monitoring water dissociation and subsequent hydrogen diffusion.