IAP Seminar

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Tuesday, 5th February 2019, 9:30 s.t.
TU Wien, Institut für Angewandte Physik, E134
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Tuning material properties: role of nanostructuring and metal/oxide interfaces on oxide reducibility

Oxide reducibility is an important property in catalysis by metal-oxides. Usually, oxides can be classified based on their bulk reducibility, i.e. the tendency to loose oxygen, generating excess electrons in the material. In this respect, SiO_2, MgO, and ZrO_2 are considered non-reducible oxides, while TiO_2, CeO_2, and Fe_2O_3 are typical reducible oxides. However, the reducibility of an oxide can be substantially modified, either by generating nanostructures (nanoparticles, nanowires, or nanofilms) or by creating an interface between the oxide and a metal. We will use ZrO_2 as a prototype of non-reducible oxides, and we will show how the properties, and in particular the reducibility, of the material can be tuned by nanostructuring or by depositing metal particles on ZrO_2 (classical heterogeneous catalysts) or, as an alternative, by growing ZrO_2 films on metal surfaces (inverse catalysts). We designed models of these systems, and by means of first principle calculations we analysed a key descriptor of the oxide reducibility, the formation energy of an oxygen vacancy. We also considered other reduction processes, including exposure to hydrogen. The ZrO_2 reducibility is dramatically reduced when the oxide is prepared in form of nanoparticles, or is interfaced with a metal. The consequences are not only on the chemical activity of the oxide surface, but also on other properties, such as the magnetic behaviour: while reduced bulk zirconia is non-magnetic, reduced zirconia nanoparticles are ferromagnetic.

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion).

Friedrich Aumayr
(LVA-Leiter)

Ulrike Diebold
(Seminar Chair)