DEPARTMENT OF CHEMISTRY AND PHYSICS OF MATERIALS

ANNOUNCEMENT

PARIS LODRON UNIVERSITÄT SALZBURG

Vortragsankündigung

Mittwoch, 10. Juni 2026, 11.15 Uhr im SR I

Prof. Dr. Bernd MEYER

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"Cooperative effects in molecular adsorption on oxide surfaces probed by density functional theory calculations"

The diverse chemical behavior of oxide surfaces, from rather inert to being very reactive, is usually attributed to the specific chemistry of their undercoordinated surface sites. However, the modification of the chemical properties of adsorption sites by the presence of adsorbates is often overlooked. For a test oxide, In_2O_3(111), I will show how the modification of the surface reactivity by induced adsorbates together with the competition of molecule-molecule with molecule-substrate interactions can lead to strong cooperative effects, i.e., the formation of configurations distinctly different from what would be expected for the adsorption of individual molecules.

Indium oxide is of high interest for transparent electrodes in electronics and has been identified as a promising catalyst with high selectivity for methanol synthesis from syngas. It is also an ideal model platform for surface science studies as the large unit cell of its most stable (111) surface offers a range of structurally similar yet different undercoordinated O and In adsorption sites. In my talk I will discuss how small variations in the local atomic environments, either already present at the pristine surface or induced by adsorbates, modify the proton affinity of the surface sites and how the emerging cooperative effects determine the adsorbate structures of water, methanol, and carbon dioxide, important intermediates in the methanol synthesis process. All results will be compared to STM and AFM data from the Diebold group (TU Wien).

[1] M. Wagner, *et int*, B. Meyer, U. Diebold, ACS Nano **11** (2017) 11531; ACS Nano **16** (2022) 21163
[2] M. Wagner, B. Meyer M. Setvin, M. Schmid, U. Diebold, Nature **592** (2021) 722