UNIVERSITÄT OSNABRÜCK

Seminar NanoScience
Vortragsankündigung

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„Defects in transition and rare-earth metal oxides investigated with the STM“

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10:00 Uhr
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The properties of oxide materials are largely governed by the presence of defects in their surface, whereby oxygen vacancies play naturally the most important role. On highly reducible oxides, such vacancies are easily formed and annihilated, being an effective means to balance the oxygen supply during a chemical reaction. Also on more inert oxides, defects influence the chemical properties, as they control the adsorption and nucleation behaviour at the surface. A detailed characterization of defects is therefore a basic requirement for elucidating the physical and chemical properties of an oxide material.

In this talk, results of a combined scanning tunnelling microscopy and density functional theory approach are presented, which provide atomic-scale insights into the nature of oxide defects. V_2O_3(0001) and CeO_2(111) films are used as model systems for highly reducible transition and rare-earth metal oxides. For both materials, the surface defects are characterized from a structural and electronic point of view. In the case of CeO_2, we present a technique to identify the localization of excess electrons that are left behind upon oxygen removal from the surface. We unambiguously demonstrate that those electrons do not necessarily occupy Ce sites that are in next-neighbour positions to the vacancy. On the vanadyl-terminated V_2O_3 (0001) surface, we explore the adsorption of Au adatoms and try to elucidate the role of surface defects in the observed binding behaviour. In contrast to common perception, Au atoms show only a small affinity to bind to vanadyl (V=O) vacancies in the vanadia surface and preferentially attach to regular V=O bridge sites. Only for O-vacancies where an active vanadium ion remains on the surface, a strong binding of Au atoms is revealed. Both studies demonstrate how theoretical and experimental methods can be used to unravel the complex and sometimes unexpected properties of oxide defects.

gez. M. Reichling