chemisch physikalische gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz,
J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag
von

Univ.Prof. Dipl.-Ing. Dr. Ulrike Diebold
Institut für Angewandte Physik, Technische Universität Wien

Organic Molecules at Oxide Surfaces

am
Dienstag, 22. März 2011, um 17.30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals

Abstract:
We have studied the adsorption of a variety of aromatic organic molecules on TiO_2 rutile (110) and anatase (101) surfaces using a combination of STM, photoemission spectroscopy, and accompanying DFT calculations performed by collaborators.

We have found that the electronic structure of catechol ($C_6H_4(OH)_2$) is intimately related to its bonding configuration. In particular, a bi-dentate species induces a gap state on rutile (110), while the monodentate species does not [1]. The molecule switches back-and-forth between a bidendate and monodentate state via facile transfer of hydrogen transfer to and from the TiO_2 surface. Hydrogen also plays a key role in the diffusion of catecholates across the surface [2].

We have also investigated the adsorption of aniline ($C_6H_5NH_2$) and azobenzene ($C_6H_5N{=}NH_5C_6$) with the goal to better understand the role of TiO_2 in the catalytic synthesis of nitroaromatics. We found that both molecules form the same superstructure on rutile (110) as well as anatase (101) surfaces, suggesting that TiO_2 is instrumental in cleaving the N=N double bond of azobenzene.

A short overview of ongoing and planned experiments on other oxide surface will also be presented.

[1] S.-C. Li et al., JACS 131 (2009) 980 - 984
[2] S.-C. Li et al., Science 328 (2010) 882 - 884
[3] S.-C. Li and U. Diebold, JACS 132 (2010) 64 - 66