TECHNISCHE UNIVERSITÄT WIEN

INSTITUT FÜR ANGEWANDTE PHYSIK
Institute of Applied Physics
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IAP-SEMINAR

ANNOUNCEMENT

Date: **Tuesday, 7.6.2016**
Time: **16:00 p.m.**
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**
yellow tower „B“, 5th floor, Sem.R. DB gelb 05 B (room number DB05L03), 1040 Wien, Wiedner Hauptstraße 8-10

Lecturer: **Roland Bliem**
TU Wien, IAP

Subject: **Single metal adatoms at the magnetite Fe_3O_4(001) surface**

Abstract: Magnetite (Fe_3O_4) is a widely abundant material with fascinating physical properties, which form the basis of its various applications, for example in biomedicine, microelectronics, or catalysis. In heterogeneous catalysis, magnetite is employed as catalyst material and as support for active particles down to the size of single atoms.
The Fe_3O_4(001) surface is a particularly promising support material for single-atom catalysis, since it is known to stabilize single Au adatoms up to 700 K. The stabilizing property is closely related to the nature of the $(\sqrt{2}\times\sqrt{2})R45°$ surface reconstruction, which is based on an ordered array of subsurface Fe vacancies and interstitials. Initially the structural model and its quantitative confirmation using low-energy electron diffraction, scanning tunneling microscopy (STM) and *ab initio* thermodynamics will be presented. Using STM, x-ray photoelectron spectroscopy and density functional theory (DFT) calculations, the metal adsorption properties will be explained on the basis of this model, showing that isolated adatoms are the stable phase for a broad selection of metals at room temperature. Regarding the high-temperature behavior, two classes of materials can be distinguished: Metals that agglomerate to clusters and those which form solid solution with magnetite, incorporating into the surface lattice. In the second part, the presentation will focus on examples of reactive metal adatoms and their interaction with relevant gases such as CO or O_2, studied using STM image sequences supported by DFT. These examples illustrate the high potential of the system and the challenges encountered in single-atom catalysis.

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

U. Diebold e.h.
(Seminar-Chairperson)

H. Störi e.h.
(LVA-Leiter)