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IAP-SEMINAR

EINLADUNG

Termin: **Dienstag, 11.10.2011 um 16:00 Uhr**
Ort: **Technische Universität Wien,**
Institut für Angewandte Physik,
Seminarraum 134A, Turm B (gelbe Leitfarbe), 5. OG
1040 Wien, Wiedner Hauptstraße 8-10

Vortragender: **Thomas Manz**
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Thema: **Theoretical Study of Charge and Spin Ordering at the Reconstructed Magnetite (001) Surface Anti-Phase Domain Boundary**

Kurzfassung

Magnetite is a mixed oxidation state material that exhibits charge and spin ordering transitions. For example, bulk magnetite is a half-metal above the Verwey transition temperature of ~120K and an insulator below this temperature [1]. Published calculations show a subsurface charge-ordering transition is associated with the magnetite 001 surface reconstruction [2,3]. Recent scanning tunneling microscopy (STM) experiments show the reconstructed magnetite 001 surface can contain surface anti-phase domain boundaries [4].

In this talk, I will discuss plane-wave density functional theory calculations performed to model the surface reconstruction anti-phase domain boundary. Common generalized gradient approximations (GGA) of the electron-electron exchange-correlation energy are known to overly delocalize electric charge. A semi-empirical on-site parameter, Ueff, was used to correct this error. The rational behind chosen Ueff values for different atoms in the system will be discussed. Net atomic charges and atomic spin moments were computed using two different atomic population analysis methods: (a) Bader's atoms-in-molecules method and (b) the recently developed Density Derived Electrostatic and Chemical (DDEC) method [5-7]. The reconstruction anti-phase domain boundary was found to be caused by charge-ordering of the Fe atoms in the first subsurface octahedral layer. Specifically, we find that for the reconstructed surface without anti-phase domain boundary the Fe atoms in the first subsurface octahedral layer are arranged in rows with alternating pairs in the +2 and +3 oxidataion states; that is, the iron atoms along a subsurface octahedral row have the repeating sequence ..FeII-FeII-FeIII-FeIII... If two different surface domains grow together during synthesis, the charge ordering may change phase at the boundary leading to the observed surface reconstruction anti-phase domain boundary. DFT+U calculations clearly show this interruption of charge ordering at the phase boundary. Finally, simulated STM images will be discussed that show the accumulation of electrons on Fe atoms in the surface octahedral layer. This accumulation of charge explains certain features of the experimental STM images. DFT+U calculations also show a phase change in the displacement of surface atoms at the anti-phase domain boundary. The magnitude of surface atom displacements is smaller for computations than for experiments, but the two are in qualitative agreement.

References:
[1] Verwey, E. J. W. *Nature* **1939**, *144*, 327-328.
[2] Lodziana, Z. *Phys. Rev. Lett.* **2007**, *99*, 206402.
[3] Pentcheva, R.; Wendler, F.; Meyerheim, H. L.; Moritz, W.; Jedrecy, N.; Scheffler, M. *Phys. Rev.Lett.* **2005**, *94*, 126101.
[4] Gareth Parkinson and Ulrike Diebold, to be published.
[5] Bader, R. F. W.; Macdougall, P. J.; Lau, C. D. H. *J. Am. Chem. Soc.* **1984**, *106*, 1594-1605.
[6] Manz, T. A.; Sholl, D. S. *J. Chem. Theory Comput.* **2010**, *6*, 2455-2468.
[7] Manz, T. A.; Sholl, D. S. *J. Chem. Theory Comput.* **2011**, in press, http://pubs.acs.org/doi/abs/10.1021/ct200539n.

Alle interessierten Kolleginnen und Kollegen sind zu diesem Seminar
(45 min mit anschließender gemeinsamer Diskussion) herzlich eingeladen.

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

H. Störi e.h.
(LVA-Leiter)