

[1] de Wette, F.W. et al.: New surface mode on the (001) surfaces of RbBr and RbI, Physical Review B, **35**, 5 (1987)

O 32.5 Tue 14:00 MA 042

**Lattice Dynamics of Cu<sub>2</sub>O: Bulk and (110) Surface** — ●KLAUS PETER BOHNEN<sup>1</sup>, ROLF HEID<sup>1</sup>, ALOYSIUS SOON<sup>2</sup>, and CATHERINE STAMPFL<sup>2</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik — <sup>2</sup>School of Physics, The University of Sydney

A number of theoretical studies have been carried out in the past to investigate the stability of various surface oxides for the O/Cu system however despite the fact that catalytic processes usually proceed at elevated temperatures stability at finite temperatures has never been studied for these systems. Modern ab-initio methods however allow for the determination of the lattice dynamics and the phononic contribution to the free energy. Using density functional perturbation theory we have studied the lattice dynamics of Cu<sub>2</sub>O-bulk as well as Cu<sub>2</sub>O(110). In calculating the free energy as function of lattice constant we obtained for the bulk a negative thermal expansion up to roughly 300 K in excellent agreement with experiments. This is due to anomalous mode Grüneisen parameters for vibrational modes in the low energy regime. Due to the anomalous behavior of the mode Grüneisen parameter the bulk system is highly unstable against variations of the lattice constant by more than 2%. To investigate the stability of the O/Cu surfaces we have investigated the lattice dynamics of Cu<sub>2</sub>O(110) as a prototype. Despite a large number of low lying modes no instability has been found. These calculations allow also for the O/Cu system for the first time for a realistic estimation of the surface free energy which is important for the determination of surface thermodynamic properties.

O 32.6 Tue 14:15 MA 042

**Electronic structure and thermodynamic stability of cubic La<sub>x</sub>Sr<sub>1-x</sub>MnO<sub>3</sub> (001) surfaces: First-principles calculations by means of hybrid density-functional theory** — ●SERGEJS PISKUNOV<sup>1</sup>, ECKHARD SPOHR<sup>1</sup>, and TIMO JACOB<sup>2</sup> — <sup>1</sup>Lehrstuhl fuer Theoretische Chemie, Universitaet Duisburg-Essen, Campus Essen, S05 V06 E15, Universitaetsstr. 5, D-45141 Essen, Germany — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany

Surface properties of La<sub>x</sub>Sr<sub>1-x</sub>MnO<sub>3</sub> (LSM) are of high scientific and technological interest due to potential application of these materials in magnetoresistive devices, spintronics, and high-temperature fuel cells. Using the hybrid exchange-correlation functional within density functional theory, we calculated the electronic structure for a wide range of cubic LSM(001) surfaces at low doping  $x \sim 1/8$ . The layered antiferromagnetic structure is found to be the most energetically favorable for all LSM(001) surfaces under study. Stability of the considered LSM surfaces has been predicted by means of the atomistic thermodynamics. Our calculations show that segregation of Sr at La(Sr)-terminated surface does not lead to its stabilization and thus is thermodynamically unlikely. On the other hand, MnO<sub>2</sub>-terminated LSM(001) can be stabilized through adsorption of atomic oxygen atop of Mn sites.

O 32.7 Tue 14:30 MA 042

**Preparation of model single crystalline aluminium oxide films suitable for scanning tunnelling microscopy** — ●SERGIY BORODIN and MICHAEL ROHWERDER — Max-Planck-Institut für Eisenforschung, Düsseldorf, Deutschland

Self assembly of organic molecules on aluminium or aluminium alloys is of increasing technical importance, e.g. for adhesion promotion and corrosion protection. For the performance of the SAMs in many cases their defect structure is of importance. However, it is difficult to obtain detailed information about the nanoscopic defect structure, as it is difficult to prepare suitable atomically flat samples that can be scanned by STM.

In this work a model thin film aluminum has been prepared under UHV conditions, whose surface is suitable for a scanning tunneling microscopy investigation, e.g. of phosphonate self-assembly on aluminium. This surface is stable even upon contact at high water exposures and hence much superior to model aluminium oxide surfaces prepared on NiAl.

O 32.8 Tue 14:45 MA 042

**Work function measurements with a combined AFM/STM setup under ultrahigh vacuum conditions at 5K on thin MgO films grown on Ag(001)** — ●THOMAS KÖNIG, GEORG HERMANN SIMON, VIOLETA ŠIMIC-MILOSEVIC, MARKUS HEYDE, and HANS-JOACHIM

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For many years metal supported thin oxide films have been investigated in the research field of heterogeneous catalysis. The properties of the thin films depend strongly on both the support and the film thickness. While thick films approach the properties of bulk material thin films exhibit their own characteristics. It has been proposed by Pacchioni et al. [1] that charging can occur by depositing metal atoms on ultrathin MgO films grown on metal supports. The charging of Au atoms on top of a thin MgO film grown on Ag(001) has been confirmed by STM measurements done by Sterrer et al. [2]. The MgO film on top of the metal support leads to a compression of the metal electrons which for a free metal spill over into the vacuum. The compression results in a reduction of the surface dipole and thus to a decrease of the work function. Here we present work function measurements on different MgO film thicknesses grown on Ag(001). The measurements have been done with our combined AFM/STM setup operating under UHV conditions at 5K. The results will be discussed and compared with theoretical calculations.

[1] L. G. Giordano et al., Phys. Rev. B **73**, 045414, 2005. [2] M. Sterrer et al., Phys. Rev. Lett. **98**, 096107, 2007.

O 32.9 Tue 15:00 MA 042

**Stress of CoO(111) on Ir(100)** — ●ZHEN TIAN, DIRK SANDER, and JUERGEN KIRSCHNER — Max-Planck Institute of Microstructure Physics

An important aspect of epitaxial oxide films is that the growth of (111) oriented films with rock salt structure leads to polar surfaces, where adjacent layers are composed of either anions or cations only. Considerable repulsive Coulomb interaction within the oxide (111) layers are therefore expected [1]. We measured the stress change during the formation of CoO(111) on Ir(100) by post-oxidation of Co films [2]. Combined structural investigations by LEED and stress measurements by the crystal curvature technique are performed. The formation of the CoO(111)-c(10×2) structure by post-oxidation of 2 monolayers Co induces a compressive surface stress change of -0.5 N/m. The epitaxial Co film prior to oxidation is under a tensile stress of +16 GPa, which is induced by the lattice misfit between fcc-Co and Ir. The formation of the CoO(111) film induces a tensile stress change of +2.1 N/m, as compared to the clean Ir(100) surface. This stress change is quantitatively ascribed to the anisotropic misfit between the c(10×2) structure of CoO(111) and Ir(100) of +0.22 % and +4.2 % along Ir[110] and Ir[110], respectively. Our stress measurements indicate that charge depolarization effects [3] might be operative on the CoO(111)-c(10×2) film.

[1] C. Noguera, J. Phys.: Condens. Matter **12** (2000) R367-R410.  
[2] C. Giovanardi, L. Hammer, and K. Heinz, Phys. Rev. B **74**, 125429 (2006).  
[3] C. Tusche, H. L. Meyerheim, and J. Kirschner, Phys. Rev. Lett. **99** (2007) 026102.

O 32.10 Tue 15:15 MA 042

**Metal-insulator transition on the V<sub>2</sub>O<sub>5</sub>(001) surface: Theory and experiment** — ●MARIA VERONICA GANDUGLIA-PIROVANO<sup>1</sup>, REMY FORTRIE<sup>1</sup>, JOACHIM SAUER<sup>1</sup>, RALF-PETER BLUM<sup>2</sup>, HORST NIEHUS<sup>2</sup>, CARSTEN HUCHO<sup>3</sup>, SHAMIL SHAIKHUTDINOV<sup>4</sup>, and HANS-JOACHIM FREUND<sup>4</sup> — <sup>1</sup>Inst. für Chemie, HU-Berlin — <sup>2</sup>Inst. für Physik, HU-Berlin — <sup>3</sup>Paul-Drude-Institut Berlin — <sup>4</sup>FHI Berlin

Several vanadium oxides undergo a metal-to-insulator transition (MIT) in the bulk, e.g., V<sub>2</sub>O<sub>3</sub> at ~150 K, VO<sub>2</sub> at 340 K, whereas V<sub>2</sub>O<sub>5</sub> is a semiconductor. Experimental evidence for a thermally induced surface insulator-metal transition (MIT) at the V<sub>2</sub>O<sub>5</sub>(001) surface at 350-400 K is presented. This surface exposes vanadyl (V=O) double rows along the [010] direction. Using density functional theory (DFT) in combination with statistical thermodynamics, the facile reduction along the rows was predicted.[1] The experimentally observed MIT transition expands preferentially in the direction of these rows. We then used the Monte Carlo method to simulate the reduced V<sub>2</sub>O<sub>5</sub>(001) surface at a given temperature and defect concentration. We typically find areas with a random distribution of isolated defects and others with up to 5 sites forming [010] oriented trenches. Using calculated band gaps for reduced V<sub>2</sub>O<sub>5</sub> structures as obtained with DFT+U, we construct band gaps maps which agree with those derived from scanning tunneling spectroscopy data; only the areas with defective rows are metallic. [1] M. V. Ganduglia-Pirovano and J. Sauer, PRB **70**, 045422 (2004). [2] R.-P. Blum, H. Niehus, C. Hucho et al., PRL. in press.