

**Stability, atomic and electronic structure of reduced  $\text{Fe}_3\text{O}_4(111)$  surfaces** — ●MARKUS PAUL<sup>1</sup>, MICHAEL SING<sup>1</sup>, DAVID SCHRUPP<sup>2</sup>, RALPH CLAESSEN<sup>1</sup>, and VICTOR BRABERS<sup>3</sup> — <sup>1</sup>Lehrstuhl für Experimentelle Physik IV, Universität Würzburg, Germany — <sup>2</sup>Lehrstuhl für Experimentalphysik II, Universität Augsburg, Germany — <sup>3</sup>Department of Physics, Eindhoven University of Technology, The Netherlands

Polar faces of ionic materials present a challenge for the determination of the atomic structure. Underlying difficulties are the relative stability and variability of such surfaces which can cause a poor reproducibility in the experiment or the coexistence of different structures on the same surface. In this work Magnetite(111) single crystal surfaces have been studied by STM, LEED and XPS under different *in situ* preparation conditions and stoichiometries, accordingly. The coexistence of several surface structures has been detected confirming only small differences in their relative stabilities. An unusual superstructure has been found for a reduced  $\text{Fe}_{1-x}\text{O}$ -like surface layer. It is explained as originating from elastic strain formation due to lateral mismatch between  $\text{Fe}_3\text{O}_4$  substrate and  $\text{Fe}_{1-x}\text{O}$ -like overlayer.

O 59.5 Thu 16:45 H41

**Stabilization of thin ZnO films by surface depolarization** — ●CHRISTIAN TUSCHE, HOLGER L. MEYERHEIM, and JÜRGEN KIRSCHNER — MPI für Mikrostrukturphysik Halle, D-06120 Halle, Germany

Heterostructures of the oxide semiconductor ZnO attracted interest for application in ultra violet laser diodes and spintronic devices. Theoretical predictions rely on detailed information on the film and interface structures. Scanning tunneling microscopy (STM) and surface x-ray diffraction (SXR) was used to study morphology and structure of ultra thin ZnO films on Ag(111).

ZnO films, 0.3 to 5 monolayers (ML) in thickness, were grown by pulsed laser deposition in  $10^{-7}$  mbar  $\text{O}_2$  atmosphere on Ag(111) at 300 K, followed by annealing at 680 K. SXR indicates that the film is (0001) oriented, and the hexagonal lattice vectors are aligned parallel with the Ag(111) surface. While single crystal (0001) or (000 $\bar{1}$ ) surfaces are polar, and extended flat regions ( $> 10$  nm) are not stable, the 2 ML thick ZnO films form a flat double-layer over the whole surface.

Stabilization is achieved by a transition of the Wurtzite- towards a graphite like structure with reduced polarity, i. e., O ions move to the plane of Zn ions: SXR shows an in-plane expansion of the ZnO lattice by 1.6% compared to bulk (3.30 Å vs. 3.25 Å), corresponding to a 7/8 coincidence with the Ag substrate (Ag: 2.89 Å). In parallel, Zn-O bonds (bulk: 1.97 Å) within the hexagonal plane shorten to 1.92 Å and intra-plane Zn-O bonds expand to 2.20 Å. The ions change their four-fold coordination (Wurtzite structure) to a three-fold one.

O 59.6 Thu 17:00 H41

**Identification of reactive oxygen sites at surfaces of  $\text{MoO}_3$  by polarization-resolved NEXAFS spectra: theoretical studies** — ●MATTEO CAVALLERI and KLAUS HERMANN — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

The identification of reactive oxygen sites at metal oxide surfaces and the characterization of their physical properties is of great importance for an understanding of the catalytic activity of such materials and, thus, for a rational design of more efficient and selective catalysts. Here we evaluate Near-Edge X-Ray Absorption Fine Structure (NEXAFS) spectra, based on density functional theory and appropriate surface clusters, to study and discriminate non-equivalent oxygen centers present at surfaces of catalytically relevant molybdenum oxides. For the (010) surface of bulk  $\text{MoO}_3$  this technique is able to unambiguously distinguish between singly coordinated molybdenyl oxygen covering the topmost molybdenum layers and other oxygen centers of similar local environment, differing only by their spatial orientation in the crystal. Theoretical predictions are also successfully used to identify and interpret characteristic features in the NEXAFS spectrum that arise from defects and oxygen vacancies<sup>1</sup>. Upon comparison between measured and computed NEXAFS spectra for different photon polarization directions it is also possible to validate proposed structures of thin  $\text{MoO}_3$  films at the Au(111) surface.

<sup>1</sup> M. Cavalleri, K. Hermann, S. Guimond, Y. Romanyshyn, H. Kuhlenbeck and H.-J. Freund, submitted to Cat. Today (2006)

O 59.7 Thu 17:15 H41

**Lattice Dynamics of  $\text{RuO}_2$ : Bulk and (110) Surface** — ●KLAUS-PETER BOHNEN<sup>1</sup>, ROLF HEID<sup>1</sup>, and OMAR DE LA PENA SEAMAN<sup>2</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik — <sup>2</sup>Department of Applied Physics, CINVESTAV-Mérida, Yucatán,

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Although  $\text{RuO}_2$  has been studied as a prototype catalyst for CO oxidation no careful study of the lattice dynamics for this material has been presented so far. Using modern ab-initio methods we obtain the phonon dispersion and the generalized density of states (GDOS). Inelastic neutron scattering experiments allow for an experimental determination of the GDOS. In contrast to what is known from structural studies, we find that the local density approximation gives a much better description of the phonon spectrum than the generalized gradient corrected form. This is also consistent with Raman measurements. Besides the bulk we have also studied the lattice dynamics for the (110) surface. Unfortunately, no complete experimental phonon study of this surface has been carried out so far, however, our results are consistent with the available experimental information. These calculations allow for the first time for the determination of the bulk and surface part of the phononic contribution to the free energy, a quantity which is essential for the determination of thermodynamic properties.

O 59.8 Thu 17:30 H41

**Tensor LEED study of the dynamics of the  $\text{NaCl}(100)$  surface** — ●JOCHEN VOGT — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

A wealth of theoretical studies dealt with the dynamics of the  $\text{NaCl}(100)$  surface, e.g. in relation to its melting behaviour, friction, or the simulation of image contrast in atomic force microscopy. Accurate experimental information on the temperature dependent vibrational amplitudes of ions in different layers is missing so far, although it could serve as a critical test for the various potential models applied to this prototype material. This contribution reports LEED experiments at various temperatures between 25 K and 300 K, in which beam intensities were recorded as a function of electron energy. The experimental  $I(E)$  data were analyzed using the tensor LEED approach. At all investigated temperatures the  $\text{NaCl}(100)$  surface exhibits the same relaxation, characterized by a static inward shift of the topmost  $\text{Na}^+$  ion of  $0.09 \pm 0.03 \text{ \AA}$ . The dynamics of the topmost layer is significantly higher than those of the second layer, where the measured amplitudes are close to literature bulk values. Above 100 K,  $\text{Na}^+$  and  $\text{Cl}^-$  ions in the topmost layer have nearly the same amplitudes, while the amplitudes of the cations in the second layer are larger than those of the anions. In this temperature range the mean square amplitudes of the ions at the surface are in good agreement with previously reported lattice dynamics studies.

O 59.9 Thu 17:45 H41

**Photon Mapping of  $\text{MgO}$  thin Films with an STM** — ●HADJ-MOHAMED BENIA, NIKLAS NILIUS, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der MPG, Berlin

The light emission from an STM junction consisting of an  $\text{MgO}$  thin film on  $\text{Mo}(001)$  and an Au tip is analysed with respect to its spatial distribution for various excitation conditions. The spectral characteristic of the light is compatible with an emission mechanism mediated by tip-induced plasmons that are excited by inelastic tunnel processes involving field emission resonances in the tip-sample gap. For  $\text{MgO}$  islands of distinct topographic height, the local emission yield can be tuned by changing the sample bias. This interrelation reflects the dependence of field emission resonances on the  $\text{MgO}$  work function, which in turn is a function of the number of  $\text{MgO}$  layers covering the Mo support.

O 59.10 Thu 18:00 H41

**Structural and electronic properties of bulk earth alkali oxides and their surfaces** — ●BJÖRN BAUMEIER, PETER KRÜGER, and JOHANNES POLLMANN — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Earth alkali oxides play a vital role in a number of technological applications, most prominently as supports in catalysis.

While structural properties of  $\text{BeO}$ ,  $\text{MgO}$ ,  $\text{CaO}$ ,  $\text{SrO}$  and  $\text{BaO}$  are quite well described within the local density approximation of density functional theory, the calculated electronic structure suffers from well-known shortcomings, most noticeably the significant underestimate of the band gap and conduction band energies. We present results of DFT calculations using self-interaction-corrected (SIC) pseudopotentials for the aforementioned earth alkali oxides. Bulk electronic properties are in very good agreement with experimental data and – where available – with results of considerably more elaborate quasiparticle calculations. To investigate the properties of nonpolar low-index surfaces of these