# O 14: Clean surfaces: Metals, semiconductors, oxides and insulators I

Time: Monday 15:00–16:45 Location: WIL B122

O 14.1 Mon 15:00 WIL B122

**Change of the surface electronic structure of Au(111) by a monolayer MgO(001) film** — •Yi Pan[1], Stefania Benedetti[2], Niklas Nilius[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [2]CNR, Istituto Nanoscienze, Centro S3, Via G. Campi 213/a, 41100 Modena, Italy

Monolayer films of MgO(001) have been prepared on an Au(111) surface and explored with scanning tunneling microscopy and spectroscopy. The symmetry mismatch between the hexagonal substrate and the squared over-layer results in the formation of a (6x1) superlattice, as revealed from the distinct stripe pattern observed in the STM. The presence of the oxide film modifies the potential situation at the interface, which induces a substantial up-shift of the Shockley-type surface band on Au(111). The resulting MgO/Au interface band is also characterized by a pseudo-gap at around 0.5 eV that opens at the position of the new Brillouin zone of the enlarged (6x1) cell. In addition, the oxide layer gives rise to a drastic decrease of the Au(111) work function, as deduced from the energy position of field-emission resonance on the bare and MgO-covered surface. The work function drop is explained by an interfacial charge transfer from the oxide film into the electro-negative gold surface.

O 14.2 Mon 15:15 WIL B122

**Electronic structure and thermodynamics of oxygen vacancies on (100) and (111) surfaces of MgO.** — •Sergey V. Levchenko, Norina Richter, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Polar metal oxide surfaces exhibit an increased sensitivity to the chemical environment due to major changes in surface stoichiometry driven by the requirement to compensate the surface charge. On top of such rearrangements, formation of surface point defects can greatly influence chemical properties of the surface. In this study, we employ density functional theory with HSE06 exchange-correlation functional with different values of the exchange screening parameter (including PBE as a limiting case) to calculate electronic structure and formation energies of neutral and charged O vacancies at the polar MgO(111) surface, which has been (and continues to be) a subject of extensive experimental and theoretical studies. The vacancies are calculated at the O-terminated octopolar reconstruction, which was predicted to be the most stable one for a wide range of O chemical potentials [1]. We use the *ab initio* atomistic thermodynamics approach [2] to estimate concentration, distribution, and charge states of the vacancies as a function of temperature, oxygen pressure, and electronic chemical potential. The properties of defects at the (111) surface are compared to the defects at the non-polar (100) termination.— [1] W. B. Zhang and B. Y. Tang, J. Phys. Chem. C 112 (2008) 3327; [2] K. Reuter and M. Scheffler, Phys. Rev. B 65, 035406 (2001); C. M. Weinert and M. Scheffler, Mat. Sci. Forum 10-12, 25 (1986)

O 14.3 Mon 15:30 WIL B122

**NC-AFM Aufnahmen von reinem und wasserstoffterminierten Diamant C(100)** — Markus Nimmrich[1], •Markus Kittelmann[1], Philipp Rahe[1], Andrew Mayne[2], Gerald Dujardin[2], Alexander von Schmidsfeld[3], Michael Reichling[3], Wolfgang Harneit[4] und Angelika Kühnle[1] — [1]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Germany — [2]Laboratoire de Photophysique Moléculaire, Université Paris-Sud, France — [3]Fachbereich Physik, Universität Osnabrück, Germany — [4]Institut für Experimentalphysik, Freie Universität Berlin, Germany

In diesem Beitrag stellen wir Ergebnisse unserer Untersuchung von hochreinem Typ IIa Diamant mit dem Nicht-Kontakt-Rasterkraftmikroskop (NC-AFM) vor. Wir präsentieren NC-AFM-Aufnahmen, die zum ersten Mal die einzelnen Wasserstoffatome der wasserstoffterminierten Diamant C (100) (2 x 1): H Oberfläche und die Kohlenstoffdimere auf der wasserstofffreien Diamant (100) (2 x 1) Oberfläche atomar aufgelöst zeigen.

Für die wasserstoffterminierte Oberfläche wird eine fast quadratische Elementarzelle abgebildet. Die beobachteten interatomaren Abstände sind in guter Übereinstimmung mit bereits publizierten Berechnungen der Diamant C (100) - (2 x 1): H Oberflächenstruktur.

Durch Entfernen des Wasserstoffs von der Diamantoberfläche wird die Probe nichtleitend. Wir stellen hochauflösende Aufnahmen vor, in denen die Kohlenstoffdimere einzeln dargestellt werden. Mit unseren Ergebnisse liefern wir einen experimentellen Nachweis für die (2 x 1)-Dimerrekonstruktion auf der nichtleitenden C (100) Oberfläche.

O 14.4 Mon 15:45 WIL B122

**Construction of an Interatomic Potential for Zinc Oxide Surfaces by High-Dimensional Neural Networks** — •Nongnuch Artrith, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Zinc oxide (ZnO) is a technologically important material with many applications, e.g. in heterogeneous catalysis. For theoretical studies of the structural properties of ZnO surfaces, defects, and crystal structures it is necessary to simulate large systems over long time-scales with sufficient accuracy. Often, the required system size is not accessible by computationally rather demanding density-functional theory (DFT) calculations. Recently, artificial Neural Networks (NN) trained to first principles data have shown to provide accurate potential-energy surfaces (PESs) for condensed systems. We present the construction and analysis of a NN PES for ZnO. The structural and energetic properties of bulk ZnO and ZnO surfaces are investigated using this potential and compared to DFT calculations.

O 14.5 Mon 16:00 WIL B122

**Electron localization in defective ceria films: An STM and DFT study** — Jan Frederik Jerratsch[1], Xiang Shao[1], •Niklas Nilius[1], Hans-Joachim Freund[1], Cristina Popa[2], M. Veronica Ganduglia-Pirovano[2], and Joachim Sauer[2] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany

Scanning tunnelling microscopy and density functional theory have been employed to identify the spatial correlation between an oxygen vacancy and the associated Ce3+ ion pair in a defective CeO2(111) film. The two Ce3+ ions can occupy different cationic shells around the vacancy (1st to 4th neighbour). The resulting variation in the chemical environment leads to a splitting of the filled Ce3+ f-levels, which is detected with STM spectroscopy. The position of the Ce3+ ion pair is also reflected in characteristic defect patterns observed in empty-state STM images, which result from the bright appearance of Ce4+ ions next to the defect while the Ce3+ remain dark. Both findings demonstrate that at least one extra electron localizes in a Ce ion that is not adjacent to the O vacancy.

O 14.6 Mon 16:15 WIL B122

**Formation and coexistence of different surface structures on heavily reduced TiO2 (110) rutile surface: STM/STS study.** — •Pavel Shukrynau, Marius Toader, Lars Smykalla, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

Cycles of Ar+ ion bombardment followed by specific temperature treatment leads to the formation and coexistence of two different phases onto single crystal TiO2 (110) rutile surface. One of the observed reconstructions is somehow similar to that cross-linked (1x2)-TiO2 structure, where the cross-link chains are perpendicular to the added rows of Ti2O3. In contrast, we observe cross-links that are rotated to 45° with respect to the <001> direction of the rows. This uncommon formation of the cross-link chains could be explained by the rearrangement of the top atoms at certain temperatures. STM topographs taken over the neighboring phase show bright rows, that run in <110> direction. Close inspection of the filled and empty images reveals zigzag arrangement of the bright protrusions within the particular line. Tunneling spectra acquired over various sites in the topographic image give the information about the bonding nature within the reconstruction. We propose the possible structural models of the coexisting phases and discuss their formation mechanisms on the base of atomically resolved STM images that were taken in both constant current and constant height modes.

O 14.7 Mon 16:30 WIL B122

**Epitaxial films of praseodymia on Si(111): controlled modification from $Pr_2O_3$ to $PrO_2$ via plasma and thermal treatment** — •Sarah Röhe[1], Andreas Schaefer[1], Volkmar Zielasek[1], Thomas Schroeder[2], and Marcus Bäumer[1] — [1]IAPC, Universität Bremen — [2]IHP, Frankfurt (Oder)

A cold RF oxygen plasma treatment is demonstrated as a successful route to prepare clean, well-ordered and stoichiometric $PrO_2$ layers on silicon which are very difficult to obtain by other techniques. As a starting point, cubic $PrO_{2-\Delta}$ films are obtained by growing hexagonal $Pr_2O_3$ on Si(111) by MBE and annealing these layers to 720 K in oxygen atmosphere. The subsequent plasma treatment is performed in a plasma cell directly attached to a UHV chamber so that samples can be transferred to XPS without breaking vacuum. The Pr 3d XP spectra show so far unobserved spectral characteristics presenting a fingerprint for $PrO_2$. The XPS data provide insight into the special role of praseodymia among the rare earth oxides. They also reveal that former XP studies of praseodymia suffered from significant reduction at the surface. Starting with $PrO_2$ films prepared by oxygen plasma, different oxidation states of praseodymia can be obtained by reducing the oxide in a controlled way via thermal treatment. Several temperature-programmed desorption peaks of $O_2$ are observed in the range from 300 to 900 K and indicate phase transitions. The different praseodymia phases are studied with respect to their activity towards CO oxidation at their surface under UHV conditions.