

O 90: Semiconductor Substrates

Time: Friday 10:30–13:15

Location: H45

O 90.1 Fri 10:30 H45

Growth Study of Thin MgO Films on Fe(001) — ●HENDRIK RONNEBURG, STEFANIE STUCKENHOLZ, CHRISTIN BÜCHNER, MARKUS HEYDE, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The electronic structure and morphology of oxide surfaces are of crucial importance for their reaction behaviour. A detailed understanding of the structure-reactivity relationship is desired for the studies in heterogeneous catalysis.

We use noncontact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) to study model catalysts, namely metal supported thin oxide film systems.

Thin MgO films can be grown on different metal substrates, e.g. Mo(001), Ag(001) or Fe(001). MgO films grown on Mo(001) and on Ag(001) have been studied in detail by scanning probe methods [1, 2]. The electronic structure and morphology of the oxide film is altered by the substrate. To further investigate this support influence on the properties of thin oxide films our present studies focus on the system of MgO grown on Fe(001).

Here we present preliminary results from our growth study of thin MgO films on Fe(100).

[1] S. Benedetti, *et al.*, Chem. Phys. Lett. **430**, 330 (2006)

[2] T. König, *et al.*, J. Phys. Chem. C **113**, 11201 (2009)

O 90.2 Fri 10:45 H45

Concentration of point defects at metal-oxide surfaces: case study of MgO (100) — NORINA A. RICHTER¹, SABRINA SICOLO², ●SERGEY V. LEVCHENKO¹, JOACHIM SAUER², and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem 14195, Germany — ²Humboldt-Universität zu Berlin, Berlin 10099, Germany

We calculate from first principles the concentration of neutral and charged oxygen vacancies on a doped MgO (100) surface at realistic (T , p_{O_2}) conditions. Vacancy formation energies are computed using hybrid density-functional theory with parameters of the exchange-correlation functional adjusted according to a basic consistency requirement on the Kohn-Sham and G_0W_0 defect transition levels. The parameters are validated by CCSD(T) calculations of formation energies for neutral vacancies using embedded cluster models. Gibbs free energies of formation are obtained using the *ab initio* atomistic thermodynamics approach [1]. We demonstrate that the concentration of surface vacancies is significantly increased due to band bending and Fermi level pinning at the surface, resulting in lower formation energies of charged vacancies.

[1] K. Reuter and M. Scheffler, Phys. Rev. B **65**, 035406 (2001); C. M. Weinert and M. Scheffler, Mat. Sci. Forum **10-12**, 25 (1986); M. Scheffler and J. Dabrowski, Phil. Mag. A **58**, 107 (1988).

O 90.3 Fri 11:00 H45

Ultra-thin ZnO films on metal substrates from first principle — ●BJOERN BIENIEK, YONG XU, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO films can be used to model catalysts or ZnO surfaces. By means of density-functional theory (DFT - PBE and the hybrid functional HSE) we investigate the structure of ultra-thin ZnO on the (111) surfaces of Ag, Cu, Pd and Pt. In contrast to the bulk, the free-standing ZnO mono-layer adopts a graphene-like structure [1]. We find that this flat structure prevails on the metal substrates and obtain coincidence structures in good agreement with experiment [2, 3]. The influence of O₂ and H₂ environments is investigated with *ab-initio* thermo-dynamics [4] and surface phase diagrams are presented. Zn- and O-point defects are stabilized in the mono-layer by the substrates that would not be present in the freestanding ZnO mono-layer. With decreasing nobility of the metal substrate, the stability of defects, in particular inter-facial O, increases and the corrugation of the film becomes more pronounced. With increasing H₂ partial pressure sparse ring structures occur in Zn poor conditions. Metal supported ultra-thin ZnO films therefore do not resemble conventional ZnO surfaces and should be regarded as distinct nano-systems in their own right.

[1] Z. C. Tu and X. Hu, PRL **94**, 035434 (2006) [2] C. Tusche *et al.*

PRL **99**, 026102 (2007) [3] G. Weirum *et al.* J. Phys. Chem. C, **114** (2010) [4] K. Reuter and M. Scheffler, PRB **68**, 045407 (2003)

O 90.4 Fri 11:15 H45

Manipulation of subsurface donors in ZnO — ●HAO ZHENG, ALEXANDER WEISMANN, and RICHARD BERNDT — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

The capability of manipulating structures at the atomic scale has become an important asset of the scanning tunneling microscope (STM). Nowadays atoms may be arranged into nanostructures with device-like functions. Usually this exquisite control is limited to adatoms. A recent exception is interstitial H in Pd, which could be moved with an STM tip. No comparable results have been reported for semiconductors where the controlled positioning of individual dopants would be desirable. We present the manipulation of interstitial Zn in ZnO, a semiconductor with extraordinary properties. Zn interstitials are of particular interest because they may be the sought-after shallow donors that lead to n-type conductance of ZnO despite its wide band gap of 3.4 eV.

O 90.5 Fri 11:30 H45

Cyclooctyne adsorption on clean and hydrogen precov-ered Si(001) surfaces — ●GERSON METTE¹, MICHAEL DÜRR^{1,2}, RUBEN BARTHOLOMÄUS³, ULRICH KOERT³, and ULRICH HÖFER¹ — ¹Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — ²Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen — ³Fachbereich Chemie, Philipps-Universität, D-35032 Marburg

The reaction of organic adsorbates on semiconductor surfaces is of special interest with respect to surface functionalization and its use in molecular electronics. Whereas several alkenes and alkynes exhibit well ordered monolayers on Si(001), second- and multilayer attachment is still a central challenge towards successful functionalization.

In this context, the adsorption of cyclooctyne on clean and hydrogen precov-ered Si(001) surfaces was investigated by means of STM. The adsorption behavior was observed to be similar at room temperature and at low surface temperature of 50 K in contrast to systems like C₂H₄/Si which adsorb via a mobile precursor state. Moreover, it was found to be insensitive to distorted, hydrogen-induced dangling-bond configurations. At high coverage, cyclooctyne forms well ordered structures on Si(001). Our results suggest a direct adsorption pathway for cyclooctyne on Si(001) most likely governed by the molecule's triple bond in combination with its high ringstrain. This should make cyclooctyne a good candidate for chemoselective cycloadditions in more complex multifunctional compounds.

O 90.6 Fri 11:45 H45

Self-assembly of cis-Oligodiacetylenes from solution — ●CHRISTIAN STEINER¹, ERIN T. CHERNICK², DAVID GESSNER¹, MAXIMILIAN AMMON¹, RIK R. TYKWINSKI², and SABINE MAIER¹ — ¹Department of Physics, University of Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany — ²Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Henkestraße 42, 91054 Erlangen, Germany

Cis-Oligodiacetylenes (ODAs) typically tend to adopt a folded, helical conformation in solution. Helical oligomers or polymers with a conjugated, chiral backbone provide a material with unique electronic and photonic properties which can be applied towards enantioselective sensing, chiral catalysis or for templating self-assembly, yielding chiral nanostructures.

The influence of the solvent on the conformation of ODAs was probed both by scanning tunneling microscopy and atomic force microscopy in ambient condition. We found that molecules solved in isopropanol aggregate in clusters, while molecules solved in tetrahydrofuran form flat films on the surface. Clusters on Mica surfaces are typically larger than on HOPG indicating that not only the solvent but also the surface charge influences the aggregation of the molecules. Molecularly resolved scanning tunneling microscopy images on HOPG suggest that in films the ODAs assemble in wire-like structures.

O 90.7 Fri 12:00 H45

The interface of III-V semiconductors to H₂O studied by reflection anisotropy spectroscopy and UPS — ●WOLF-DIETRICH ZABKA^{1,2}, MATTHIAS M. MAY^{1,2}, OLIVER SUPPLIE^{1,2}, HELENA STANGE^{1,2}, CHRISTIAN HÖHN¹, HANS-JOACHIM LEWERENZ^{1,3}, and THOMAS HANNAPPEL^{1,4,5} — ¹Helmholtz-Zentrum Berlin, Institute for Solar Fuels — ²Humboldt-Universität zu Berlin, Institut für Physik — ³California Institute of Technology, Pasadena, USA — ⁴Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — ⁵CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

III-V semiconductors are a promising absorber material class for solar-driven water splitting [1]. The interface between the semiconductor and H₂O is crucial for stability as well as charge transfer efficiency to the electrolyte [2,3].

For a better understanding of this interface, we perform model-experiments applying H₂O-adsorption in UHV to the surface of GaP(100) and InP(100) prepared by metalorganic vapour phase epitaxy (MOVPE). The influence of adsorbed water on III- and V-rich surfaces was examined with reflection anisotropy spectroscopy (RAS) and ultraviolet photoelectron spectroscopy (UPS). The two surface terminations show substantially different responses to H₂O. A comparison to results for UHV-cleaved surfaces [3] tries to illuminate the role of hydrogen-termination for these MOVPE-prepared surfaces.

[1] H. Döscher et al., *ChemPhysChem* **13**: 2899 (2012); [2] B. Wood et al., *The Journal of Chemical Physics* **136**: 064705 (2012); [3] O. Henrion et al., *Surface Science* **457**: L337 (2000).

O 90.8 Fri 12:15 H45

STM Observation of Krypton Adsorbed on Graphite — ●RAPHAEL BINDEL, TOMOHIRO MATSUI, and HIROSHI FUKUYAMA — Department of Physics, Graduate School of Science, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Physisorption of a Krypton monolayer on graphite in the $\sqrt{3}x\sqrt{3}R30$ commensurate phase is investigated by low-temperature scanning tunneling microscopy (STM) at $T < 100$ mK. Former experiments have shown the visibility of Krypton on Graphite in STM images [1]. We observe the growth of the Kr monolayer directly. Moreover, the Krypton adsorption site is determined to be the hollow site of the Carbon lattice by using the lateral boundary between Graphite and islands of the Krypton commensurate phase. In partial agreement with density functional theory calculations [1], the $4p$ and $5s$ -states of the Krypton atoms appeared in STM images recorded at different voltages for the occupied as well as for the unoccupied states.

O 90.9 Fri 12:30 H45

Formation of Lu silicide on Si (111)-7x7 surface: STM/PES study at room temperature and low coverage — ●PAVEL SHUKRYNAU¹, XU YING¹, LARS SMYKALLA¹, MARTIN VONDRACEK², and MICHAEL HIETSCHOLD¹ — ¹Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — ²Institute of Physics Academy of Sciences of the Czech Republic, Cukrovarnická 10, CZ 162 53 Prague, Czech Republic

Interaction of very small amounts of lutetium with Si (111)-7x7 reconstructed surface was investigated in detail using combination of Scanning Tunneling Microscopy/Spectroscopy and Photoelectron Spectroscopy. Two distinct types of nanoclusters were found in the initial growth of the Lu/Si interface: the clusters of the first type have well defined globular shape with the average size of about 1 nm and are

tightly bound to the underlying substrate. Other type of clusters is not homogeneous, showing a motion inside one half of the 7x7-unit cell. Analysis of photoelectron spectra of the Si 2p core levels shows core level binding energy shifts and intensity variations of Si surface related components, which clearly indicate that the reaction starts already at room temperature. Comparison of tunneling spectra with valence band PES data allows to determine the electronic structure of adsorbed species locally and suggests the formation of Lu-rich silicide.

O 90.10 Fri 12:45 H45

AlGaIn/GaN based pH-sensitive field-effect transistors for nonaqueous solutions — ●JOHANNES ANZT¹, VOLKER CIMALLA¹, WILFRIED PLETSCHEN¹, and OLIVER AMBACHER^{1,2} — ¹Fraunhofer Institute for Applied Solid State Physics, Freiburg, Germany — ²Laboratory for Compound Semiconductor Microsystems, University of Freiburg, Germany

The purpose of this work is to characterize ion-sensitive field effect transistors (ISFETs) based on AlGaIn/GaN heterostructures for measurements in nonaqueous solutions. For example, organic solvents offer larger potential windows for electrochemical techniques. Moreover, the pH value in biofuel is an important parameter to characterize quality. While ISFET sensors have already shown excellent sensing properties in aqueous solutions, pH measurements in nonaqueous solutions are faced to several challenging obstacles. Nonaqueous solutions often have low conductivity and the preparation of buffer solutions can be limited by solubility of the constituents. By definition, pH-scales in different solvents or solvent mixtures are not equal, thus, their pH-values ($\text{pH} = -\lg a(\text{H}^+)$) are not comparable. For example, reactivity at $\text{pH} = 0$ in liquid ammonia is by far lower than at $\text{pH} = 0$ in acetic acid. As the pH-ISFET response directly depends on the surface potential, which in turn is directly related to the activity of protons, it offers a possibility to get a universal measuring device with an alternative universal pH-scale.

O 90.11 Fri 13:00 H45

Heteroepitaxial growth of GaP on Si(111) substrates for III-V nanowire solar cells — ●AGNIESZKA PASZUK^{1,2}, WEIHONG ZHAO^{1,2}, MATTHIAS STEIDL^{1,2}, SEBASTIAN BRÜCKNER^{1,2}, ANJA DOBRICH², JOHANNES LUCZAK², PETER KLEINSCHMIDT^{2,3}, HENNING DÖSCHER^{1,2}, and THOMAS HANNAPPEL^{1,3} — ¹Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Ilmenau — ²Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — ³CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Erfurt

III-V nanowires provide opportunities to realize high efficiency solar cells. We intend to grow nanowires by metal organic vapor phase epitaxy (MOVPE) on III-V/Si(111) templates to benefit from silicon as a low cost substrate. As a buffer layer we use GaP, since it is almost lattice matched to silicon. To achieve successful nanowire growth on GaP/Si(111) it is required to prepare GaP(111)B surfaces. A contamination-free transfer system enables us to study the MOVPE prepared surfaces with various surface science tools. To understand the heteroepitaxial growth of GaP on Si(111) we studied homoepitaxial GaP(111)A and B surfaces as a reference. Different characteristic surface reconstructions visible in low energy electron diffraction (LEED) enable identification of the GaP polarity. For growth on Si(111), changing the Si surface termination we can control the resulting GaP polarity.