

## O 31: Clean surfaces II

Time: Tuesday 10:30–13:00

Location: A 060

O 31.1 Tue 10:30 A 060

**Characterisation of a ceria film on Si(111) with non-contact atomic force microscopy** — ●REINHARD OLBRICH<sup>1</sup>, HANS HERMANN PIPER<sup>1</sup>, MARVIN ZOELLNER<sup>2</sup>, THOMAS SCHROEDER<sup>2</sup>, and MICHAEL REICHLING<sup>1</sup> — <sup>1</sup>Universität Osnabrück, Germany — <sup>2</sup>IHP Frankfurt (Oder), Germany

A 180nm thick film of ceria deposited on Si(111) is studied with atomic force microscopy operated in the non-contact mode (NC-AFM) and Kelvin probe force microscopy (KPFM). The thin film is prepared by annealing to different temperatures in an ultra-high vacuum environment. Up to a temperature of 845 K, pyramidal triangular structures are observed. In a temperature range from 515 K to 780 K, 6 to 12 nm high spikes appear between the triangle structures. After annealing the film to 930 K and higher temperatures flat terraces and step structures develop on the film surface that are similar to structures observed on CeO<sub>2</sub>(111) surfaces of bulk crystals. Annealing temperatures over 1130 K causes a decomposing of the thin film. Sputtering the ceria film and annealing at 1110 K generates the best results with clear terraces and step structures. The KPFM measurement reveals a positive local charge at step edges and a lower charge on the terraces.

O 31.2 Tue 10:45 A 060

**Structural, electronic and optical properties of the two isomers of Si(111)2x1** — ●CLAUDIA VIOLANTE<sup>1</sup>, ADRIANO MOSCA CONTE<sup>1</sup>, FRIEDHELM BECHSTEDT<sup>2</sup>, and OLIVIA PULCI<sup>1</sup> — <sup>1</sup>ETSF, Dept. of Physics University of Rome Tor Vergata — <sup>2</sup>IFTO, Friedrich Schiller Universität, Jena, Germany

The Si(111)2x1 surface, which appears on cleaved surfaces at low and room temperature, has been among the most studied semiconductor surfaces ever. Although apparently simple, it shows several intriguing and not completely understood features. The atomic structure of the Si(111)2x1 surface has been known for decades to consist of Pandey chains, that can tilt with two possible directions, generating two almost energetically degenerate structures called isomers: the Si(111)2x1 negative buckling and the Si(111)2x1 positive buckling. Although it is currently believed that for a sample of Si(111)2x1 at room temperature the most stable configuration is the positive buckling structure, it has been recently shown by STS measurements that for highly n-doped Si(111)2x1, at low temperature, both positive and negative isomers may coexist on the surface. A confirmation of this experimental observations could come from the study of optical properties of these two isomers. In this talk we will show and discuss the results of our theoretical simulations for the calculation of structural, electronic and optical properties (RAS spectra) of the two structures, obtained by ab-initio calculations within the most reliable state-of-the-art methods based on density functional theory and many-body perturbative techniques.

O 31.3 Tue 11:00 A 060

**Vibrational spectra of reconstructed Si(100) surfaces** — ●CHARLES H. PATTERSON — School of Physics, Trinity College Dublin, Dublin 2, Ireland

We present calculations of vibrational spectra of IR-active modes at the Si(100) (2x1), p(2x2) and c(4x2) surfaces and the (2x1)-H surface. Previous calculations of phonons at these surfaces have not included scattering cross-sections. In contrast to existing hypotheses regarding relative scattering cross-sections for vibrational motions parallel or perpendicular to the surface, we find that the largest scattering cross-sections for the clean surfaces are for motions parallel to the surface. This is because parallel motions of chemically unsaturated dimers are accompanied by large charge transfer between dimer atoms which is relatively weakly screened by the less polarisable bulk semiconductor. Results of calculations are compared to HREELS data for the clean and H-covered Si(100) surfaces and some suggestions for new experiments are made.

O 31.4 Tue 11:15 A 060

**STM measurements on MOVPE-prepared germanium and silicon surfaces** — ●JOHANNES LUCZAK<sup>1</sup>, PETER KLEINSCHMIDT<sup>1,4</sup>, SEBASTIAN BRÜCKNER<sup>1,2</sup>, HENNING DÖSCHER<sup>1,2</sup>, OLIVER SUPPLIE<sup>1</sup>, ENRIQUE BARRIGÓN<sup>3</sup>, and THOMAS HANNAPPEL<sup>1,2,4</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — <sup>2</sup>TU Ilmenau, Institut für Physik, Fachge-

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An important requirement to achieve low defect densities in the III-V epilayers deposited on group IV substrates is a suitable substrate surface preparation prior to heteroepitaxy. Generation of double layer steps on Si(100) or Ge(100) is desirable for subsequent anti-phase domain-free heteroepitaxy of III-V semiconductors. A contamination-free MOVPE-to-UHV transfer system allowed us to analyze different surfaces with various UHV based surface-sensitive techniques such as x-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM). STM measurements on Si(100) showed the formation of D\_A or D\_B - double-layer steps on a surface with an intermediate offset of 2° in [011], depending on the process parameters. STM measurements on Ge(100) showed single-layer steps after homoepitaxial growth on substrates with 0.2° offset in [011] direction, and double-layer steps after deoxidation on substrates with 6° offset in [011].

O 31.5 Tue 11:30 A 060

**Spectroscopy of single donors at ZnO(0001) surfaces** — ●HAO ZHENG<sup>1</sup>, JÖRG KRÖGER<sup>2</sup>, and RICHARD BERNDT<sup>1</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

ZnO has been widely investigated as a material for piezo-, micro-, and opto-electronic devices. Although the band-gap of ZnO in the wurtzite structure is as large as 3.4eV, undoped material exhibits n-type conductivity at room temperature. The conductivity has been attributed to native defects such as interstitial Zn, Zn with O vacancies, Zn with substitutional N, and H impurities. Despite its importance for applications the origin of the residual conductance is still controversial. Here, donors near the polar (0001) surface of nominally undoped ZnO were investigated with scanning tunneling microscopy at 5K. Spatially resolved spectroscopy reveals single and double charging. Equidistant peaks in spectra of ionized donors are attributed to polaron excitation. The data are consistent with doping due to Zn interstitials or complexes. Support by the DFG via SFB 855 is acknowledged.

O 31.6 Tue 11:45 A 060

**Construction of High-Dimensional Neural Network Potentials for Surfaces: Applications to Copper and Zinc Oxide** — ●NONGNUCH ARTRITH, BJÖRN HILLER, and JÖRG BEHLER — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Molecular dynamics simulations of large systems critically depend on the accurate description of the underlying potential energy surface (PES). First-principles methods like DFT can provide very accurate energies and forces, but at high computational costs. Therefore, the development of more efficient potentials is a very active field of research. High-dimensional Neural Networks (NN) trained to first-principles data have been shown to provide accurate PESs for systems containing a single atomic species, while they are several orders of magnitude faster than electronic structure calculations. Now, we have generalized this method to multicomponent systems with arbitrary chemical composition. This is achieved by introducing physically motivated terms to deal with long-range interactions and charge transfer. Here we report the capabilities of the NN method for systems containing a single atomic species as well as for multicomponent systems. We present structural energy differences, vacancy formation energies, and surface energies for different copper and zinc oxide surfaces. The predicted geometries, energies, forces, and atomic charges are in excellent agreement with reference DFT calculations.

O 31.7 Tue 12:00 A 060

**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 hybrid inorganic/organic interfaces, ZnO is becoming more and more wide spread as inorganic component. To prevent charging or conductivity problems in surface sensitive characterization techniques such as scanning tunneling microscopy or photoemission

spectroscopy, metal supported ultra-thin ZnO films can be used as model systems. By means of PBE density-functional theory (DFT) calculations we investigate to what extent ultra-thin ZnO on the (111) surfaces of Ag, Cu and Pd resembles the properties of bulk ZnO surfaces or if it should be regarded as a distinct nanosystem in its own right [1]. Free standing ZnO mono-layer thin films deviate from the wurtzite structure of the bulk material and adopt a planar, graphite-like geometry, in agreement with previous calculations [2]. By inspecting the stress/strain curve of the freestanding mono-layer the expected commensurability condition for different substrates can be estimated. The PBE calculations reveal that the ZnO/metal interaction is weak and a  $8 \times 9$  reconstruction on Ag (111) is most stable [3]. The results will be analyzed in terms of the underlying electronic structure and the effect of the exchange-correlation functional and the thickness of the ZnO layers will be addressed. [1] C. Freysoldt *et al.*, Phys. Rev. Lett. **99**, 086101 (2007), [2] Z. C. Tu and X. Hu, Phys. Rev. B **74**, 035434 (2006), [3] C. Tusche *et al.*, Phys. Rev. Lett. **99**, 026102 (2007)

O 31.8 Tue 12:15 A 060

**Preparation of vicinal Ge(100) surfaces in hydrogen ambient** — ●OLIVER SUPPLIE<sup>1</sup>, SEBASTIAN BRÜCKNER<sup>1,2</sup>, ENRIQUE BARRIGÓN<sup>3</sup>, HENNING DÖSCHER<sup>1,2</sup>, ANJA DOBRICH<sup>1</sup>, CLAAS LÖBBEL<sup>1</sup>, JOHANNES LUCZAK<sup>1</sup>, PETER KLEINSCHMIDT<sup>1,4</sup>, and THOMAS HANNAPPEL<sup>1,2,4</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — <sup>2</sup>TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — <sup>3</sup>Instituto de Energía Solar, Universidad Politécnica de Madrid, E-28040 Madrid — <sup>4</sup>CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Vicinal Ge(100) is the established substrate for III-V nucleation regarding high efficiency opto-electronic devices such as multi-junction solar cells. We studied vicinal Ge(100) surfaces prepared by H<sub>2</sub> annealing in metalorganic vapor phase epitaxy (MOVPE) environment prior to heteroepitaxy. A contamination-free MOVPE-to-UHV transfer system allowed to correlate in situ reflection anisotropy spectroscopy (RAS) and surface science techniques. Annealing in H<sub>2</sub> removed oxides and carbon from the substrates as confirmed by X-ray photoemission spectroscopy. Low energy electron diffraction patterns indicated a  $(2 \times 1)$  majority surface reconstruction domain. The presence of coupled Ge-H monohydride was confirmed via Fourier-transform infrared spectroscopy. The RA spectrum of the hydrogen terminated Ge(100) surface featured characteristic differences compared to the RA spectrum of UHV-prepared clean Ge(100) in literature [1].

[1] Rossow *et al.*, JVSTB**18**(2000)2229

O 31.9 Tue 12:30 A 060

**Non-polar and semipolar InN surfaces** — ●ABDERREZAK BELLABES, JÜRGEN FURTHMÜLLER, and FRIEDHELM BECHSTEDT — Friedrich-Schiller-Universität Jena

Using density-functional-based total-energy calculations and the LDA-1/2 method to compute approximately quasiparticle band structures, we have studied clean relaxed InN surfaces with vanishing or small polarity. More in detail, the c-plane, a-plane, m-plane, and r-plane surfaces have been investigated. In contrast to the polar faces, which allow Fermi level pinning, the projected fundamental bulk gap of about 0.71 eV is free of surface states in the nonpolar cases. Consequently, freshly cleaved InN surfaces cannot lead to a surface accumulation layer. The different electronic structures modify the surface dipole and hence the ionization energy and electron affinity significantly when varying the surface normal from [0001] via [11-22] and [10-10] or [11-20] to [000-1].

O 31.10 Tue 12:45 A 060

**Imaging and manipulation of ferroelectric domains by STM and STS** — ●MAIK CHRISTL<sup>1</sup>, STEFAN FÖRSTER<sup>1</sup>, HANNES BAYER<sup>1</sup>, and WOLF WIDDRA<sup>1,2</sup> — <sup>1</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — <sup>2</sup>Max Planck Institute of Microstructure Physics, Halle, Germany

Piezoresponse force microscopy (PFM) has emerged as a basic tool for imaging and domain engineering on ferroelectric materials, however the lateral resolution is limited down to several nanometers [1].

Here we present an alternative approach of characterizing ferroelectric domain structures by using the scanning tunneling microscope (STM). Epitaxial BaTiO<sub>3</sub> films of various thickness which have been grown under ultra high vacuum conditions on a Pt(100) substrate [2] have been studied by STM and STS at room temperature. DI/dV maps allow to identify the out-of-plane domain structure in the BaTiO<sub>3</sub> films as prepared. Upon applying higher STM bias voltages, the ferroelectric polarization can be reversed and domain structures will be written. With STS a clear contrast between positively and negatively poled areas becomes visible. Additionally, downward polarized areas appear higher in the STM topography. The manipulated areas are stable for days. All STM data will be compared with PFM measurements of the same sample.

[1] M. Alexe and A. Gruverman, *Nanoscale Characterisation of Ferroelectric Materials*, Springer, Berlin Heidelberg **2004**.[2] S. Förster, M. Huth, K.-M. Schindler, and W. Widdra, *J. Chem. Phys.* **135**, 104701 **2011**.