

## O 17: Semiconductor Substrates

Time: Monday 16:00–19:15

Location: PHY C 213

O 17.1 Mon 16:00 PHY C 213

**Structural sensitivity of the electromechanical coupling at Si surfaces** — ●SANDRA HOPPE<sup>1</sup>, ANJA MICHL<sup>1,2</sup>, JÖRG WEISSMÜLLER<sup>2,3</sup>, and STEFAN MÜLLER<sup>1</sup> — <sup>1</sup>Institute of Advanced Ceramics, Hamburg University of Technology, Germany — <sup>2</sup>Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany — <sup>3</sup>Institute of Materials Physics and Technology, Hamburg University of Technology, Germany

Electromechanical coupling describes a relation between a material's mechanical and electronic properties. It has been found for various metal surfaces that an applied strain leads to a change in the work function. While this phenomenon has been studied for silicon nanowires and silicene, surprisingly, no results are available for clean silicon surfaces. We investigated the electromechanical coupling at the silicon (100) and (111) surfaces via density functional theory by calculating the response of the ionization potential and the electron affinity to different types of strain. The highest occupied and the lowest unoccupied molecular orbital (HOMO and LUMO) were obtained from the surface states within the surface band gap. We find large negative response parameters and a high sensitivity of the strain response to surface relaxations. This can be attributed to the directional bonds in covalent semiconductors and discussed in terms of volume and surface contributions to the response of the surface dipole potential and the electronic structure to strain. While we find a considerable volume influence on the dipole potential, the response of HOMO and LUMO seems to be dominated by the local reconstruction geometry.

O 17.2 Mon 16:15 PHY C 213

**Simultaneous nc-AFM/STM characterization of subsurface defects on B:Si(111)- $\sqrt{3}\times\sqrt{3}$  surface** — ●EVAN SPADAFORA<sup>1</sup>, JAN BERGER<sup>1</sup>, PINGO MUTOMBO<sup>1</sup>, MYKOLA TELYCHKO<sup>1</sup>, MARTIN ONDRACEK<sup>1</sup>, MARTIN SVEC<sup>1</sup>, ZSOLT MAJZIK<sup>1</sup>, ALASTAIR MC LEAN<sup>2</sup>, and PAVEL JELINEK<sup>1</sup> — <sup>1</sup>Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — <sup>2</sup>Department of Physics, Queen's University, Kingston, Ontario, Canada

B:Si(111)- $\sqrt{3}\times\sqrt{3}$  surface has gained a lot of interest in surface science, due to its prominent electronic and structural properties. Compared to bare silicon surface, this system has reduced chemical reactivity, which makes it a suitable candidate for deposition of molecular complexes without a risk of their decomposition. Here we will report combined nc-AFM/STM measurements using qPlus sensor with atomic resolution of the B:Si(111)- $\sqrt{3}\times\sqrt{3}$  surface supported by total energy DFT calculations. STM reveals slight modulation of the tunneling current over surface area, which we attributed to presence of subsurface boron defects. We combine KPFM and lock-in STS measurements with large-scale DFT calculations to characterize position of boron subsurface defects and their influence on surface electronic structure.

O 17.3 Mon 16:30 PHY C 213

**In situ Scanning Tunneling Microscopy investigation of layered superlattices [(VSe<sub>2</sub>)<sub>n</sub>1.06[(TaSe<sub>2</sub>)<sub>n</sub>]** — ●PAVEL SHUKRYNAU<sup>1</sup>, RYAN ATKINS<sup>2</sup>, DAVE C. JOHNSON<sup>2</sup>, and MICHAEL HIETSCHOLD<sup>1</sup> — <sup>1</sup>Institute of Physics, Technische Universität Chemnitz, Reichenhainer Straße 70, D-09107 Chemnitz, Germany. — <sup>2</sup>Materials Science Institute and Chemistry Department, University of Oregon, Eugene, Oregon 97403, USA

Variable Temperature Scanning Tunneling Microscopy (VT STM) was used to investigate local structural and electronic properties of the cleaved surface of [(VSe<sub>2</sub>)<sub>n</sub>1.06[(TaSe<sub>2</sub>)<sub>n</sub>]] layered compound. The original uppermost layer dissipates into small domains of 50x50 nm in size or more. In a region where three domains are in contact, a small triangular area with a side up to 5 nm is usually found, exhibiting a dark depression. The detailed inspection of the interior of the domain reveals a local ordering in a hexagonal-like pattern with rare inclination of surface defects. The observed structure is somehow similar to those obtained previously on other transition metal-chalcogenide surfaces. We were not able to identify unambiguously the chemical identity of the surface layer in STM scans. However, tunneling spectroscopy measurements distinctly show the dominance of the metal atoms in the topmost layer rather than the chalcogen ones.

O 17.4 Mon 16:45 PHY C 213

**Adsorption of Tetrahydrofuran and Diethylether on the Si(001) surface studied by means of STM, XPS and UPS** — ●MARCEL REUTZEL<sup>1</sup>, GERSON METTE<sup>1</sup>, MICHAEL DÜRR<sup>1,2</sup>, ULRICH KOERT<sup>3</sup>, and ULRICH HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — <sup>2</sup>Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany — <sup>3</sup>Fachbereich Chemie, Philipps-Universität, D-35032 Marburg

A promising possibility to compete with the challenges of miniaturization in semiconductor device physics is the functionalization of inorganic semiconductor surfaces with organic molecules. It is thus important to understand the basic adsorption mechanisms of different classes of organic molecules. In this contribution, we investigate the adsorption properties of tetrahydrofuran and diethylether on the Si(001) surface as representatives for the functional group of ethers. We find a complex adsorption scheme which is similar for the two molecules.

At 50 K, a dative bond is formed via the donation of electron density of an oxygen lone pair into the D<sub>down</sub> orbital of the c(4x2) reconstructed Si(001) surface. Heating the sample to 300 K leads to a surface mediated ether cleavage which results in covalently bonded adsorbates on two neighboring dimer rows. While the ring opening reaction of tetrahydrofuran leads to a bridging Si-O-(CH<sub>2</sub>)<sub>4</sub>-Si configuration, the linear diethylether is cleaved and leads to Si-O-C<sub>2</sub>H<sub>5</sub> and Si-C<sub>2</sub>H<sub>5</sub> adsorbates. The scission of diethylether further enables a tip induced intrarow hopping of the (-C<sub>2</sub>H<sub>5</sub>) fragment.

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**Switching single molecules by STM voltage pulses on the Si(100) surface** — ●ANJA NICKEL<sup>1</sup>, JÖRG MEYER<sup>1</sup>, ROBIN OHMANN<sup>1</sup>, CHRISTIAN JOACHIM<sup>2</sup>, GIANAURELIO CUNIBERTI<sup>1</sup>, and FRANCESCA MORESCO<sup>1</sup> — <sup>1</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — <sup>2</sup>CNRS, CEMES, 29 rue J. Marvig, 31055 Toulouse, France

For the development of electronics down to atomic scale, it is of fundamental importance to build atomic-size interconnections in a planar geometry and to be able to controllably switch between different connection paths. Dangling bond wires build on the H:Si(100) are presently intensively investigated as promising candidates to build such interconnections. In this frame, we have investigated by scanning tunneling microscopy (STM) at low temperature Acetylbiphenyl molecules on the Si(100) surface. STM images show that the molecules adsorb along the dangling bond rows of the silicon. By applying voltage pulses with the STM tip, we demonstrate that single Acetylbiphenyl molecules can be reversibly switched between two different configurations. The experiment shows that Acetylbiphenyl is a suitable molecule to be used as molecular latch on a dangling bond based atomic scale circuit.

O 17.6 Mon 17:15 PHY C 213

**Initial-stage oxidation products on Si(111)-(7x7) in AFM and STM** — JO ONODA<sup>1</sup>, ●MARTIN ONDRACEK<sup>2</sup>, AYHAN YURTSEVER<sup>3</sup>, PAVEL JELINEK<sup>1,2</sup>, and YOSHIKI SUGIMOTO<sup>1</sup> — <sup>1</sup>Graduate School of Engineering, Osaka University, Suita, Osaka, Japan — <sup>2</sup>Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — <sup>3</sup>The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka, Japan

Studying the defects that form on a silicon surface in the initial stages of oxidation is important from the technological point of view and resolving the existing controversies regarding the structure of these defects can also contribute to better understanding the experimental techniques that were used in the studies. We investigated structures that appear in the initial oxidation stage of the Si(111)-(7x7) surface using the combined techniques of non-contact atomic force microscopy (AFM) and scanning tunneling microscopy (STM). We identified the defects resulting from initial oxidation as the *ins*×1 and *ins*×2 structures (1 or 2 oxygen atoms in backbonds of Si adatom) and the secondary oxidation product as the *ad-ins*×3 structure (3 oxygen atoms in the backbonds and 1 on top). We excluded the presence of adsorbed O<sub>2</sub> molecules on the surface. We used *ab initio* simulations with a diverse range of tip models to interpret the experimental data and to clarify the mechanisms that lead to the observed forces and tunneling currents.

O 17.7 Mon 17:30 PHY C 213

**In situ study of water adsorption on InP(100) surfaces** — ●MATTHIAS M. MAY<sup>1,2</sup>, HANS-JOACHIM LEWERENZ<sup>1,3</sup>, and THOMAS HANNAPPEL<sup>1,4</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Institute of Solar Fuels — <sup>2</sup>Humboldt-Universität zu Berlin, Institut für Physik — <sup>3</sup>California Institute of Technology, Pasadena, USA — <sup>4</sup>TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik

Photoelectrochemical water splitting with semiconductors promises to harvest solar energy directly and efficiently in the form of chemical energy. The most critical part of potential devices is the solid-electrolyte interface, which has to enable efficient charge-transfer and simultaneously block corrosion.

III-V semiconductors such as GaP or InP are an interesting light absorber material class, but their surface has to be designed appropriately for solar water splitting applications.[1] We perform water (oxygen) adsorption experiments on atomically well-defined InP(100) surfaces prepared by metal-organic vapour phase epitaxy. Monitoring the adsorbate-induced surface modifications of different surface reconstructions with reflection anisotropy spectroscopy and photoelectron spectroscopy, we aim to develop criteria for the design of III-V electrode surfaces.[2] We find that In-rich,  $(2 \times 4)$  reconstructed and  $p(2 \times 2)/c(4 \times 2)$  reconstructed, P-rich surfaces exhibit a distinctly different initial interaction with the adsorbates, which could explain why In-rich InP(100) photocathodes perform so well.

[1] Hannappel et al., in *Photoelectrochemical Water Splitting*, RSC Publishing (2013). [2] May et al., *New J. Phys.* **15**:103003 (2013).

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**Frustrated self-assembly of shape-persistent star molecules on HOPG** — ●STEFAN-S. JESTER, EVA SIGMUND, LISA M. RÖCK, and SIGURD HÖGER — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Star-shaped organic molecules with a rigid backbone and flexible side chains adsorb at the solution/solid interface to form self-assembled 2D nanopatterns. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures and thus an insight on the driving forces of their formation. We investigate the role of alkoxy side chain length on the adsorption patterns: Different dense and porous adsorbate patterns are observed, and for chain length  $n = 12$ , frustrated self-assembly leads to hierarchically organized superstructures. Up to 10 molecules form triangular aggregates which pack densely into hexagonal patterns with very large (15.5 nm) lattice constants. [1] S.-S. Jester, E. Sigmund, L. M. Röck, S. Höger *Angew. Chem. Int. Ed.* **2012**, *51*, 8555.

O 17.9 Mon 18:00 PHY C 213

**Ultra-thin ZnO on Metal Substrates as ZnO Surface Model** — ●BJOERN BIENIEK, OLIVER T. HOFMANN, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz Haber Institut der MPG, 14195 Berlin

In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO can be used as model systems. However, it is not clear to what degree the ZnO films resemble the surfaces of ZnO or whether they exhibit significantly different properties. We investigate the structure of ultra-thin ZnO films (1 to 4 layers) on the (111) surfaces of Ag, Cu, Pd, and Pt by means of density-functional theory. The free-standing ZnO monolayer adopts an  $\alpha$ -BN structure. This structure prevails on the metal substrates, and we obtain coincidence structures in good agreement with experiment [1, 2, 3]. Thicker ZnO layers adopt a wurtzite structure. The films exhibit a large random corrugation, which can be regularized by hydrogen adsorption. A hydrogen overlayer with 50% coverage is formed at chemical potentials that range from low vacuum to ultra-high vacuum  $H_2$  pressures. For the Ag substrate both  $\alpha$ -BN and wurtzite ZnO films are accessible in this pressure range, while for Cu wurtzite films are favoured. The surface structure and the density of states of these hydrogen passivated ZnO thin films agree well with those of the bulk ZnO(0001)- $2 \times 1$ -H surface. [1] C. Tusche *et al.* PRL **99**, 026102 (2007) [2] Y. Martynova *et al.*, J. Cat., **301**, 227-223 (2013) [3] G. Weirum *et al.* J. Phys. Chem. C, **114** (2010)

O 17.10 Mon 18:15 PHY C 213

**A photoelectron diffraction study of the Fe/GaAs(4x2)-interface** — ●DOMINIQUE HANDSCHAK, FRANK SCHÖNBOHM, TOBIAS LÜHR, CHRISTOPH KEUTNER, ULF BERGES, and CARSTEN WESTPHAL — Exp. Physik 1/DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

In this study we investigate a system of a  $(4 \times 2)$ -reconstructed GaAs(001) substrate with an Fe adsorbate. This system is applied in the field of spintronics, which use the GMR (giant magnetoresistance) effect. Especially the interface between these two layers has a strong influence on the efficiency of the effect. The method of x-ray photoelectron diffraction (XPD) is an excellent tool for investigating this system, because it is chemical and interface sensitive. The angle-resolved measurement yield structural information due to scattering and diffraction effects of the photoelectron. The GaAs substrate is found in the well ordered  $(4 \times 2)$ -reconstructed structure. XPD pattern of Ga 3d and As 3d reveal that the reconstruction is not lifted due to the Fe deposition. The Fe/GaAs interface is formed by a pyramid-like structure of the iron layers. The strongest lateral shift is found in the first Fe-monolayer with regard to the GaAs substrate and decreases evenly to zero with every additional monolayer towards the surface. Thereby the topmost layers are well bcc-ordered with the Fe-lattice constant of  $a(\text{Fe}) = 2.866 \text{ \AA}$ .

O 17.11 Mon 18:30 PHY C 213

**Epitaxial growth of the topological insulator  $\text{Bi}_2\text{Se}_3$  on Si(111): Growth mode, lattice parameter, and strain state** — ●M. VYSHNEPOLSKY<sup>1,2</sup>, C. KLEIN<sup>1</sup>, A. HANISCH-BLICHARSKI<sup>1</sup>, and M. HORN-VON HOEGEN<sup>1</sup> — <sup>1</sup>Department of Physics, Universität Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany — <sup>2</sup>Present address: Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The epitaxial growth of  $\text{Bi}_2\text{Se}_3$  films on Si(111), prepared by co-deposition of selenium (Se) and bismuth (Bi) at 200-250°C, was studied by in-situ high resolution spot profile analysis low energy electron diffraction (SPA-LEED), ex-situ atomic force microscopy (AFM) and x-ray diffraction (XRD). The first  $\text{Bi}_2\text{Se}_3$  layer grows as complete quintuple layer and covers the Si substrate before the next layer nucleates. Its lateral lattice parameter is increased by 1% compared with the value of  $a_{||} = 4.136 \text{ \AA}$  for a 6-nm-thick film. With increasing film thickness, a continuous change of the lattice parameter is observed to an asymptotic value of  $a_{||,\infty} = 4.134 \text{ \AA}$ , which is explained by a van der Waals-like bonding between the  $\text{Bi}_2\text{Se}_3$  film and the Si substrate [1]. The films are atomically smooth without small angle mosaics or small angle rotational domains. The precise determination of thus determined lateral and the vertical lattice parameter of  $c = 28.65 \text{ \AA}$  reveal that films grown at higher temperature exhibit smaller lattice parameters which is attributed to an increased density of Se vacancies. Bulk defects in the film cause a parabolic increase of the width of the diffraction peaks in XRD. [1] M. Vyshnepolsky *et al.*, Appl. Phys. Lett. **103**, 111909 (2013)

O 17.12 Mon 18:45 PHY C 213

**STM study of thin terbium-silicide layers on Si(111)** — ●MARTIN FRANZ, ROBERT KOHLHAAS, and MARIO DÄHNE — Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany

The growth of rare earth silicides on silicon surfaces leads to the formation of very interesting structures such as self-organized metallic nanowires on the Si(001) and the Si(557) surface [1]. On Si(111), the formation of nanoclusters is observed at very low coverages [2], while at higher coverages two- and three-dimensional layers form [3].

In this work the growth and the atomic structure of Tb silicide films on Si(111) in the coverage regime from submonolayers to several monolayers were studied using scanning tunneling microscopy. In this regime various superstructures were identified. At submonolayer coverages first nanoclusters form before a  $2\sqrt{3} \times 2\sqrt{3}$  superstructure is observed. For Tb coverages exceeding 0.5 ML the  $1 \times 1$  superstructure of the  $\text{TbSi}_2$  monolayer appears additionally, and at coverages exceeding one monolayer the three-dimensional  $\text{Tb}_3\text{Si}_5$ -multilayer is observed. Furthermore, elongated islands showing a  $2 \times 1$  reconstruction on top are found.

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[1] M. Dähne and M. Wanke, J. Phys.: Condens. Matter **25**, 014012 (2013).

[2] M. Franz *et al.*, Surf. Sci. **609**, 215 (2013).

[3] I. Engelhardt *et al.*, Surf. Sci. **600**, 755 (2006).

O 17.13 Mon 19:00 PHY C 213

**Surface characterization of arsenic terminated Si(111) substrates prepared in MOVPE for III-V nanowire solar cells** — ●WEIHONG ZHAO<sup>1</sup>, AGNIESZKA PASZUK<sup>1</sup>, MATTHIAS STEIDL<sup>1</sup>, SEBASTIAN BRÜCKNER<sup>1</sup>, OLIVER SUPPLIE<sup>1</sup>, ANJA DOBRICH<sup>2</sup>, PETER KLEINSCHMIDT<sup>1,3</sup>, and THOMAS HANNAPPEL<sup>1,2,3</sup> — <sup>1</sup>Technische Uni-

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III-V nanowires grown on Si(111) substrates by metal-organic vapor phase epitaxy (MOVPE) enable a promising new solar cell concept meeting the demands of high-quality-low-cost photovoltaics. GaP buffer layers grown on Si(111) substrates represent suitable quasi-substrates since GaP is almost lattice-matched to Si. Apparently,

preparation of atomically flat Si (111) surfaces is an essential step for adjacent GaP hetero-epitaxy. However, little is known about preparation and surface properties of Si(111) surfaces in MOVPE with H<sub>2</sub> ambient. A contamination-free transfer system enabled us to study the MOVPE prepared surfaces with numerous UHV based surface science tools. A dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces. Varying the Si(111) surface preparation could control the polarity of the adjacent GaP layer. With the confirmation of FTIR, STM and LEED, we successfully established a controlled arsenic termination procedure during the epitaxy.