O 30: Semiconductor Surfaces

Time: Tuesday 10:30–12:45 Location: S053

Topical Talk O 30.1 Tue 10:30 S053

Surface Phase Transitions in Atomistic Detail and with Femtosecond Resolution — •Wolf Gero Schmidt — Universität Paderborn

Ab initio molecular dynamics on ground and excited-state potential energy surfaces may be used to gain deep insight in the driving forces and mechanisms of surface phase transitions and can greatly assist the interpretation of experimental data. This is illustrated in my talk using two prominent examples: (i) Photoholes localized at the Brillouin zone boundary of the In/Si(111)(8x2) surface are shown to drive an ultrafast (8x2) $\longrightarrow$ (4x1) phase change that is accompanied by an insulator-metal transition [1,2]. (ii) Thermal excitation of the Au/Si(553)(1x6) surface leads to soft Au chain vibrations that reduce transiently the Au electron affinity, which lowers the barrier for a $sp^2 + p \longrightarrow sp^3$ hybridization change of Si step edge atoms. This leads eventually to an order-disorder phase transition and the formation of a two-dimensional spin liquid [3].

[1] T Frigge et al., Nature 544, 207 (2017).
[2] CW Nicholson et al., Science 362, 821 (2018).
[3] C Braun et al., PRL 124, 146802 (2020).

O 30.2 Tue 11:00 S053

Dimer coupling energies of the Si(001) surface examined by SPA-LEED — •Christian Brand, Giriraj Jnawali, Jonas Fortmann, Mohammad Tajik, Alfred Hucht, Peter Kratzer, Hamid Mehdipour, Björn Sothmann, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

Though the surface of Si(001) belongs to the most famous in the world still some of its properties and phenomena are unrevealed. Si(001) exhibits buckled dimers in the topmost layer, arranged in dimer rows, and thus forming a (2×1) reconstruction at room temperature. Upon cooling the structure undergoes an disorder-order transition to the $c(4\times2)$ reconstructed ground state. High-resolution SPA-LEED (Spot Profile Analyzing - Low Energy Electron Diffraction) was used to quantify the structural change along the transition upon heating from low to high temperatures. Rapid cooling in the regime of critical slowing down formed a so-called domain structure with typical size of ~ 14 nm. The data is analyzed in the framework of the anisotropic 2D Ising model and complemented by density functional theory calculations. We determined a phase transition temperature of $T_c = 190.6$ K, critical exponents β, γ, and ν of the Ising model and the coupling constants $J_\parallel = (-24.9\pm1.3)$ meV and $J_\perp = (-0.8\pm0.1)$ meV of the Si dimers by solving Onsager's equation and evaluating the correlation length ratio of the two directions.

O 30.3 Tue 11:15 S053

Reduced contact resistance to gallium nitride by plasma-assisted atomic layer deposition — •Maximilian Christis — Walter Schottky Institut, Technische Universität München

Gallium nitride is an industrially relevant III-V semiconductor that draws significant attention for a range of both established and emerging applications, including for light emitting diodes, power electronics, photocatalysis, and sensing. Established contacting schemes for GaN rely on wet-chemical surface preparations and post-metallization high-temperature (≥ 600°C) annealing processes, which complicate fabrication and may adversely affect device performance. Here, we present a low-temperature gas-phase process (200 °C) that reduces the Schottky barrier height and the contact resistivity at the GaN/metal interface. In particular, we employ H2 plasma-enhanced atomic layer deposition (ALD) that creates an ultimately thin, homogeneous AlOx monolayer using oxygen from the native gallium oxide as oxidant. This AlOx coating reduces the surface band bending and results in Ohmic current-voltage characteristics for n-doped GaN contacted by Ti metal. In ongoing work, we are also exploring how the monolayer AlOx ALD approach can be applied to improve contacts to p-doped GaN in combination with high work function metals. Among the various applications that could benefit from this low thermal budget contact fabrication strategy, we are investigating how such metal/semiconductor structures impact the electrocatalytic performance of n-GaN/Pt cathodes for water splitting.

O 30.4 Tue 11:30 S053

Distance dependance and lateral change of electrostatic forces between Pb-islands and wetting layer on Pb/Si(111)-(7x7) — Ben Lottenburger, •Paul Philip Schmidt, Daniel Rothhardt, Manuel Schulze, and Regina Hoffmann-Vogel — Universität Potsdam, Institut für Physik und Astronomie, Experimentelle Physik kondensierter Materie

Pb islands on silicon show a wide range of interesting properties, such as explosive island growth [1,2]. Previous work has already been able to explain some features, such as the unusual height distribution of the islands[3,4]. To understand this system in more detail, we have investigated the differences in the electrostatic interaction between the tip and the Pb islands on one side and the Pb-containing wetting layer on the other side. We have used scanning force microscopy in the non-contact frequency modulation mode and bias distance measurements in ultrahigh vacuum at ˜120K. The Si has been cleaned by direct current heating. Subsequently, Pb has been vapor deposited. The Frequency shift as a function of tip-sample distance has been measured on both Pb islands and the wetting layer. The differences in force and work function between have been investigated both. [1] Hershberger et al, PRL 113, 236101 (2014). [2] Huang et al, PRL 108, 026101 (2012). [3] Hupalo et al, PRB 65, 115406 (2001). [4] Späth et al, PRL 124, 016101 (2020)

O 30.5 Tue 11:45 S053

Growth of well-ordered K3C60 thin films on Bi2Se3 — •Michael Herb and Isabella Gierz — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

The molecular solid K3C60 is a BCS-type superconductor with a critical temperature of 20K [1]. More intriguingly, K3C60 powder exposed to strong mid-infrared driving fields exhibits the optical properties of a transient superconductor [2] possibly up to room temperature [3] and with nanosecond lifetimes [4]. The microscopic mechanism behind these observations remains poorly understood. We want to shed light onto this issue by measuring the transient band structure of driven K3C60 using time- and angle-resolved photoemission spectroscopy (tr-ARPES). These experiments cannot be performed on the originally used K3C60 powder as they require large, well-ordered K3C60 single crystals. Therefore, we investigate the growth of K3C60 thin films on different substrates using low-energy electron diffraction (LEED) and ultraviolet photoemission spectroscopy (UPS). We provide evidence for well-ordered growth on Bi2Se3, enabling future tr-ARPES studies on the material.

O 30.6 Tue 12:00 S053

Structure and origin of antiphase domains and related defects in thin GaP epilayers on As-modified Si(100) — •Franz Niklas Knoop[1], Agnieszka Paszuk[2], Benjamin Borkenhagen[1,3], Oliver Supplie[2,4], Manali Nandy[2], Gerhard Lilienkamp[1], Peter Kleinschmidt[2], Thomas Hannappel[2], and Winfried Daum[1] — [1]IEPT, TU Clausthal — [2]Institute of Physics, TU Ilmenau — [3]Fallstein Gymnasium Osterwieck — [4]Physics Department, HU Berlin

The deposition of low-defect III-V-layers on Si(100) is impaired by the formation of antiphase domains (APDs) in the epilayer. We study the origin and formation of APDs and related defects in thin GaP buffer layers on nearly-single-domain, As-modified Si(100) substrates. By comparing results obtained by low energy electron microscopy (LEEM), AFM, STM and scanning Auger electron microscopy, we identify two different types of APD-related defects in the GaP layer and trace these defects back to residual minority (2x1) domains of the Si substrate. GaP growth on minority domain terraces with widths in the range 40-100 nm gives rise to APDs of comparable lateral dimensions. The observation of trench-like defects in the epilayer extending down to the surface of the substrate indicates that homogeneous layer-by-layer growth of GaP is impeded on narrow terraces (<20 nm) of the (2x1)-reconstructed minority domain of the substrate. We propose that insufficient nucleation of GaP on these terraces leads to the formation of trenches, while on wider minority terraces APDs are formed by 3D-like growth.

O 30.7 Tue 12:15 S053

Adsorption of CO and CO_2 on the Y-stabilized ZrO_2(100)

surface — •Shuang Chen, Xiaojuan Yu, Eric Sauter, Alexei Nefedov, Stefan Heissler, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

Understanding the stabilization mechanism of the Y- stabilized zirconia (YSZ) (100) surface has triggered a great debate over the past 30 years. In this work, we focused on a fundamental study on the surface structure of YSZ(100) by polarization-resolved infrared reflection absorption spectroscopy (IRRAS), in combination with grazing-emission X-ray photoelectron spectroscopy (XPS). The combined IR and XPS results allowed to gain detailed insight into the adsorption of carbon monoxide and carbon dioxide on YSZ(100) over a large coverage range from submonolayer to multilayers. The experimental data were further analyzed based on the density functional theory (DFT) calculations.

O 30.8 Tue 12:30 S053

Starting from a Fixed Geometry: Real-Time XPS Investigation of a Surface Reaction with Controlled Molecular Configurations — •Timo Glaser[1], Christian Länger[1], Julian Heep[1], Jannick Meinecke[2], Mathieu Silly[3], Ulrich Koert[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik und Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [3]Synchrotron SOLEIL, 91192 Gif sur Yvette, France

The relative orientation between two reactants can have a major influence on the reactivity and on the products of a chemical reaction. In gas-surface chemistry with well-defined single-crystal surfaces, the orientation and configuration of one reactant is fixed by the surface, but still the reacting gas molecules can impact on the surface in all possible orientations. Here we show how to constrain the relative orientation of both reactants by attaching a reactive group (ether) via a linker (cyclooctyne) on a single crystal surface. This keeps the reacting group in a highly-constrained configuration close to the surface. We demonstrate this concept for ether cleavage on silicon (001), the surface analogue of an S_N2 reaction. The kinetics of the further reaction of the ether group with the silicon surface is studied by means of real-time XPS using synchrotron radiation. We find both a low-energy barrier and a low prefactor, which we discuss in terms of the constrained starting configuration of the ether group. As this configuration represents the starting point of a low-energy pathway, it gives direct experimental access to the underlying reaction mechanism.