O 74: Poster Metal and Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Wednesday 18:00–20:00 Location: P2

O 74.1 Wed 18:00 P2

Lithium adsorption on Cu(111) for anodeless lithium ion batteries — •Darius Hübner — Universität Ulm, Institut für theoretische Chemie, Oberberghof 7, 89081 Ulm

Anodeless batteries in which the anode is created upon the first charging are of strong current interest as they avoid processing and cost concerns as well as lead to an increased safety. In order to contribute to the understanding of the the viability of copper charge collectors in anodeless Lithium ion batteries, we studied the deposition of lithium on a Cu(111) substrate using periodic density functional theory calculations.

We find that the lattice mismatch between lithium and copper leads to the formation of a fcc lithium structure with fewer atoms per layer than the copper substrate. Additionally, this lithium structure shows remarkably lower surface diffusion barriers compared to a standard bcc lithium surface. As an enhanced surface mobility is supposed to suppress dendrite growth, this suggests a reduced formation of dendrites in the initial steps of the anode formation.

O 74.2 Wed 18:00 P2

Spin-State Switching of Indium-Pthalocyanine on Pb(100) — Niklas Ide, Arnab Banerjee, •Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Kiel, Deutschland

Indium(III) phthalocyanine chloride, deposited on Pb(100), is investigated using a scanning tunnelling microscope at cryogenic temperatures. The chloride ions dissociate, leaving behind indium phthalocyanine (InPc), which is observed in two distinct configurations: the metal ion oriented either towards (↓) or away from (↑) the substrate. The study reveals isolated molecules and islands which exhibit a $\sqrt{65} \times \sqrt{65}, \mathrm{R} \pm 30^\circ$ superstructure, characterized by a unit cell containing four inequivalent molecules, one in the InPc↑ state and three in the InPc↓ state at different sites. Variations in the conductance spectra of the lowest unoccupied molecular orbital are observed, depending on the adsorption sites and azimuthal orientations of the complexes. Notably, only the InPc↑ molecules within the islands exhibit Shiba states, signifying the presence of a localized spin. Electron extraction allows for the conversion of both isolated complexes and molecules in islands from the InPc↑ to InPc↓ state. This transition is accompanied by a change in their spin state, as evidenced by the disappearance of the Shiba states.

O 74.3 Wed 18:00 P2

On-surface fabrication of cesium tin halide nanostructures deviating from the perovskite $\mathbf{ABX_3}$ structure — Madad Abbasli, Dina Wilks, Carsten Busse, and •Robin Ohmann — University of Siegen, Siegen, Germany

We demonstrate that evaporation of the precursor molecules CsBr and $SnBr_2$ onto an atomically clean gold surface not only leads to the expected stoichiometric $CsSnBr_3$ structure, but also yields a range of other distinct structures. The experiments were conducted in ultra-high vacuum and investigated by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). When deposited on Au(111), we observe a flower structure with hexagonal symmetry tentatively assigned to Cs_2SnBr_6, a ladder structure, a stripe pattern, a honeycomb structure, and a large square structure. The emergence of these structures depends on surface coverage - either submonolayer or multiple monolayers - and on the relative proportions of the two precursor molecules. In contrast, on Au(100) these structures are not observed, suggesting that the interface is playing a crucial role. The structures are compared with those formed by depositing either CsBr or $SnBr_2$ on Au(111). While a honeycomb structure can also be formed with $SnBr_2$ alone, the other structures bear no resemblence to either pure component. Thus, they are assigned to structures involving specific ratios of Cs, Sn and Br deviating from the standard ABX_3 structure. The structural variability underscores the importance of precise deposition conditions and interface selection in the fabrication of perovskite materials.

O 74.4 Wed 18:00 P2

Band alignment at InP/$\mathbf{TiO_2}$ interfaces from density-functional theory — Isaac Azahel Ruiz Alvarado[1], Christian Dressler[2], and •Wolf Gero Schmidt[1] — [1]Universität Paderborn, Germany — [2]TU Ilmenau, Germany

The natural band alignments between indium phosphide and the titanium dioxide polymorphs rutile, anatase and brookite as well as amorphous titania are calculated from the branch point energies of the respective materials. Type-I alignment is predicted, irrespective of the type of titania interfacing with InP. The actual band offset may differ, however, from the natural band alignment depending on the microscopic structure of the interface. Supercell calculations are performed for the interface between P-rich InP(001) surface and amorphous titania thin films. The valence band offset increases substantially compared to the natural band alignment, while the conduction band offset is reduced, resulting in nearly aligned conduction bands. Depending on the interface properties, both type-I and type-II interfaces are observed in the simulations. The results show that with careful control of the microscopic interface structure and the atomic order of the titania film a very wide range of band alignments becomes accessible.

O 74.5 Wed 18:00 P2

Structure of tellurium phases on Ni(111) and Ni(111)-(1 × 1)-2C (graphene) — •Alexander Wegerich, Gwyn R. Thomas, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Using quantitative LEED-IV analyses, STM and DFT, we examine Te on Ni(111) to understand the interactions and emerging structures. For $\Theta_{\mathrm{Te}} = 0.33\,\mathrm{ML}$ a $\left(3 \times \sqrt{3}\right)_{\mathrm{rect}}$-2Te superstructure is identified. For $\Theta_{\mathrm{Te}} = 0.40\,\mathrm{ML}$ this changes to a $\left(5 \times \sqrt{3}\right)_{\mathrm{rect}}$-4Te superstructure. As LEED-IV analyses reveal, these superstructures are identical to those that can be observed for the Te/Cu(111) system [1], albeit with different stacking and reduced Te-Metal bond length.

In addition, we also present our first results regarding Te on the well-known Ni(111)-(1 × 1)-2C (graphene) structure [2, 3]. The presence of Te reduces the thermal stability of the graphene on Ni(111). At annealing temperatures above 570 K the graphene begins to dissolve and structures for the Te/Ni(111) system emerge. In the course of our studies, we also determined the Ni(111)-(1 × 1)-2C (graphene) structure by LEED-IV analysis and obtained picometer accuracy by virtue of a low Pendry R-factor of R = 0.10.

[1] T. Kißlinger et al., Phys. Rev. B **104**, 155426 (2021)
[2] J. Lahiri et al., New J. Phys. **13**, 25001 (2011)
[3] Y. Gamo et al., Surface Science **374**, 61-64 (1997)

O 74.6 Wed 18:00 P2

An atomistic analysis of the carpet growth of KCl across Ag(111) step edges — •Anna Juliana Kny[1], Adam Sweetman[2], and Moritz Sokolowski[1] — [1]Clausius Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [2]School of Physics and Astronomy, University of Leeds, UK

Thin alkali halide (AH) films of 2-3 atomic layer thickness, grown on metal substrates, are widely used for studying decoupled molecules by scanning tunneling microscopy. For many combinations of AH and metal surface, a continuous growth of the AH layer across step edges of the substrate is observed, which is called carpet growth. Here, we report a first atomistic analysis of the layer distortions in the carpet growth region of KCl layers at Ag(111) step edges.[1] STM measurements were performed at room temperature and with Cl anions decorated W-tips which yield a high atomic resolution. We find that the AH layer distorts locally and in a non-uniform manner within a short lateral distance of four unit cells, when it grows across the Ag step. Furthermore, we find that the Ag(111) surface adapts to the AH layer, as the carpet growth is accompanied by a straightening of the Ag steps along the <110> direction and a splitting of higher Ag steps into multiple mono-atomic ones. These mono-atomic Ag steps allow for the carpet growth if the distance between them is larger than 13 Å, while a carpet growth across higher or closer Ag steps was not observed.[1]

Supported by the DFG through the research training group 2591, the Royal Society, and the ERC.

[1] A.J. Kny et al., J. Phys. Chem. Letters (2024), under revision.

O 74.7 Wed 18:00 P2

Epitaxial growth of bismuthene-based transition metal compounds — •Holger Diehm, Bing Liu, Simon Moser, Jörg Schäfer, and Ralph Claessen — Würzburg-Dresden Cluster of Excellence ct.qmat and Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany

This work explores the fabrication of alloy phases between bismuthene - a fully planar honeycomb structure of bismuth atoms on a silicon carbide (0001) substrate - and 3d transition metals (TMs).

Bismuthene is a promising candidate for quantum spin Hall (QSH) effect at room-temperature [1] that shows interacting 1D spin-polarized electrons in a metallic edge channel [2]. While topological protection of the edge channels can be lifted by edge coupling [3], interfacing it with ordered TM-rich phases could locally introduce magnetic moments. This provides a novel platform to explore the effects of broken time-reversal symmetry and its potential impact on the topological phase.

Our work focusses on epitaxially grown bismuthene, garnished with manganese, chromium or cobalt. While bismuthene on silicon carbide shows a rt(3) x rt(3) surface reconstruction in low energy electron diffraction (LEED), incorporation of transition metals causes an additional 3 x 3 phase. In addition, scanning tunneling microscopy (STM) is used to analyze the surface structure on an atomic level.

This study paves the way for both fundamental research and application-oriented development in spintronics.

[1] Science 357, 287 (2017); [2] Nat. Phys. 16, 47 (2020); [3] Nat. Commun. 13, 3480 (2022).