O 43: Poster: Semiconductor Substrates - Adsorption

Time: Tuesday 18:15–20:30 Location: Poster A

O 43.1 Tue 18:15 Poster A

Preparation and characterization of monolayer Thallium films on Si(110) — •Pascal Grenz[1], Philipp Eickholt[1], Anke Beck-Schmidt[1], Koji Miyamoto[2], Kazuyuki Sakamoto[3], and Markus Donath[1] — [1]Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchroton Radiation Centre, Japan — [3]Department of Nanomaterials Science, Japan

Surface states of thin Thallium-layers on Sillicon are strongly influenced by spin-orbit-interaction (SOI), leading to peculiar spin textures. One example is the Tl/Si(110)-(1x1) surface with C_1h symmetry a non vortical Rashba spin structure in the occupied states has been observed[1]. For the unoccupied states a large spin splitting along $\bar{\Gamma}\bar{X}$ with an out-of-plane spin polarization is predicted. A well prepared surface is cruical for the investigation of the unoccupied electronic structure with spin- and angle-resolved inverse photoemission (SRIPE). In this contribution, we present different preparation methods and discuss the influence of those on the crystallographic and electronic surface structure.

[1] E. Annese *et al.*, Phys. Rev. Lett. **117**, 016803 (2016)

O 43.2 Tue 18:15 Poster A

Preparation and Characterization of a Monolayer Thallium on Si(110) — •Pascal Grenz[1], Philipp Eickholt[1], Anke Beck-Schmidt[1], Koji Miyamoto[2], Kazuyuki Sakamoto[3], and Markus Donath[1] — [1]Instiute of Physics, Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchroton Radiation Centre, Japan — [3]Department of Nanomaterials Science, Chiba University, Japan

Surface states of thin thallium-layers on silicon are strongly influenced by spin-orbit-interaction (SOI) leading to peculiar spin textures. One example is the Tl/Si(110)-(1x1) surface, with C_{1h} symmetry, where a non vortical Rashba spin structure in the occupied electronic states has been observed [1]. For the unoccupied states a large spin splitting along $\bar{\Gamma}\bar{X}$ with an out-of-plane spin polarization is predicted.

A well prepared surface is cruical for the investigation of the unoccupied electronic structure with spin- and angle-resolved inverse photoemission (SRIPE). In this contribution, we present different preparation methods and discuss the influence of those on the crystallographic and electronic surface structure.

[1] E. Annese *et al.*, Phys. Rev. Lett. **117**, 016803 (2016)

O 43.3 Tue 18:15 Poster A

Preparation and Characterization of a Monolayer Thallium on Si(110) — •Pascal Grenz[1], Philipp Eickholt[1], Anke Beck-Schmidt[1], Koji Miyamoto[2], Kazuyuki Sakamoto[3], and Markus Donath[1] — [1]Instiute of Physics, Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchroton Radiation Centre, Japan — [3]Department of Nanomaterials Science, Chiba University, Japan

Surface states of thin thallium layers on Si(111) are strongly influenced by spin-orbit-interaction leading to peculiar spin textures [1]. A further interesting example is the Tl/Si(110)-(1x1) surface, where a nonvortical Rashba spin structure was observed in the occupied electronic states at **k**-points with C_{1h} symmetry [2]. For the unoccupied states, a large spin splitting is predicted along $\bar{\Gamma}\bar{X}$ with an out-of-plane spin polarization. A well-prepared surface is crucial for the investigation of the surface bands. In this contribution, we report on different preparation methods and discuss their influence on the crystallographic and electronic surface structure.

[1] S.D. Stolwijk *et al.*, Phys. Rev. Materials **1**, 064604 (2017)
[2] E. Annese *et al.*, Phys. Rev. Lett. **117**, 016803 (2016)

O 43.4 Tue 18:15 Poster A

Hexacene generated by deoxygenation on passivated silicon — •Frank Eisenhut[1], Justus Krüger[1], Dmitry Skidin[1], Seddigheh Nikipar[1], José M. Alonso[2], Enrique Guitián[2], Dolores Pérez[2], Dmitry A. Ryndyk[1,3], Diego Peña[2], Gianaurelio Cuniberti[1], and Francesca Moresco[1] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, 01069 Dresden, Germany — [2]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, 15782-Santiago de Compostela, Spain — [3]Bremen Center for Computational Materials Science (BCCMS), Universität Bremen, 28359 Bremen, Germany

On-surface synthesis represents a successful strategy to form designed molecular structures on an ultra-clean metal substrate. On non-metallic substrates, on the other hand, on-surface synthesis would allow the electrical decoupling of the resulting molecule from the surface, making possible the application of this powerful synthesis approach to electronics and spintronics. Here, we demonstrate that the on-surface generation of hexacene by surface-assisted reduction, already observed on Au(111), can be performed on the H-passivated Si(001) surface. The reaction, observed by scanning tunneling microscopy, is probably driven by the formation of Si-O complexes on the dangling bond defects. Supported by DFT calculations, we investigate the interaction of hexacene with the passivated silicon surface, and with single silicon dangling bonds.

O 43.5 Tue 18:15 Poster A

Cobalt-Pyrphyrin on Cu_2O(111): A promising system for photocatalytic water splitting — •Lisa Grad, Fabio Cossalter, Wolf-D. Zabka, Stephan Schnidrig, Benjamin Probst, Roger Alberto, Zbynek Novotny, Matthias Hengsberger, and Jürg Osterwalder — University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Photocatalytic water splitting presents a sustainable way to store solar energy in the form of chemical bonds. For large-scale use, the combination of molecular catalysts supported on abundant substrates is a viable approach. We investigate one such model system: Cobalt-Pyrphyrin (CoPyr) [1] adsorbed on the Cu_2O(111) surface.

Cu_2O(111) is a p-type semiconductor with downward band bending. This property is conserved after adsorbing a layer of CoPyr [2]. The related electrical field supports charge separation by accelerating excited electrons from the Cu_2O to the interface from where they can relax to unoccupied states of CoPyr. There are two different reconstructions of the Cu_2O(111) surface observed: (1x1) and $(\sqrt{3}\times\sqrt{3})$R30°. The structure and stoichiometry of these different surface reconstructions and their influence on electrical properties are still not fully understood, but are expected to influence the surface band bending and charge carrier dynamics. Our current effort centers on investigation of these properties using angle-resolved X-ray photoelectron spectroscopy and time-resolved two-photon photoemission.

[1] Joliat et al., Dalton Transactions 2016 45(4), 1737-1745
[2] Leuenberger et al., Nano Letters 2017 17 (11), 6620-6625

O 43.6 Tue 18:15 Poster A

The adsorption and dimererisation of Co-Salen molecules on NaCl(100) — •Rasmus Jakobsen — University College London, London, United Kingdom

In this work, we investigate the interactions of magnetic molecules with bulk insulating surfaces. These systems are of interest due to their potential uses in fields such as molecular electronics and magnetism. In particular the self-assembly of the transition metal-organic complex of Co-Salen ((Co(C16H14N2O2)) with the NaCl(100) surface, is investigated. Experimentally, this have been measured using non-contact atomic force microscopy (NCAFM) by our collaborators A. Schwarz at University of Hamburg. Co-Salen is deposited and adsorbed as individual molecules onto NaCl(100). However, room temperature measurements show two different morphologies consisting of Co-Salen dimer building blocks; a nanowire and nanocrystallite structure. How these structures form and the reasons for their relative stabilities is unknown. In previous studies, Density Functional Theory (DFT) was used to provide an unambiguous determination of the adsorption geometry of a single molecule. To continue this work, the self-assembly process has been investigated using a combined approach of DFT, semi empirical methods and empirical force fields, studying various aspects of the system such as the adsorption process of multiple molecules, step adhesion and dimerization of the molecule on the surface.