

O 16: Surface State Spectroscopy II

Time: Monday 15:00–18:00

Location: H4

O 16.1 Mon 15:00 H4

Unoccupied band structure of MgO/Ag(100) — ●REBECCA PÖSCHEL, GIANLUCA DI FILIPPO, ANDREJ CLASSEN, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Magnesium oxide films were prepared by evaporating magnesium on a well-defined Ag(100) single crystal kept at 440 K in $5 \cdot 10^{-7}$ mbar oxygen. Films of different thicknesses between 1 ML to 20 ML were deposited on the crystal. The samples were studied by monochromatic angle-resolved two-photon photoelectron spectroscopy (photon energies 3.05 eV - 3.38 eV and 4.56 eV - 4.71 eV) and by angle-resolved vacuum ultra-violet photoelectron spectroscopy (photon energy 21.2 eV). Due to the negative electron affinity of MgO the conduction band minimum is observed near the low-energy cut-off and the valence band maximum near the high-energy cut-off within same UPS spectrum. We determined the evolution of the band gap with increasing film thickness and had a more detailed look at the dispersion of the conduction band minimum and the valence band maximum for a 5 ML and 20 ML thick film. For films up to 10 ML we found an unoccupied surface state with a binding energy of 1.24 eV relative to vacuum level which shows a free-electron-like dispersion.

O 16.2 Mon 15:15 H4

Interfaces of h-BN on Ag(111) and Ag/Cu(111) — ●MARTIN SCHWARZ¹, MANUELA GARNICA¹, DANIELE STRADI², JOHANNES V. BARTH¹, and WILLI AUWÄRTER¹ — ¹Physik Department E20, Technische Universität München, James Franck Str. 1, 85748 Garching, Germany — ²Department of Micro- and Nanotechnology, Center for Nanostructured Graphene, Technical University of Denmark, Denmark

Silver has attracted increasing interest as a substrate for heteroepitaxial layers, since the growth of a silicene layer on its (111) face has been demonstrated [1]. We explored different synthesis methods of hexagonal boron nitride (h-BN) layers on silver substrates. Beside the direct growth of h-BN on Ag(111), Ag intercalation on the BN/Cu(111) system [2] was investigated. The quality of the resulting layers has been examined by high-resolution scanning tunneling microscopy while the electronic structure of the Ag surface upon 2D layer growth has been studied by scanning tunneling spectroscopy and first-principle calculations. We demonstrate that the adsorption of the 2D layer alters the surface potential and has an impact on the binding energy of the Shockley-state which shifts towards higher energies.

[1] Lalmi, B. et. al. Appl. Phys. Lett., 2010, 97, 223109

[2] Joshi, S. et. al. Nano Lett., 2012, 12, 5821-5828

O 16.3 Mon 15:30 H4

A XPS/XPD study of the topological insulator BiTe — ●PHILIPP ESPETER^{1,2}, SVEN DÖRING^{2,3}, MARKUS ESCHBACH³, MATTHIAS GEHLMANN^{2,3}, CHRISTOPH KEUTNER^{1,2}, CHRISTOPHER KOHLMANN¹, DOMINIQUE KRULL^{1,2}, LUKASZ PLUCINSKI³, ULF BERGES^{1,2}, CLAUS M. SCHNEIDER³, and CARSTEN WESTPHAL^{1,2} — ¹Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, D-44227 Dortmund, Germany — ²DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — ³Forschungszentrum Jülich, D-52425 Jülich

Three-dimensional topological insulators are considered being a new state of quantum matter. They show an electronic bulk band structure with an insulating gap while they also possess metallic and highly spin-polarized surface states. Since the most interesting effects occur at the surface of topological insulators, a precise knowledge of the surface morphology and structure is crucial to understand its electronic structure.

In this study, we demonstrate a surface structure investigation of the weak topological insulator Bi₁Te₁ by means of photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD). These measurements provide chemical as well as structural information of the sample surface.

The XPD pattern reveal that twelve different surface terminations are present on top of the sample. Furthermore, we monitored slight scaling effects and a shifting of individual Bi and Te layers.

O 16.4 Mon 15:45 H4

X-ray spectroscopic studies of the electronic structure of chromium based p-type transparent conducting oxides — ●EMMA NORTON^{1,2}, LEO FARRELL^{1,2}, STEPHEN CALLAGHAN¹, CORMAC MCGUINNESS¹, IGOR SHVETS^{1,2}, and KARSTEN FLEISCHER^{1,2} — ¹School of Physics, Trinity College, University of Dublin, Dublin 2, Ireland — ²Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)

The valence band structure of p-type transparent oxides - crystalline Mg_xCr_{2-x}O₃ and nanocrystalline Cu_xCrO_y - is analysed as a function of incoming photon energy. Comparisons with crystalline CuCrO₂:Mg are made, the best performing p-type transparent conducting oxide to date. The valence band of both p-type transparent conducting oxides show striking similarities to measurements on crystalline CuCrO₂ with all films showing that chromium states compose the top of the valence band, highlighting the important role of the Cr-O octahedra on the electronic structure.

O 16.5 Mon 16:00 H4

In operando strain-dependent HAXPES of VO₂ thin films on piezoelectric PMN-PT — ●ARNDT QUER¹, KERSTIN HANFF¹, MATTHIAS KALLAENE¹, ADRIAN PETRARU², LARS-PHILIP OLOFF¹, HERMANN KOHLSTEDT², and KAI ROSSNAGEL¹ — ¹Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — ²Department of Nanoelectronics, University of Kiel, 24143 Kiel, Germany

The class of transition-metal oxides provides candidate materials for the realization of so-called Mottronic devices that make use of ultrafast and energy-efficient switching between distinct states of correlated electrons.

A paradigmatic material is VO₂, which undergoes a first-order structural transition from a low-temperature monoclinic phase to a high-temperature rutile phase at a transition temperature of about 340 K and simultaneously switches from insulating to metallic behavior by a five orders of magnitude resistance jump.

Interestingly in VO₂ films, insulator-to-metal transition can be tuned to some degree.

Here we use hard x-ray photoelectron spectroscopy (HAXPES) to directly study the electronic structure changes in VO₂ films on PMN-PT substrates as a function of temperature and in situ applied lattice strain.

Our results show clear changes in shape and position of the core level induced by strain and ferroelectric influence at the device-interface of the PMN-PT substrate.

O 16.6 Mon 16:15 H4

Rashba Spin-Orbit Coupling in the Presence of Ferroelectricity: Ultrathin Bi-films on BaTiO₃ (001) — ●PETER LUTZ, TIM FIGGEMEIER, HENDRIK BENTMANN, and FRIEDRICH REINERT — Experimentelle Physik VII and Röntgen Research Center for Complex Materials (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The merging of two different material systems with specific physical properties provides a promising way to explore unique and new functionalities. In the case of ultrathin Bismuth (Bi) films on Barium Titanate (BTO) it was theoretically shown that the electric polarization of the ferroelectric substrate allows to manipulate the Rashba split Bi 6p states at the Fermi level [1]. By highly-ordered film growth we experimentally realized the formation of spin-orbit split surface states on ferroelectric BTO. The electronic structure looks similar to the one of pure Bi(111) or Bi/Si(111) but the films on BTO grow in thicknesses down to two bilayers [2]. This enables an enhanced coupling between the substrate and the Bi states. In our angle-resolved photoelectron spectroscopy (ARPES) data we investigated changes in the electronic structure of the electronic states when the ferroelectric substrate is driven through its structural phase transition [3]. Due to its capability of manipulating spin split states Bi/BTO may be regarded as a model system in realizing spintronic devices.

[1] H. Mirhosseini et al., Phys. Rev. B, 81, 073406, (2010) [2] T. Hirahara et al., Phys. Rev. Lett., 97, 146803 (2006) [3] W. Zhong et al., Phys. Rev. Lett., 73, 1861 (1994)

O 16.7 Mon 16:30 H4

Giant Circular Dichroism in Soft X-Ray Photoemission From Non-Magnetic Solids — ●O. FEDCHENKO¹, K. MEDJANIK², S. CHERNOV¹, D. KUTNYAKHOV¹, B. SCHÖNHENSE³, M. ELLGUTH¹, A. OELSNER⁴, S. DÄSTER⁵, Y. ACREMANN⁵, J. VIEFHAUS⁶, W. WURTH^{6,7}, T.R.F. PEIXOTO⁸, P. LUTZ⁸, C.-H. MIN⁸, F. REINERT⁸, J. BRAUN⁹, J. MINÁR⁹, H. EBERT⁹, H.J. ELMERS¹, and G. SCHÖNHENSE¹ — ¹Uni-Mainz — ²Max IV Lab, Lund, Sweden — ³Imperial College London, UK — ⁴Surface Concept GmbH, Mainz — ⁵ETH Zürich, Switzerland — ⁶DESY, Hamburg — ⁷CFEL, Uni-Hamburg — ⁸Uni-Würzburg — ⁹TU-München

We report on the first measurements of circular dichroism in the angular distribution (CDAD) of photoelectrons from W(110) in the soft X-ray range. The experiment was performed at beamline P04 of PETRA III, providing circularly-polarized photons in a wide energy range from 260-2400eV [1]. The novel technique of ToF k-microscopy [2] is ideal for the study of dichroism. The CDAD asymmetry is surprisingly large and reaches almost 100% in some regions. It can thus be used as tool for circular polarimetry throughout the soft X-ray range. CDAD shows a pronounced dependence on photon energy and k-vector. It depends on matrix elements and relative phases of partial waves, has previously been shown using conventional electron spectrometers [3].

Funded by BMBF (05K13UM2, 05K13GU3)

[1] Viefhaus et al., Nucl. Instrum. Meth. A710,151 (2013), [2] Chernov et al., Ultramicroscopy, (2015) doi:10.1016/j.ultramicro.2015.07.008, [3] Schönhense et al., Surf. Sci., 251 (1991).

O 16.8 Mon 16:45 H4

Effects of orbital composition in a pair of spin-orbit-split surface bands at Tl/Ge(111) — ●PH. EICKHOLT¹, P. KRÜGER², S.D. STOLWIJK¹, A.B. SCHMIDT¹, and M. DONATH¹ — ¹Physikalisches Institut, Universität Münster, Germany — ²Institut für Festkörpertheorie, Universität Münster, Germany

Surface states of the Tl/Si(111)-(1 × 1) [1-3] and Tl/Ge(111)-(1 × 1) surfaces are strongly influenced by spin-orbit-interaction (SOI), leading to peculiar spin textures. Our setup for spin- and angle-resolved inverse photoemission allows us to study the unoccupied spin-orbit-split surface states within the whole Brillouin zone. In general, the surface electronic structures of both systems are very similar. In particular, surface states with comparable properties are found along $\bar{\Gamma}\bar{K}$, independent of the substrate. Close to the \bar{M} point, however, the spin splitting between a pair of surface states at Tl/Ge(111)-(1 × 1) is considerably smaller than the splitting of the equivalent surface resonances at Tl/Si(111)-(1 × 1) – despite the fact that the former ones are more localized at the heavy Tl atoms. The difference in spin splitting is counter-intuitive since SOI in these systems is mainly due to the heavy Tl atoms and, in addition, Ge is heavier than Si. In this talk, we will show that a peculiar combination of SOI and hybridization [4] gives rise to the surprising differences observed in the experiment.

- [1] S.D. Stolwijk *et al.*, Phys. Rev. Lett. **111**, 176402 (2013)
- [2] S.D. Stolwijk *et al.*, Phys. Rev. B **90**, 161109(R) (2014)
- [3] S.D. Stolwijk *et al.*, Phys. Rev. B **91**, 245420 (2015)
- [4] S.N.P. Wissing *et al.*, Phys. Rev. B **91**, 201403(R) (2015)

O 16.9 Mon 17:00 H4

Many body effects on Cr(001) surfaces: An LDA+DMFT study — ●MALTE SCHÜLER^{1,2}, STEFAN BARTHEL^{1,2}, MICHAEL KAROLAK³, MATTHIAS BODE⁴, ALEXANDER I. POTERYAEV⁵, ALEXANDER I. LICHTENSTEIN⁶, MIKHAIL I. KATSNELSON⁷, GIORGIO SANGIOVANNI³, and TIM O. WEHLING^{1,2} — ¹Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — ²Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — ³Institut für Theoretische Physik, Universität Würzburg, Germany — ⁴Lehrstuhl für Experimentelle Physik II, Universität Würzburg, Germany — ⁵M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg, Russia — ⁶Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — ⁷Radboud University of Nijmegen, Institute for Molecules and Materials, Nijmegen, The Netherlands

The electronic structure of the Cr(001) surface with its sharp resonance at the Fermi energy is the topic of many experimental and theoretical works. It is so far unclear and controversially debated whether the origin of this resonance is an orbital Kondo or an electron-phonon coupling effect. We have combined ab-initio density functional calculations with dynamical mean field simulations to calculate the orbitally resolved spectral function and show that they agree well to (I)PES data. We conclude that the combination of the realistic description of the electronic structure and the dynamic treatment of local Coulomb

interaction is necessary to describe the complex many body effect in d_{z^2} and $d_{xz/yz}$ orbitals, which forms the low energy resonance.

O 16.10 Mon 17:15 H4

Electronic correlations in two-dimensional surface triangular lattices — ●FLORIAN ADLER¹, GANG LI², ANDRZEJ FLESZAR², FELIX REIS¹, WERNER HANKE², JÖRG SCHÄFER¹, and RALPH CLAESSEN¹ — ¹Physikalisches Institut und Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — ²Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We have examined the electronic structure of two related adatom systems, namely the $\sqrt{3} \times \sqrt{3}$ reconstructions of Sn on SiC(0001) and the γ -phase of Pb on Si(111). In either case, the adatoms form a congeneric two-dimensional triangular lattice on their respective substrate, leaving one dangling bond unsaturated. Despite the half-filled surface band, both systems end up in a Mott insulating state due to electronic correlations. In order to grasp the emerging physics, we have analyzed their spectral functions using angle-resolved photoemission spectroscopy.

Interestingly, one clearly observes a qualitatively different distribution of spectral weight within the lower Hubbard band of the two systems. Depending on the strength of local and non-local Coulomb interactions as well as spin interactions, each system responds differently to the frustration imposed by the triangular geometry of the substrate. This results in a possible charge or spin order, which sets its fingerprint on the symmetry and weight distribution of the k-resolved spectral function. The responsible order mechanism can then be tracked down with the help of many-body calculations. First studies on the spectral functions and a comparison between the two systems will be presented.

O 16.11 Mon 17:30 H4

Interdependence of adsorption site and charge distribution in a single donor-acceptor molecule adsorbed on an ionic crystal — ●TOBIAS MEIER¹, RÉMY PAWLAK¹, SHIGEKI KAWAI¹, SHI-XIA LIU², YAN GENG², PROKOP HAPALA³, PAVEL JELÍNEK³, ALEXIS BARATOFF¹, SILVIO DECURTINS², ERNST MEYER¹, and THILO GLATZEL¹ — ¹Department of Physics, University of Basel, Switzerland — ²Department of Chemistry and Biochemistry, University of Bern, Switzerland — ³Institute of Physics, Academy of Sciences of Czech Republic, Prague, Czech Republic

Electron donor-acceptor molecules are promising candidates for molecular electronic devices since they may generate separated electron-hole pairs upon absorption of photons or rectify electrical currents. Relevant properties of such complexes do not only depend on their intrinsic donor-acceptor character, but can also be modified by their interaction with the underlying surface. We used TTF-dppz [1], a fused pi-conjugated donor-acceptor molecule, deposited on insulating NaCl films on Cu(111). To investigate the interplay between the atomic structures of TTF-dppz and NaCl, we performed high-resolution STM and AFM measurements at 5 K. The charge distribution above individual molecules has been studied by local contact potential mapping [2,3]. We observed two different charge distributions which strongly depend on the adsorption site of the molecule. The results have been correlated with density functional theory calculations. [1] C. Jia et al., Chem. Eur. J. **13**, 3804 (2007)., [2] S. Kawai et al., ACS Nano **7**, 9098 (2013)., [3] B. Schuler et al., Nano Lett. **14**, 3342 (2014).

O 16.12 Mon 17:45 H4

Two air- and water- stable ionic liquids in the presence of TaF5 and NbF5. Photoelectron Spectroscopy Study — ●ANNA DIMITROVA¹, MARIT WALLE¹, MARCEL HIMMERLICH¹, STEFAN KRISCHOK¹, ADRIANA ISPAS², and ANDREAS BUND² — ¹Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, Deutschland — ²Technische Universität Ilmenau, FG Elektrochemie und Galvanotechnik, Deutschland

Electroplating from Ionic Liquids has a great potential for deposition of metals and alloys with a Nernst potential below that of water decomposition. In order to control the electrochemical processes, an understanding of intra- and outer molecular interactions which take place before the metal electrochemical reduction is required. To this end we used Photoelectron Spectroscopy as a tool to study the electronic structure and the local environment of the atoms in thin films of a binary mixture - Ionic Liquids and TaF5 or NbF5. Two ionic liquids with a common anionic part were used: 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide, [BMP][Tf2N] and

3-propyl-1-methyl-imidazolium bis(trifluoromethylsulfonyl)imide, [PMIm][Tf₂N], in which TaF₅ and NbF₅ were separately dissolved in a different stoichiometry. In order to avoid the fast oxidation of both of the metal salts, the sample preparation and transportation to the

Ultra-High Vacuum Chamber was done in an O₂-free atmosphere. In this study the surface chemical compositions at different ionic liquid-to-metal salt concentration are discussed and compared with previous data, where ambient conditions were used for sample preparation.