O 66: Electronic Structure of Surfaces

Time: Wednesday 18:15–21:00 Location: Poster A

O 66.1 Wed 18:15 Poster A

XMCD of 3d adatoms on Bi_2Te_3 and Bi_2Te_2Se: experiment and ab initio theory — Martin Vondracek[1], •Jan Honolka[1], Cinthia Piamonteze[2], Jonas Warmuth[4], Matteo Michiardi[3], Philip Hofmann[3], Khajetoorians Alexander Ako[4], Jens Wiebe[4], Roland Wiesendanger[4], Tim Wehling[5], Jan Minar[6], Hubert Ebert[6], Jian-Li Mi[3], Bo B. Iversen[3], and Markus Dunst[6] — [1]Inst. of Physics ASCR, Prague, Czech Republic — [2]PSI, Switzerland — [3]iNano, Aarhus University, Denmark — [4]INF, University of Hamburg, Germany — [5]Inst. of Theo. Physics, University of Bremen, Germany — [6]LMU München, Germany

The chalcogenide 3D topological insulator Bi_2Te_3 obeys time-reversal symmetry, and hosts a linear dispersive, topological surface state around the Gamma point[1]. It is predicted, that magnetic adatoms can break time-reversal symmetry, thereby generating an energy gap at the Dirac point of the otherwise topologically protected surface states[2]. Here we summarize experimental XAS and XMCD results of single $3d$ adatoms Ni, Fe, and Cu on Bi_2Te_3 and Bi_2Te_2Se surfaces. While Cu shows a d^{10} electronic configuration, we find a significant resonant Ni $L_{2,3}$ intensity in XAS, however no magnetic dichroism within the detection limit. The results are compared to ab initio theory. Calculated equilibrium positions of adatoms and their host structure show strong relaxation effects. d-shell occupancies and magnetic properties are extracted. Moreover, we present simulated resonant spectral shapes. [1] M. Z. Hasan and C. L. Kane, Reviews of Modern Physics 82, 3045 (2010). [2] Y. L. Chen et al., Science 329, 659 (2010).

O 66.2 Wed 18:15 Poster A

STM study on the electronic properties of the Vanadium (100) (1x5) surface reconstruction — •Andreas Topp[1], Berthold Jäck[1], Matthias Eltschka[1], Markus Etzkorn[1], Christian Ast[1], and Klaus Kern[1,2] — [1]Max-Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

Vanadium has recieved comparibly little attention in surface science, despite the interesting superconducting properties, since its superconducting phase offers a high critical temperature with moderate critical fields [1]. The (1×5) reconstuction of the Vanadium (100) surface has been studied by means of AES, ARPES, STM topography, LEED and DFT [2, 3]. The influence of oxygen in forming this reconstuction has been of special interest. Here, we use scanning tunneling microscopy to investigate the local electronic structure of the (1×5) reconstruction with atomic scale precision. By reporting on conductance measurements between $0 - 1\,\mathrm{V}$, we can show that the local density of states strongly varies within the reconstruction.

[1] S.Sekula and R.Kernohan, Phys. Rev. B **5**, 904 (1972)
[2] R.Koller *et al.*, Surf. Sci. **480**, 11 (2001)
[3] M.Kralj *et al.*, Surf. Sci. **526**, 166 (2013)

O 66.3 Wed 18:15 Poster A

Force and Kelvin Probe Measurements on Confined Electronic States inside Quantum Resonators — •Fabian Queck[1], Florian Albrecht[1], Alastair McLean[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston, Ontario, Canada, K7L 3N6

On closed-packed surfaces of noble metals such as Cu(111) surface state electrons form a nearly free electron gas in two dimensions. The electrons are scattered from step-edges, point defects and adsorbates giving rise to standing wave patterns, which can be engineered by so-called quantum corrals [1]. The standing wave patterns gives rise to long range interactions between adsorbates [2] and should therefore be associated with measurable forces between scatterers.

Here we make an attempt to directly measure these forces with atomic force microscopy and to measure the possible changes of the local contact potential difference generate by the modulation of the surface local density of states associated with the standing wave patterns.

[1] M. F. Crommie, C. P. Lutz, and D. M. Eigler. Confinement of Electrons to Quantum Corrals on a Metal Surface. Science, 262(5131), 218-220, 1993.

[2] J. Repp. Rastertunnelmikroskopie und -spektroskopie an Adsorbaten auf Metall und Isolatoroberflaechen. PhD thesis, Freie Universitaet Berlin, 2002.

O 66.4 Wed 18:15 Poster A

Three-dimensional band mapping and spin-polarized states in the phase change material $Ge_2Sb_2Te_5$ — •Marcus Liebmann[1], Christian Pauly[1], Jens Kellner[1], Jos Boschker[2], Rui Ning Wang[2], Evangelos Golias[3], Jaime Sanchez-Barriga[3], Oliver Rader[3], Raffaella Calarco[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin — [3]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin

We present an angle-resolved photoemission (ARPES) study of the ternary phase change material $Ge_2Sb_2Te_5$, epitaxially grown on Si(111) in the metastable cubic phase, transferred in-situ in ultra-high vacuum from the molecular beam epitaxy system to the analysis chamber. This material serves, e.g., in DVDs as a fast switchable material (1 ns) between the metallic cubic and an insulating amorphous phase. Recently, the observation of an inverted valence band provided evidence of non-tivial $\mathbb{Z}_2$ topology [1], opening up the perspective of ns-switching between a topological crystalline and an insulating amorphous phase. We performed a three-dimensional mapping of the band structure by variation of the photon energy (15-31 eV) and found the center of the bulk valence band about 130 meV below the Fermi energy and away from the center of the Brillouin zone. A spin polarization of nearly 100% close to the Fermi energy has been observed by spin-polarized ARPES. We show a detailed analysis of the involved states near the Fermi energy contributing to the transport.

[1] C. Pauly *et al.*, Appl. Phys. Lett. **103**, 243109 (2013).

O 66.5 Wed 18:15 Poster A

Manipulation and control of electronic properties of Si:P δ-layers — •Federico Mazzola[1], Craig Polley[3], Jill Miwa[2], Michelle Simmons[4], and Justin Wells[1] — [1]NTNU, Norwegian University of Science and Technology — [2]Department of Physics and Astronomy, Aarhus University — [3]MAX-IV Laboratory, Lund, Sweden — [4]Centre for Quantum Computation & Communication Technology School of Physics The University of New South Wales

Many body interactions play a fundamental role for material properties such as conductivity, scattering and transport of carriers. In particular, electron-phonon- coupling (EPC) has been attracting interest because is thought to be a prerequisite for superconductivity.

δ-doping in Si, which consists in placing a highly conductive P layer just beneath the Si surface, constitutes an important step for quantum computer architectures allowing for the possibility of shrinking the scale of devices down to the atomic scale, with a single atom transistor and atomic scale nanowire having been demonstrated.

Here I will introduce ARPES and Resonant-PES characterization and explain how such a technique can be used to understand many-body interactions in the electronic band-structure of Si:P δ-layers and to characterize the dimension of this new hybrid system. In particular, we will introduce a characterization of the electronic confinement of a sub-surface state and we will study how such a state is affected by many-body interactions.

O 66.6 Wed 18:15 Poster A

Elementary contributions to the resistivity of a thin Bi_2Se_3 film — •Sebastian Bauer, Paul Graf, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We present scanning tunneling potentiometry (STP) measurements on a 14 QL Bi_2Se_3 film on Si(111) using a multiprobe STM [1]. STP gives us simultaneously microscopic information about the topography and the electrochemical potential of the topological insulator (TI) Bi_2Se_3 while a lateral current flows through the Bi_2Se_3 film. The microscopic (nm-scale) sheet conductance of the Bi_2Se_3 film is evaluated by STP yielding a value of 1.8 mS. This is very close to the value of our macroscopic (μm-scale) measurements (2.1 mS) also found by other groups [2]. Despite the topological protection of the Bi_2Se_3 surface state [3], we observe sharp voltage drops on the Bi_2Se_3 surface, located at Bi_2Se_3 step edges. The step edges contribute to the total resistance of the surface by a resistivity of 0.9 Ω·cm at each step edge of a quintuple layer, reducing the sheet conductance of the TI film [4].

[1] A. Bannani, C. A. Bobisch, and R. Möller, Rev. Sci. Instrum. 79, 083704 (2008). [2] A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [3] M. Hazan and C. L. Kane, Rev. Mod. Phys. 82, 3045-3067 (2010). [4] S. Bauer and C. A. Bobisch, in revision.

O 66.7 Wed 18:15 Poster A

Manipulating the surface conductivity of Bi_2Se_3 by Bi ad-islands — •Paul Graf, Sebastian Bauer, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We studied the microscopic (nm-scale) electron transport on the surface of thin films of the topological insulator Bi_2Se_3 [1],[2] by scanning tunneling potentiometry (STP) [3] using a multiprobe STM [4]. Especially, we analyzed the impact of Bi ad-islands to the electron transport, i.e. the electrochemical potential of the Bi_2Se_3 film. In addition, the macroscopic (μm-scale) conductivity was determined by a two point measurement. Since the surface state of Bi_2Se_3 is topologically protected, small defects on the surface like the bismuth bilayer islands are predicted not to disturb the current flow through the Bi_2Se_3 film significantly. We find that both, the microscopic and the macroscopic conductivity of the Bi_2Se_3 film increases after adding bismuth bilayer islands to the surface. This effect can be explained by electron donation from the bismuth ad-islands to the Bi_2Se_3 film [5]. The impact of scattering of conduction electrons at the Bi ad-islands to the local surface potential will be discussed.

[1] C. L. Kane und E. J. Mele, Phys. Rev. Lett. 95, p. 146802 (2005). [2] H. Zhang et. al., Nat. Phys. 5, p. 438 (2009). [3] P. Muralt et. al., Appl. Phys. Lett. 48, p. 514 (1986). [4] A. Bannani, C. A. Bobisch and R. Möller, Rev. Sci. Instrum. 79, 083704 (2008). [5] M. Chen et. al., Appl. Phys. Lett. 101, p. 081603 (2012)

O 66.8 Wed 18:15 Poster A

Core-resonant double photoemission from palladium films — •Ilya Kostanovskiy, Frank Schumann, Zheng Wei, Yuri Aliaev, and Jürgen Kirschner — Max Planck Institute of Microstructure Physics, Halle, Germany

We present a core-resonant double photoemission study from palladium films with synchrotron radiation. In an MVV Auger process a 3d (M) core level electron is excited and the subsequent decay involves two 4d (V) valence electrons. This process provides access to the electron-electron interactions in the valence band. We measured Pd 3d photoelectrons in coincidence with the Auger MVV electrons by means of linear polarized light. We selected two polarization directions perpendicular to each other. In contrast to single electron photoemission we observe a polarization dependence not only for the photo electrons, but also for the Auger line. This effect can be quantitatively explained within a simple model.

Additionally, we present the sum energy spectra which display a simple triangular-like line shape. It resembles a self convolution of a constant density of states. Our results will be compared with theoretical descriptions of the Auger decay. These either implement an electron-electron interaction within the valence band or use atomic multiplet theory.

O 66.9 Wed 18:15 Poster A

Rashba-splitting in thin Bi-films on a Au(111)-surface — •Dominik Jungkenn[1], Sebastian Jakobs[1,2], Stepan Tsirkin[3], Andreas Ruffing[1], Eugene Chulkov[3], Mirko Cinchetti[1], Stefan Mathias[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [3]Donostia International Physics Center (DIPC), Depto. de Fisica de Materiales and Centro Mixto CSIC-UPV/EHU, Facultad de Ciencias Quimicas, UPV/EHU, 20018 San Sebastian, Spain

The combination of large spin-orbit coupling and a broken inversion symmetry at the surface or interface of a crystal leads to a spin-dependent splitting of the band structure (Rashba-effect [1]), which is of great interest in the growing field of spintronics. The Rashba-effect was observed in different systems with varying splitting magnitudes, e.g surface states, quantum-well states and topological insulators. Here, we investigate the strongly Rashba-type spin-orbit split system Bi/Au(111) using low energy electron diffraction (LEED) and angle resolved photoemission spectroscopy (ARPES). Our results exhibit a spin-split band structure with a so far unrivaled large Rashba parameter (α_R = 4.78 eVÅ) for a coverage below 1 monolayer (ML). The results are supported by DFT calculations that reproduce our observations in good agreement.

[1] Yu. A. Bychkov, E. I. Rashba. JETP, 39(2), 78-81 (1984)

O 66.10 Wed 18:15 Poster A

Analysis of the Band Dispersions of the Bilayer Ruthenate $Sr_3Ru_2O_7$ around the High Symmetry Points — •Arlette S. Ngankeu[1,2], Emanuela Carleschi[1], Bryan P. Doyle[1], Volodymyr B. Zabolotnyy[3], Timur K. Kim[4], Ivana Vobornik[5], Manju Unnikrishnan[5], Rosalba Fittipaldi[6], Mario Cuoco[6], Antonio Vecchione[6], and Sergey V. Borisenko[3] — [1]University of Johannesburg (South Africa) — [2]Aarhus University (Denmark) — [3]IFW Dresden (Germany) — [4]Diamond Light Source (United Kingdom) — [5]IOM-CNR TASC Laboratory Trieste (Italy) — [6]CNR-SPIN and Department of Physics, University of Salerno (Italy)

We have investigated the formation of heavy d electron quasiparticles in $Sr_3Ru_2O_7$ by analysing the dispersion of the low-energy states around the high symmetry points Γ and X of the first Brillouin zone. This study was performed at the BESSY 1^3 ARPES endstation. We report the existence of flat bands giving rise to van Hove singularities (vHS) in the DOS in closed proximity to the Fermi level, associated to the γ_2, α_2 and δ Fermi surface sheets. These vHS are deemed to be responsible for the appearance of the multiple metamagnetism observed in the system. Our results also show signatures of strong correlation effects characterised by the peak-dip-hump line shape of the dispersive states. Finally, we have noted the presence of bands not predicted by electronic structure calculations, which might be band replicas ascribed to the reconstruction of the sample surface.

O 66.11 Wed 18:15 Poster A

Low temperature scanning tunneling microscopy investigation of the phase change material Ge2Sb2Te5 — •Jens Kellner[1], Christian Pauly[1], Marcus Liebmann[1], Jos Boschker[2], Volker Deringer[3], Raffaella Calarco[2], Richard Dronskowski[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Paul Drude Institut für Festkörpelektronik, Berlin, Germany — [3]Institute of Inorganic Chemistry, RWTH Aachen University, Germany

We present a scanning tunneling microscopy (STM) study of the phase change material GST-225 (GST), epitaxially grown on Si(111) in the metastable cubic phase, transferred in-situ in ultrahigh vacuum from the molecular beam epitaxy system to the STM. Despite the fact that GST is already commercially used, there is still no complete understanding of the ultra fast switching speed, the strong resistance change and the high endurance of the Ge-Sb-Te alloys. One contribution to such a theory is an atomic scale understanding of the electronic properties of GST. V. Deringer modeled the surfaces by cutting slabs from the hexagonal bulk cells of GST followed by relaxation. The relaxed structure features a number of octahedral and tetrahedral Ge bonds which can be distinguished in the density of states (DOS) projections. We detected the differential conductivity of such states by scanning tunneling spectroscopy at 0.4 K leading to an identification of different bonding configurations.

O 66.12 Wed 18:15 Poster A

Tuning the Fermi energy to the Dirac point in the ternary topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ — •Jens Kellner[1], Markus Eschbach[2], Jörn Kampmeier[3], Martin Lanius[3], Gregor Mussler[3], Lukasz Plucinski[2], Markus Liebmann[1], Detlev Grützmacher[3], Claus Schneider[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-6), Germany — [3]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-9), Germany

A topological insulator (TI) has a bulk energy gap but conducting helical surface states. In order to make use of these states, e.g. in transport devices or for creating exotic quasiparicles like Majorana Fermions, one has to tune the Fermi energy (E_F) close to the Dirac point (E_D) within the band gap. However, currently used TI materials e.g. Bi_2Te_3 and Sb_2Te_3 have major drawbacks. For Bi_2Te_3, E_D is buried in the bulk valence band (BVB) and E_F is located in the bulk conduction band (BCB). Whereas with Sb_2Te_3, E_D is in the bulk energy gap and E_F is located in the BVB. Mixing the two compounds leads to a ternary system $(Bi_{1-x}Sb_x)_2Te_3$ where charge compensation is achieved and the position of E_D can be tuned [1].We were able to synthesize $(Bi_{1-x}Sb_x)_2Te_3$ thin films for 0.94<x<0.96 by molecular beam epitaxy (MBE), transferred in-situ in ultrahigh vacuum from the MBE system to the photoemission setup. Angle resolved photoemission spectroscopy shows that E_F and E_D are congruent and no bulk bands intersect E_F. [1] J. Zhang, Nat. Comm. 2, 574 (2011)

O 66.13 Wed 18:15 Poster A

Two-photon photoemission from $GeSb_2Te_4$ — •Sebastian Otto, Philipp Rosenzweig, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time- and angle-resolved, polarization-dependent two-photon photoemission is used to study the electronic structure and dynamics at the surface of $GeSb_2Te_4$. The topological surface state is centered at 0.45 eV above the Fermi level due to intrinsic p-doping. The valence band, the two lowest conduction bands and an image-potential state are identified. Measurements with circularly polarized light show the expected change of sign in the circular-dichroism asymmetry at the Dirac point. The dichroism depends only on the circular polarization of the probe pulse, which indicates an indirect filling from the conduction band. The second conduction band shows a negative dispersion similar to $SnSb_2Te_4$ [1] and Sb_2Te_3 [2].

[1] D. Niesner, S. Otto, V. Hermann and Th. Fauster, Phys. Rev. B **89**, 081404(R) (2014)

[2] J. Reimann, J. Güdde, K. Kuroda, E. V. Chulkov and U. Höfer, Phys. Rev. B **90**, 081106(R) (2014)

O 66.14 Wed 18:15 Poster A

Double photoemission from surfaces: intensity relations — •Yuri Aliaev, Frank Oliver Schumann, Ilya Kostanovski, Gianluca Di Filippo, Zheng Wei, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The emission of an electron pair upon single photon absorption requires a finite electron-electron interaction. This makes double photoemission a particulary sensitvie tool to study the electron correlation in matter. This is supported by a recent theoretical work which predicts that the pair intensity is a direct reflection of the correlation strength.[1] In order to explore the validity of this we performed a study on a variety of materials. Among them are noble metals, transition metals and insulators. The latter include transition metal oxides like CoO and NiO which are also termed highly correlated. We find an increased pair emission rate of NiO and CoO compared to the metals which reaches factor of 10. This enhancement is photon energy depedent. It is highest at 23.7 eV and decreases monotonically as a function of the photon energies. At 60 eV the intensity levels for the oxides and metals are largely identical.

We also discovered that an increase of the coincidence intensity is accompanied by an increase in the singles count rate. This demonstrates that the pair emission is an efficient process at surfaces contributing up to 15% to the single electron emission. Our experimental results demonstrates that the correlation strength can be accessed by double photoemission.

[1] B.D. Napitu, J. Berakdar, Phys. Rev. B **81**, 195108. (2010)

O 66.15 Wed 18:15 Poster A

Electronic structure of spintronic materials investigated with laser-based high-resolution angle-resolved photoemission — •Pika Gospodaric, Markus Eschbach, Lukasz Plucinski, Ewa Mlynczak, Mathias Gehlmann, Sven Döring, and Claus Michael Schneider — Forschungzentrum Jülich GmbH, Peter Grünberg Institute (PGI-6), 52425 Jülich, Germany

In this contribution we will present the first experimental results obtained with the new setup for high resolution angle resolved photoemission spectroscopy (ARPES) operated with laser light. The existing lab-based ARPES system was upgraded with a 6 eV photon source based on the fourth harmonic generation of fundamental 1.5 eV ultrashort pulsed laser beam from a commercial Ti:Sa oscillator. A small spot size of 100 microns can be achieved on the sample, whereas the short pulses allow time-resolved measurement as a future application. The system offers electronic structure investigation of surfaces with possibility to control the polarization of light and thus enables detection of differential absorption of left and right circular polarized light, i.e. circular dichroism (CD), which can be observed in spin polarized energy bands. Calibrations were performed on Au(111)and Cu(111) single crystal surfaces which exhibit clear parabolic surface states in the center of their Brillouin zone. Investigation of the spin texture of the Dirac cone in the 3D topological insulator Sb2Te3 was performed using CD.

O 66.16 Wed 18:15 Poster A

Subsurface contributions in epitaxial rare-earth silicides — •Olaf Lübben[1], Jorge I. Cerdá[2], Alexander N. Chaika[3], and Igor V. Shvets[1] — [1]Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), School of Physics, Trinity College, Dublin 2, Ireland — [2]Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Cantoblanco, 28049 Madrid, Spain — [3]Institute of Solid State Physics RAS, Chernogolovka, Moscow district 142432, Russia

Metallic thin films of heavy rare-earth silicides epitaxially grown on Si(111) substrates have been widely studied in recent years because of their appealing properties: unusually low values of the Schottky barrier height, an abrupt interface, and a small lattice mismatch. Previous studies also showed that these silicides present very similar atomic and electronic structures. Here, we examine one of these silicides (Gd_3Si_5) using scanning tunneling microscopy (STM) image simulations that go beyond the Tersoff-Hamann approach. These simulations strongly indicate an unusual STM depth sensitivity for this system.

O 66.17 Wed 18:15 Poster A

Ultrafast time and angle resolved photoemission spectroscopy measurements using high harmonic radiation above 70eV photon energy and sub-1eV resolution at 10kHz repetition rate — •Jürgen Schmidt[1], Alexander Guggenmos[1,2], Soo Hoon Chew[1], and Ulf Kleineberg[1,2] — [1]LMU München, Fakultät für Physik, Am Coulombwall 1, 85748 Garching — [2]MPQ, Hans-Kopfermann-Str. 1, 85748 Garching

High harmonic generation has established as the standard tool for ultrafast time resolved photoelectron spectroscopy experiments to study electron dynamics on gases and solids. Angle resolved measurements additionally give insight into the momentum space of the electrons and provide full information about the band structure dynamics. These measurements benefit from sources with high repetition rate on the one hand and high photon energies on the other hand in order to be able to also address core-like electron states which revealed insight into the temporal dynamics of the photoemission process [1]. Here we show that our source produces harmonic radiation between 70 and 100eV at a repetition rate of 10kHz with sufficient flux for angle resolved photoemission experiments [2] and we report about time resolved measurements on various metal surfaces excited by few-cycle NIR pulses. [1] Cavalieri et al., Nature 449, 1029 (2007) [2] Schmidt et al., Rev. Sci. Instrum., to be submitted