O 13: Electronic Structure of Surfaces II

Time: Monday 15:00–18:15 Location: MA 041

Invited Talk O 13.1 Mon 15:00 MA 041

Advanced spin-resolved momentum microscopy — •Christian Tusche — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Angle resolved photoemission spectroscopy (ARPES) is an universal tool to probe the electronic structure of solids. Conventional electron spectrometers measure the distribution of photoelectrons in a limited angular interval, which makes complete mapping of band structures a time consuming task. Here, we discuss the recent approach to this issue by momentum microscopy. A momentum microscope captures the complete 2π solid angle of emission directions into a high resolution (k_x, k_y) image of the full surface Brillouin zone of a solid. This efficient measurement scheme intrinsically provides comprehensive quantitative information beyond high-symmetry directions.

Of particular importance is the spin of the electron, that gives rise to phenomena like ferromagnetism, spin-polarized surface states, and the discovery of new material classes like topological insulators. So far, however, the spin was only inefficiently probed in photoemission experiments, resulting in a rather low figure of merit (10^{-4}) for spin-resolved ARPES. This longstanding problem is defeated by introducing the novel concept of spin-resolved momentum microscopy: In combination with an imaging spin filter, we measure more than 5000 spin-resolved points in the full $k_{||}$-space, simultaneously. We will discuss examples ranging from the spin-resolved Fermi surface of ferromagnets to highly polarized states in topological insulators.

O 13.2 Mon 15:30 MA 041

Strongly anisotropic spin-orbit splitting in a 2-dimensional electron gas — •Matteo Michiardi[1], Marco Bianchi[1], Maciej Dendzik[1], Jill Miwa[1], Moritz Hoesch[2], Timur K. Kim[2], Peter Matzen[1], JianLi Mi[3], Martin Bremholm[3], Bo Brummerstedt Iversen[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, United Kingdom — [3]Center for Materials Crystallography, Department of Chemistry, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

Near-surface two-dimensional electron gases (2DEG) on the topological insulator Bi_2Te_2Se are induced by electron doping and studied by angle-resolved photoemission spectroscopy. A pronounced spin-orbit splitting is observed for these states. The k-dependent splitting is strongly anisotropic to a degree where a large splitting can be found in the $\bar{\Gamma}\bar{M}$ direction while the states are hardly split along $\bar{\Gamma}\bar{K}$. We show that this strong anisotropy can be explained by expanding the $\mathbf{k}\cdot\mathbf{p}$ hamiltonian for 2DEGs to include the possibility of band structure anisotropy as well as both isotropic and anisotropic third order Rashba splitting. The interplay of band structure, higher order Rashba effect and tuneable doping offers the opportunity to engineer not only the size of the spin-orbit splitting but also its direction.

O 13.3 Mon 15:45 MA 041

Epitaxial Sb_2Te_3/Bi_2Te_3 heterostructures: a new (route to) topological p-n junction — •Markus Eschbach[1], Ewa Mlynczak[1], Jens Kellner[2], Jörn Kampmeier[1], Martin Lanius[1], Christian Weyrich[1], Gregor Mussler[1], Natalya Demarina[1], Thomas Schäpers[1], Lukasz Plucinski[1], Detlev Grützmacher[1], Markus Morgenstern[2], and Claus M. Schneider[1] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institut, 52425 Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, 52074 Aachen, Germany

Recently, in the field of 3D Topological Insulators various attempts have been carried out to tune the chemical potential and, more specifically, the Dirac point to a desired energetic position i.e. to engineer the electronic bandstructure for the purpose of designing future spintronic devices. Here we show the first direct experimental proof, by angle-resolved photoemission, of the realization of a topological p-n junction made of a heterostructure of two different 3D TI materials Bi_2Te_3 and Sb_2Te_3 grown on Si(111). In the experiment we observe an energetic shift of the entire electronic structure of about 200 meV when decreasing the upper Sb_2Te_3 layer from a thickness of 25 QL to 6 QL. On one hand, we consider surface doping and the creation of a ternary alloy at the surface and on the other hand the creation of a depletion region and a built-in electric field at the interface of the two TI materials to be responsible for the shift. The latter contribution is supported by solving Schrödinger and Poisson equations self-consistently for a 1D model system.

O 13.4 Mon 16:00 MA 041

Spin-resolved electronic structure of BiTeI — •Henriette Maass[1], Christoph Seibel[1], Hendrik Bentmann[1], Christian Tusche[2], Taichi Okuda[3], Thiago Peixoto[1], Oleg Tereschchenko[4], Jürgen Kirschner[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Max-Planck-Institut für Mikrostrukturphysik, Am Weinberg 2, D-06120 Halle — [3]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan — [4]Institute of Semiconductor Physics, 636090, Novosibirsk, Russia

The non-centrosymmetric lattice structure and large spin-orbit interaction in bismuth tellurohalides lead to large Rashba-type spin-splittings in the bulk and surface electronic structure of these materials. The resulting spin structure is predicted to be highly dependent on the orbital character of the electronic states [1]. Deploying a spin- and angle- resolving photoelectron spectrometer based on very-low-energy electron diffraction [2] and a momentum microscope with an imaging spin filter [3] we investigated the photoelectron spin polarization of the surface band structure of BiTeI for a subset of energies and momenta. Our experiments reveal a peculiar spin-structure yielding evidence for an orbital dependence of the Rashba-splitting. In particular we find evidence for a correlation between the photoelectron spin and the orbital character of the Rashba surface band.

[1] Z. Zhu *et al.*, New J. Phys. **15**, 023010, (2013)
[2] T. Okuda *et al.*, Rev. of Sci. Instr. **82**, 103302, (2011)
[3] C. Tusche *et al.*, Ultramicroscopy **130**, 70-76, (2013)

O 13.5 Mon 16:15 MA 041

Electronic and spin structure of topological surface state in Sn-based ternary topological insulators — •Maia G. Vergniory[1], Tatyana V. Menshchikova[2], Igor V. Silkin[3], Yuri M. Koroteev[3], Sergey V. Eremeev[3], and Evgueni V. Chulkov[4] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, 06120 Germany — [2]Tomsk State Univeristy, Tomsk, 634050 Russia — [3]Institute of Strength and Materials Science, Siberian Branch, Tomsk, 634021 Russia — [4]Donostia International Physics Center, Donostia-San Sebastian, 20018 Spain

We report the bulk and surface electronic properties and spin polarization of a new rich family of Sn-based ternary complex topological insulators studied by means of first principles calculations. These compounds exist in different stoichiometries: SnxAyBz (A:Sb and Bi) (B: Te and Se). The crystal structure of these compounds is characterized by alternating along hexagonal axis quintuple, septuple and nonuple layer van der Waals bonded building blocks. We reveal that the bulk band gap in these systems is about 100 meV and the spin polarization near the Dirac point is up to 85%. Within the same family, for some of these compounds, which crystal structure has ionic-covalent bonded Bi2Te3 and crystalline topological insulator SnTe atomic layers within building block, the complex SOI-induced bulk band inversion caused by competition of band inversions in Bi2Te3 and in SnTe layers occurs and results in inherently nonlinear dispersion of the topological surface state.

O 13.6 Mon 16:30 MA 041

Warping Effects on Spin and Electronic Structure of the Topological Surface State in α-Sn — •M. R. Scholz[1], A. Fleszar[2], G. Li[2], F. Adler[1], S. Glass[1], L. Dudy[1], J. Aulbach[1], S. Muff[3], J.-H. Dil[3], M. Bianchi[4], M. Michiardi[4], P. Hofmann[4], W. Hanke[2], R. Claessen[1], and J. Schäfer[1] — [1]Phys. Inst. and RCCM, Univ. Würzburg — [2]Inst. f. Theo. Physik u. Astronomie, Univ. Würzburg — [3]Swiss Light Source, Paul-Scherrer-Institut Villigen — [4]Aarhus University

The strain-induced insulating phase of α-Sn was proposed to be of non-trivial topology in 2007 [1] and subsequently experimentally established by our group in 2013 [2]. Soon after the discovery of the topological insulators of the Bi_2X_3 family of materials the influence of

the 3-fold symmetry of the crystal on spin texture and electronic structure of the topological surface state (TSS) has been dicussed, and is still a subject of current research. Here, we want to report on a detailed investigation of the influences of the diamond lattice symmetries on the TSS in α-Sn. Our results from angle-resolved photoemission show that the TSS deviates from the ideal shape of a Dirac cone with circular constant energy contours. Moreover, spin-resolved photoemission reveals a lifting of the perpendicular locking of spin and momentum similar to the case of Bi_2X_3, while, in contrast, the spin remains fully within the surface plane. The experimental results are in nice agreement with our own DFT calculations. [1] Fu and Kane Phys. Rev. B **76**, 045302 (2007); [2] Barfuss et al., Phys. Rev. Letters **111**, 157205 (2013)

O 13.7 Mon 16:45 MA 041

Probing the Surface Properties of the Topological Insulator $TlBiSe_2$ by Photoelectron Diffraction, Scanning Tunneling Spectroscopy and Ab-Initio Theory — •Eike F Schwier[1], Clément Didiot[2], Kenta Kuroda[3], Roland Stania[4,5], Jun Zhang[5], Elia Razzoli[2], Mao Ye[1], Hideaki Iwasawa[1], Matthias Muntwiler[5], Philipp Aebi[2], Akio Kimura[6], Kenya Shimada[1,6], Hirofumi Namatame[6], and Masaki Taniguchi[1,6] — [1]Hiroshima Synchrotron Radiation Center, Japan — [2]U Fribourg, Switzerland — [3]U Marburg, Germany — [4]U Zürich, Switzerland — [5]PSI, Villigen, Switzerland — [6]U Hiroshima, Japan

It was recently found that the cleaved surface of the 3D topological insulator $TlBiSe_2$ is decorated with island-like structures[1]. In our study we deployed a combination of photoelectron diffraction (PED) as well as ab-initio theory and scanning tunneling spectroscopy to probe the properties of the surface. By comparing our PED measurements with multiple scattering calculations and taking into account different surface topographies we were able to unambiguously answer the question of the islands chemical composition and to estimate the island-substrate out-of-plane lattice constant. Using ab-initio calculations, we were further able to explain the emergence of the surface core-level shift in Tl 5d by comparing different surface terminations and Tl coverages. We will also present results from STS measurements on and between the islands in order to shine some light on the islands influence on the Dirac cone formation and its spin polarization.

[1] K. Kuroda et al., PRBB 88, 245308, 2013.

O 13.8 Mon 17:00 MA 041

Spin-orbit interaction and Dirac cones in d orbital noble metal surface states — •Ryan Requist[1], Polina M. Sheverdyaeva[2], Paolo Moras[2], Sanjoy K. Mahatha[3], Carlo Carbone[2], and Erio Tosatti[1,3,4] — [1]International School for Advanced Studies,Trieste, Italy — [2]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy — [3]International Centre for Theoretical Physics, Trieste, Italy — [4]IOM-CNR – Democritos, Trieste, Italy

We report a joint photoemission/ab initio study of spin-orbit effects in the deep d orbital surface states of a 24-layer Au film grown on Ag(111) and a 24-layer Ag film grown on Au(111), singling out a conical intersection (Dirac cone) in a large surface-projected gap at the time-reversal symmetric $\overline{M}$ points. Unlike the often isotropic dispersion at $\overline{\Gamma}$ point Dirac cones, the $\overline{M}$ point cones are strongly anisotropic. An effective $\mathbf{k}\cdot\mathbf{p}$ is derived to describe the anisotropic Rashba band splitting and spin polarization near the Dirac cone, and we discuss multiband tight binding models for surface states with spin-orbit interactions.

O 13.9 Mon 17:15 MA 041

Rashba splitting of graphene-covered Au(111) revealed by quasiparticle interference mapping — •Mikhail Fonin, Philipp Leicht, Julia Tesch, Felix Blumenschein, Philipp Erler, and Luca Gragnaniello — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Although the Rashba-split bands are readily visible in angle-resolved photoemission, their observation at the local scale employing quasiparticle interference (QPI) mappings is challenging. Here, we report on low-temperature scanning tunneling microscopy/spectroscopy measurements on epitaxial graphene flakes on Au(111). Careful analysis of the QPI maps allows the discrimination between the electronic systems of graphene and Au(111). Beyond the scattering vectors, which can be ascribed to the elastic scattering within each of the systems, we clearly observe QPI features related to the scattering process between graphene states and the Au(111) surface state. This additional interband scattering process at the graphene/Au(111) interface allows the direct quntitative determination of the magnitude of the Rashba splitting of the Au(111) surface state, which cannot be evaluated from QPI measurements on pure Au(111). This experiment demonstrates a new local spectroscopic approach to investigate the band structure of surfaces with Rashba splitting.

O 13.10 Mon 17:30 MA 041

Microscopic theory of the residual surface resistivity of Rashba electrons — •Juba Bouaziz[1], Stefan Blügel[1], Hiroshi Ishida[2], and Samir Lounis[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]College of Humanities and Sciences, Nihon University, Sakura-josui, Tokyo 156, Japan

A microscopic expression of the residual electrical resistivity tensor is derived in linear response theory for Rashba electrons scattering at a magnetic impurity with cylindrical or non-cylindrical potential. We investigated the specific case of an Fe adatom deposited on Au(111) surface [1] and studied the evolution of the diagonal and off-diagonal elements of the resistivity tensor as function of the magnetization direction of the impurity and of the spin-orbit strength. We found that the longitudinal residual resistivity leads to an anomalous magnetoresistance while the transversal one to a planar Hall effect. In the limit of no spin-orbit interaction and a non-magnetic impurity of cylindrical symmetry the expression of the residual resistivity of a two-dimensional electron-gas has the same simplicity and form as for the three-dimensional electron gas [2] and can also be expressed in terms of scattering phase shifts.

[1] S. Lounis *et al.* Phys. Rev. Lett. **108**, 207202 (2012)
[2] J. Friedel, NuovoCimento Suppl. **7**, 287 (1958)

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O 13.11 Mon 17:45 MA 041

Unconventional surface reconstruction of Na_2IrO_3 with persistent energy gap — •Felix Lüpke[1,2], Soham Manni[3,4], Steven C. Erwin[5], Igor I. Mazin[5], Philipp Gegenwart[4], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [3]I. Physikalisches Institut, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [4]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86159 Augsburg, Germany — [5]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA

Na_2IrO_3 is an intriguing material for which theoretical predictions, so far unverified, have been made that the surface of Na_2IrO_3 should exhibit a clear signature of the quantum spin Hall effect. We studied the surface of Na_2IrO_3 using scanning tunneling microscopy, spectroscopy and density-functional theory calculations. We observed two types of surface terminations with different surface periodicity and Na content. By comparing bias-dependent experimental topographic images to simulated images, we determined the detailed atomistic structure of both observed surfaces. The found dramatic structural changes are highly unusual and cast doubt on any prediction of surface properties based on bulk electronic structure. Indeed, we found no indication of the predicted quantum spin Hall behavior.

O 13.12 Mon 18:00 MA 041

Initial stages of the Fe2ZrSi Heusler alloy formation — •Katerina Horakova[1], Jan Honolka[1], Jan Lancok[1], Vladimir Chab[1], and Petr Sajdl[2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, 182 21 Prague 8, Czech Republic — [2]Institute of Chemical Technology Prague, 166 28 Prague 6, Czech Republic

We measured the electronic structure of clean Zr (0001) surfaces before and after adsorption of submonolayer coverages of Si and Fe atoms. Measurements were done using k-space microscopy. Our aim is to study the initial stages of the formation of Fe2ZrSi Heusler alloys on this surface. Our work is motivated by a passivation process of zirconium, widely used in the nuclear power industry. Fe and Si are deposited sequentially on the clean Zr surface. The structure of the surface was analysed by LEED and XPS. Different chemical states of Zr were found as a function of temperature and the composition. On a clean surface we detected two different chemical states of the Zr, one corresponding to the metal Zr, and the second to the bond with

hydrogen naturally trapped in the bulk. After Si deposition, a slight annealing at 400°C of the Si layer produces a new quasicrystalline structure connected with strong changes of the electronic structure at Ef. These changes are probably a result of Zr-Si-H bonding. The deposition of Fe and subsequent annealing produces a disordered layer only.