O 55: Electronic Structure and Spin-Orbit Interaction II

Time: Wednesday 16:00–19:15 Location: H42

O 55.1 Wed 16:00 H42

Hexagonal warping effects in the spin-split electronic structure of the $BiAg_2$ surface alloy — •Hendrik Bentmann[1,2], Mattia Mulazzi[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe, Germany

Whereas the Rashba-model predicts an isotropic spin-orbit (SO) splitting and an in-plane spin orientation for the electronic states in a two-dimensional electron gas (2DEG), the anisotropic lattice symmetries in a real system can lead to significant deviations from this scenario. Based on angle-resolved photoemission experiments, we discuss such effects for the surface states of the $BiAg_2$ surface alloy, a prototype model system for SO effects in 2DEGs. The dispersion of the surface states shows a pronounced hexagonal warping which is accurately captured by $k{\cdot}p$-theory taking into account the C_{3v}-symmetry of the surface. Additionally, we find threefold modulations in the photoemission intensity giving hints on the influence of the lattice symmetry on the orbital character of the electronic states. We compare our results on $BiAg_2$ with similar effects in the surface electronic structure of the topological insulator $Bi_2Te_3(0001)$.

O 55.2 Wed 16:15 H42

Single Dirac-cone on the Cs-covered topological insulator surface $Sb_2Te_3(0001)$ — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Sebastian Fiedler[1,2], Christian Junger[1,2], Chul-Hee Min[1,2], Kazuyuki Sakamoto[3], Friedrich Reinert[1,2], and Kenya Shimada[4] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522, Japan — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

In contrast to more prominent topological insulator (TI) materials like Bi_2Te_3 and Bi_2Se_3 the surface electronic structure of naturally p-type Sb_2Te_3 is comparably unexplored. Using angle-resolved photoelectron spectroscopy (ARPES) we measured the occupied electronic structure of clean and Cs-covered $Sb_2Te_3(0001)$. The surface-doping-induced band bending results in a non-rigid shift of the electronic valence band features leaving the Dirac-point right above the Fermi-level. The influence of the adatoms is compared to effects of metal adsorption on other TI surfaces. Furthermore we identify a trivial, Rashba-split surface state by photon-energy-dependent ARPES and studied its spin-character using spin-resolved ARPES.

O 55.3 Wed 16:30 H42

Determining the Rashba splitting of $BiCu_2$/Cu(111) by STS via interband scattering — •Manuel Steinbrecher[1], Hasmik Harutyunyan[1], Christian R. Ast[2], and Daniel Wegner[1] — [1]Physikalisches Institut and CeNTech, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Max Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Rashba systems are a promising class of materials for use in spintronics applications. They are characterized by surface states that are spin-split in k-space due to strong spin-orbit coupling. Well-known Rashba systems under recent investigation are alloys on noble metal surfaces. We have examined one of these surface alloys, Bi/Cu(111), by STM and STS measurements. By evaluating standing waves of the Rashba-split surface states, we have expanded an elegant method for measuring surface-state dispersions and compared the results with ARPES measurements and DFT calculations. For occupied states, we have found multiple intra- and interband scattering channels that enable the quantitative determination of band dispersions including the Rashba splitting. The results are in very good agreement with ARPES data and demonstrate the usefulness of this strategy to determine the band structure of Rashba systems. The lack of possible scattering channels will be discussed in terms of spin polarization and hybridization effects. We will provide an outlook on results regarding unoccupied states where DFT predictions mostly lack experimental verification.

O 55.4 Wed 16:45 H42

Theory of spin-orbit coupling at LaAlO3/SrTiO3 interfaces and SrTiO3 surfaces — •Zhicheng Zhong — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

The theoretical understanding of the spin-orbit coupling (SOC) effects at $LaAlO_3/SrTiO_3$ interfaces and $SrTiO_3$ surfaces is still in its infancy. We perform first-principles density-functional-theory calculations and derive from these a simple tight-binding Hamiltonian, through a Wannier function projection and group theoretical analysis. We find striking differences to the standard Rashba theory for spin-orbit coupling in semiconductor heterostructures due to multi-orbital effects: by far the biggest SOC effect is at the crossing point of the xy and yz (or zx) orbitals; and around the Γ point a Rashba spin splitting with a cubic dependence on the wave vector $\vec{k}$ is possible.

O 55.5 Wed 17:00 H42

Strong correlations at topological insulator surfaces and the breakdown of the bulk-boundary correspondence — •Manuel Schmidt — RWTH Aachen, Deutschland

The criteria for strong correlations on surfaces of three-dimensional topological insulators are discussed. Usually, the Coulomb repulsion at such surfaces is too weak for driving a phase transition to a strongly correlated regime. I discuss a mechanism and possibilities of its experimental implementation by which the strength of the Coulomb interaction can be tuned over a wide range. In the strongly interacting regime, the surface states are gapped, even though the topological classification of the bulk band structure predicts gapless surface states.

O 55.6 Wed 17:15 H42

Bi/Ag(111) - A "Bird's Eye View" - Spin-resolved Band Structure above the Fermi Level — •Sune N. P. Wissing[1], Anke B. Schmidt[1], Fabian Zinser[2], Klaus Kern[2], Christian R. Ast[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Max-Planck-Institut für Festkörperforschung Stuttgart, Germany

We studied the unoccupied electronic structure of the surface alloy Bi/Ag(111) $(\sqrt{3}\times\sqrt{3})\,R30°$ with scanning tunneling spectroscopy and spin- and angle-resolved inverse photoemission. The adsorption of heavy elements on noble-metal surfaces results in surface alloys, which exhibit surface states with large Rashba-type spin splittings. Detailed information about the occupied electronic structure is available from various angle-resolved photoemission studies. Above the Fermi level, we have identified several unoccupied states with significant spin dependence. We determined their nature regarding symmetry and bulk vs. surface character as well as their energy vs. momentum dispersion and their spin dependence. We will discuss our results in the light of theoretical calculations [1].

[1] G. Bihlmayer *et al.*, PRB **75**, 195414 (2007)

O 55.7 Wed 17:30 H42

Rashba-Type Spin-Split Surface: $(\sqrt{3}\times\sqrt{3})$Bi/Ag(111)$R30°$ — •Lydia El-Kareh, Paolo Sessi, Thomas Bathon, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We report on low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) investigations of the $(\sqrt{3}\times\sqrt{3})$Bi/Ag(111)$R30°$ surface alloy, that has been reported to show a giant Rashba-Bychkov (RB) effect [1,2]. Comparison of our STS data with photoemission experiments and first principle calculations [3] allow the identification of two downward dispersing spin-split surface states with onsets at $-100\,\mathrm{meV}$ and $+725\,\mathrm{meV}$ with respect to the Fermi level. Bias-dependent quasi-particle interference maps reveal a striking energy dependence of scattering processes at step edges and around impurities. Based on a detailed analysis of the obtained data we will discuss the band dispersion and spin topology of both bands.

[1] C. R. Ast *et al.*, Phys. Rev. Lett. **98**, 186807 (2007).
[2] C. R. Ast *et al.*, Phys. Rev. B **75**, 201401(R) (2007).
[3] G. Bihlmayer *et al.*, Phys. Rev. B **75**, 195414 (2007).

O 55.8 Wed 17:45 H42

Unoccupied surface state of Tl/Si(111): Rotating spin and gi-

ant splitting — •Sebastian D. Stolwijk[1], Kazuyuki Sakamoto[2], Anke B. Schmidt[1], Peter Krüger[3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Graduate School of Advanced Integration Science, Chiba University, Japan — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

Spin-resolved inverse photoemission experiments reveal the unoccupied electronic structure along the $\bar{\Gamma}\bar{\mathrm{K}}$ direction of the Tl/Si(111)-(1×1) surface. Our recently developed **RO**tatable **S**pin-polarized **E**lectron source (ROSE) enables measurements of the in-plane and out-of-plane component of the polarization vector. With this, we identify a spin-orbit split surface state, whose polarization vector rotates from the usual Rashba direction to the direction perpendicular to the surface upon approaching the $\bar{\mathrm{K}}$ point. This effect can be simply understood as a consequence of the 2D symmetry of the hexagonal system [1]. Remarkably, the spin-orbit split surface state shows almost complete out-of-plane polarization with opposing sign at the $\bar{\mathrm{K}}$ and $\bar{\mathrm{K}}'$ point. Moreover, the spin-orbit split surface state exhibits a giant splitting in energy of more than 0.5 eV. Our results are supported and discussed on the basis of calculations within the GW approximation including spin-orbit coupling. Charge distributions of the surface state reveal that the giant splitting is due to a strong localization close to the Tl atom.

[1] K. Sakamoto et al., Phys. Rev. Lett. **102**, 096805 (2009)

O 55.9 Wed 18:00 H42

Origin of Rashba-splitting in the quantized subbands at the Bi_2Se_3 surface — •Hadj Mohamed Benia[1], Alexander Yaresko[1], Andreas P. Schnyder[1], Jürgen Henk[2], Chentiang Lin[1], Klaus Kern[1,3], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Institut für Physik -Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg, D- 06099 Halle (Saale), Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We study the band structure of the Bi_2Se_3 topological insulator (111) surface using angle-resolved photoemission spectroscopy (ARPES). We examine the situation where two sets of quantized subbands exhibiting different Rashba spin-splitting are created via bending of the conduction (CB) and the valence (VB) bands at the surface. We show that the potential gradients at both 2DEGs are similar and therefore not responsible for the splitting discrepancy. On the other hand, first principles calculations show that the contribution of Bi 6*p* states to the VB is clearly smaller than to the CB. Therefore, and since Bi 6*p* states are characterized by a strong spin-orbit coupling (SOC), the spin-splitting discrepancy is traced back to a difference in the SOC strength.

O 55.10 Wed 18:15 H42

Visualizing Anderson Localization of Non-Interacting Electrons — Fabian Zinser[1], Maurits W. Haverkort[1], Sune N. P. Wissing[2], Anke B. Schmidt[2], Markus Donath[2], Klaus Kern[1], and •Christian R. Ast[1] — [1]MPI für Festkörperforschung, 70569 Stuttgart — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

Randomness destroys translational invariance resulting in exponential spatial localization of wave functions through quantum interference. This effect — known as Anderson localization — is a universal property of waves, which has been observed directly in light and matter. In electron systems, Anderson localization has been studied mostly indirectly in transport experiments through metal-insulator transitions or conductance fluctuations. This complicates theoretical descriptions as, e. g., calculating the conductance remains a challenging task despite highly sophisticated models. Using the Bi_xPb_{1-x}/Ag(111) mixed surface alloy, we go beyond averaged quantities both in theory and experiment. We measure simultaneously chemical composition and local electronic structure linking experiment and theory on the most fundamental level: we demonstrate the atomically resolved observation of spatial wave function localization for a mixed surface alloy — a purely two-dimensional electron system in a static disordered potential. We then use the chemical composition as the structural input for the "original" real space Anderson tight-binding model which allows us to directly compare the locally resolved wave functions in experiment and theory with remarkable agreement.

O 55.11 Wed 18:30 H42

Spin Polarized Photoemission from Bi2Te3 and Sb2Te3 Topological Insulator Thin Films — •Lukasz Plucinski[1,2], Alexei Herdt[1,2], Gustav Bihlmayer[3], Gregor Mussler[4], Sven Döring[2], Detlev Grützmacher[4], Stefan Blügel[3], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institute PGI-6, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [3]Peter Grünberg Institute PGI-1, Forschungszentrum Jülich, 52428 Jülich, Germany — [4]Peter Grünberg Institute PGI-9, Forschungszentrum Jülich, 52428 Jülich, Germany

Spin polarized photoemission spectra from surfaces of Bi2Te3 and Sb2Te3 thin films show up to 45% in-plane spin polarization in the Dirac cone near the Fermi level, which is consistent with the dedicated ab initio theoretical results which find spin polarization in the order of 40-50% when averaged over the surface quintuple layer with the exponential depth profile related to the scattering mean free path of the VUV photoelectrons. Furthermore a non-zero out-of-plane spin polarization component is found in the Bi2Te3 hexagram Fermi surface.

We will discuss the spin-orbit entanglement mechanism behind the non-100% spin polarization in topologically protected surface states, and propose possible surface engineering solutions to increase the spin polarization of the Dirac cone in films grown by the MBE. Furthermore we will compare analytical band structure models with the DFT-based slab calculations.

O 55.12 Wed 18:45 H42

Electron dynamics of the topological insulator Bi_2Te_2Se — •Daniel Niesner[1], Thomas Fauster[1], Oleg Tereshchenko[2,4], Konstantin Kokh[3,4], and Evgueni Chulkov[5] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 A3, 91058 Erlangen — [2]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — [3]Institute of Geology and Mineralogy, 630090 Novosibirsk, Russia — [4]Tomsk State University, 634050 Tomsk, Russia — [5]Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain

In addition to the conventional Dirac cone, bismuth chalcogenides exhibit a high-lying topological surface state (TSS) in a projected bulk bandgap 1...1.5 eV above the Fermi level [1].

Bichromatic two-photon photoemission (2PPE, $h\nu = 1.65\,\mathrm{eV} + 4.65\,\mathrm{eV}$) was employed to follow the transient occupation of this state and the conduction band (CB*) above it. In addition, an image-potential state (IPS) is observed at a similar final-state energy. From a careful analysis of the polarization- and the time-dependence of the 2PPE data, the lifetimes of the single states are deconvolved. They amount to 25 fs (IPS), 22 fs (TSS) and 13 fs (CB*). Also, a linear energy-dependence of the decay rate of the conduction band below the TSS is found, as it is characteristic for layered materials [2].

[1] D. Niesner *et al.*, Phys. Rev. B 86, 205403 (2012)
[2] S. Xu *et al.*, Phys. Rev. Lett. 76, 483 (1996)

O 55.13 Wed 19:00 H42

Computing the LDOS for a disordered 2DEG with Rashba-type spin orbit interaction — Jascha Ulrich[1], Serge Florens[2], •Markus Morgenstern[1], Daniel Hernangomez[3], and Thierry Champel[3] — [1]2. Physikalisches Institut B, RWTH Aachen — [2]Institut Néel, CNRS/UJF, Grenoble — [3]LPMMC, CNRS/UJF, Grenoble

We present the application of a recent formalism developed by Serge Florens and Thierry Champel for the description of the single-electron dynamics under high magnetic fields in smoothly varying potential landscapes to systems with Rashba-type spin-orbit interaction subject to disorder both in the electrostatic potential $V(\vec{r})$ and the Rashba parameter $\alpha(\vec{r})$. Assuming an electrostatic disorder potential $V(\vec{r})$ and a Rashba parameter $\alpha(\vec{r})$ in the plane of the two-dimensional electron gas which vary locally linear on the scale of the magnetic length l_B and working in the high-field limit of negligible Landau level mixing, we present a compact formula for the temperature-broadened local density of states $\rho^{\mathrm{STS}}(\omega, \vec{r})$ as measured in an STS experiment according to the popular Tersoff-Hamann formula for setups with constant tip density of states. The resulting expression can efficiently be evaluated numerically by Fourier transform methods on home computers for arbitrary electrostatic and Rashba disorder maps. Explicit analytic expressions for limiting cases of zero temperature and constant Rashba parameter are given. We discuss the effects of the electrostatic potential and Rashba fluctuations on the electron dynamics and the form of the local density of states.