O 8: Electronic Structure and Spin-Orbit Interaction I

Time: Monday 10:30–13:00 Location: GER 38

O 8.1 Mon 10:30 GER 38

Depending on how you look at it - (un)conventional spin topology in the unoccupied band structure of Bi/Ag(111) — •Sune N. P. Wissing[1], Anke B. Schmidt[1], Christian R. Ast[2], Hossein Mirhosseini[3], Jürgen Henk[4], and Markus Donath[1] — [1]Westfälische Wilhelms-Universität Münster, Germany — [2]Max-Planck-Institut für Festkörperforschung Stuttgart, Germany — [3]Johannes Gutenberg-Universität Mainz, Germany — [4]Martin-Luther-Universität Halle-Wittenberg, Germany

We report on the challenge to determine the spin of the electronic structure out of a spin-polarized (inverse) photoemission experiment. For this purpose, we present a study on the unoccupied electronic structure of Bi/Ag(111) with spin- and angle-resolved inverse photoemission. Above the Fermi level, we identify several states with distinct spin character.

We focus our attention on the two p_{xy}-derived surface states. For the downward dispersing $m_j = 1/2$ state, theoretical calculations [1] predict a complex spin topology, where the spin polarization changes sign at the band maximum. Our experimental findings, however, indicate a spin splitting compatible with the conventional Rashba model. To shed more light on this issue, we investigated the spin topology with the help of first-principles electronic-structure and photoemission calculations. We will discuss the dependence of the measured spin topology on the polarization of the emitted light and the symmetry of the involved electronic states.

[1] G. Bihlmayer *et al.*, Phys. Rev. B **75**, 195414 (2007)

O 8.2 Mon 10:45 GER 38

Spin-flip scattering in the surface bands of $BiAg_2$/Ag(111) — •Gustav Bihlmayer[1], Lydia El-Kareh[2], Matthias Bode[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Since its discovery, the surface alloy $BiAg_2$/Ag(111) has attracted considerable attention due to the 'giant Rashba' splitting in the occupied surface bands. Recently, also the unoccupied part of the spectrum was investigated by scanning tunneling microscopy. But, although theory predicted a rather complex spin-texture of these bands [1], the quasiparticle interference patterns seem compatible with a conventional Rashba-type spin-polarization of these bands [2]. Close examination of the spin- and orbital resolved bandstructures obtained by density functional theory show, that the orbital structure allows spin-flip scattering processes that can reconcile experimental evidence with theoretical predictions. Our calculations and experiments show that this behavior is not only characteristic for the Bi-based surface alloy, also in the $PbAg_2$/Ag(111) system these spin-flip scattering events are observed. The same mechanism also blocks quasiparticle interference in forward scattering, while other scattering events are explicitly forbidden by time-reversal symmetry.

[1] G. Bihlmayer et al., Phys. Rev. B **75**, 195414 (2007)
[2] L. El-Kareh et al., Phys. Rev. Lett. **110**, 176803 (2013)

O 8.3 Mon 11:00 GER 38

Rashba-split surface states of $(\sqrt{3} \times \sqrt{3})$Pb/Ag(111)$R30°$ — •Lydia El-Kareh[1], Gustav Bihlmayer[2], Arne Buchter[3], Hendrik Bentmann[3], Friedrich Reinert[3], Stefan Blügel[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We report on a combined low-temperature scanning tunneling spectroscopy (STS), angle-resolved photoemission spectroscopy (ARPES), and density functional theory (DFT) investigation of the $(\sqrt{3} \times \sqrt{3})R30°$ Pb/Ag(111) surface alloy which provides a giant Rashba-type spin-splitting [1,2]. By means of STS and quantum interference mapping we determined the band onsets, splitting strengths, and dispersions for two Rashba-split bands. The unambiguous assignment of scattering vectors is achieved by comparison to ARPES measurements. The detailed analysis of the spin and orbital character of both bands as obtained by DFT calculations allows to solve an apparent deviation between experimentally observed scattering events and the theoretically predicted spin polarization [3].

[1] D. Pacilé *et al.*, Phys. Rev. B **73**, 245429 (2006).
[2] G. Bihlmayer *et al.*, Phys. Rev. B **75**, 195414 (2007).
[3] L. El-Kareh *et al.*, Phys. Rev. Lett. **110**, 176803 (2013).

O 8.4 Mon 11:15 GER 38

The Unoccupied Band Structure of Pb/Ag(111) — •Katharina T. Ritter, Sune N. P. Wissing, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Surface alloys of heavy elements on noble metal fcc(111) surfaces are known to exhibit strongly Rashba-split band structures. Especially the surface alloys with $(\sqrt{3} \times \sqrt{3})R30°$ reconstruction have been in the focus of theoretical and experimental reasearch. So far, most experimental data result from photoemission experiments and hence are limited to the occuppied electronic states.

Here, we perform spin- and angle-resolved inverse photoemission to access the unoccupied band structure of Pb/Ag(111). Above the Fermi level, we identify several states with distinct spin dependence. We determine their nature concerning symmetry, bulk vs. surface character, energy vs. momentum dispersion, and spin character. As we recently also investigated the related surface alloy Bi/Ag(111), we will compare the results of both systems and analyse systematic changes accompanying the reduction of the number of valence electrons of the adsorbate by one.

O 8.5 Mon 11:30 GER 38

Bulk and surface Rashba states in ferroelectric GeTe: combined experimental and theoretical SX-ARPES study — H. Volfova[1], J. Krempasky[2], H. Dill[2], V. Strocov[2], J. Braun[1], H. Ebert[1], K. Hricovini[6], R. Calarco[3], R. Bertacco[4], S. Picozzi[5], and •Jan Minar[1] — [1]LMU Munich, Munich, Germany — [2]PSI, Villigen, Switzerland — [3]PDI Berlin, Germany — [4]Politecnico Milano, Italy — [5]CNR-SPIN L'Aquila, Italy — [6]Universite de Cergy-Pontoise, France

The recent theoretical investigations of Picozzi et al. [1] predicted a huge Rashba effect originating from bulk states in ferroelectric GeTe, which spin polarisation can be switched by reversing its ferroelectric polarisation. However, detailed experimental and theoretical studies of the electronic structure by means of the angle resolved photoemission (ARPES) are until now missing. Here we present a combined theoretical and experimental study of the electronic structure of GeTe investigated with the aid of the bulk sensitive soft X-ray (SX)-ARPES [2]. It will be shown that a proper description of the photoemission process is necessary to understand the experimental results. These effects are included in the one-step model of photoemission implemented in the SPR-KKR package [3], which presents clear evidence for the predicted bulk Rashba state. [1] Di Sante et al., Andvanced materials 25, 509 (2013) [2] A. Gray, J. Minar et al., Nat. mat. 10, 759 (2011) [3] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011)

O 8.6 Mon 11:45 GER 38

Chiral magnetism of magnetic adatoms from Rashba electrons — •Juba Bouaziz[1], Manuel dos Santos Dias[1], Abdelhamid Ziane[2], Mouloud Benakki[2], Stefan Blügel[1], and Samir Lounis[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Laboratoire de Physique et Chimie Quantique, Faculté des Sciences, Université Mouloud Mammeri, 15000 Tizi-Ouzou, Algeria

We investigate chiral magnetic long-range interactions among adatoms mediated by surface states spin-splitted by spin-orbit coupling. Using the Rashba model, the tensor of exchange interactions is extracted wherein a two-ion anisotropy term is found besides the usual isotropic exchange interaction (J) and the Dzyaloshinskii-Moriya interaction (DM). The inter-adatom distance controls the strength of these terms which we exploit to design chiral magnetism in Fe nanotructures on Au(111) surface. In contrast to [1], we include without approximation the contribution of the integrable singularity observed at the extremum of the dispersion curve. When the magnetic moments are out-of-plane, we demonstrate within a simple approach that J and DM are respec-

tively related to superpositions of the out-of-plane and in-plane components of the skyrmionic magnetic waves induced by the adatoms in the surrounding electron gas [2].

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

[1] H. Imamura *et al.* Phys. Rev. B **69**, 121303 (2004)
[2] S. Lounis *et al.* Phys. Rev. Lett. **108**, 207202 (2012)

O 8.7 Mon 12:00 GER 38

Quasiparticle spin-interference by scattering off magnetic atoms on metal surfaces with spin orbit coupling — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, David S. G. Bauer, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present density-functional calculations of the quasiparticle interference at surfaces due to scattering off magnetic adatoms. Our focus is on $3d$ impurities on Au(111) where the spin-orbit coupling (SOC) causes a Rashba-type splitting of the surface state. The spin polarization of the quasiparticle waves shows a non-collinear texture because of SOC. We investigate the dependence of the polarization on the orientation of the impurity magnetic moment. We compare to previous model-based results [1] and discuss the relation to the scattering properties of the impurity, taking into account the non-zero probability of time-reversed transitions due to the magnetic moment. In our calculations we employ the KKR-Green function method for the electronic structure and scattering properties at defects [2]. We acknowledge financial support from the DFG (SPP-1666) and from the Virtual Institute Topological Insulators of the Helmholtz Association and computational support from the JARA-HPC Supercomputing Center at the RWTH Aachen.

[1] S. Lounis, A. Bringer, and S. Blügel, Phys. Rev. Lett. **108**, 207202 (2012).
[2] S. Heers, PhD Thesis, RWTH Aachen (2011); D.S.G. Bauer, PhD Thesis, RWTH Aachen (2013).

O 8.8 Mon 12:15 GER 38

Giant splitting of unoccupied surface resonant state on Tl/Si(111) — •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]Department of Nanomaterials Science, Chiba University, Chiba 263-8522, Japan — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The Tl/Si(111)-(1 × 1) surface features outstanding properties - a unique spin pattern in momentum space and an unoccupied surface state with giant spin splitting at the $\bar{\mathrm{K}}$ point [1,2]. In this contribution, we focus on the unoccupied surface electronic structure along the $\bar{\Gamma}\bar{\mathrm{M}}$ direction. Spin- and angle-resolved inverse photoemission experiments with sensitivity to the in-plane and out-of-plane components of the spin polarization vector are conducted with the help of our recently developed **RO**tatable **S**pin-polarized **E**lectron source (ROSE). Along $\bar{\Gamma}\bar{\mathrm{M}}$ only in-plane polarization is found. Moreover, we identify a spin-orbit-split surface resonant state, which exhibits a Rashba-type splitting. Remarkably, the size of the Rashba splitting is comparable to the giant splitting found for the Bi/Ag(111) surface [3].

[1] K. Sakamoto et al., Phys. Rev. Lett. **102**, 096805 (2009)
[2] S. D. Stolwijk et al., Phys. Rev. Lett. **111**, 176402 (2013)
[3] C. Ast et al., Phys. Rev. Lett. **98**, 186807, (2007)

O 8.9 Mon 12:30 GER 38

Spin-split surface states in the unoccupied electronic structure of Tl/Ge(111)-(1x1) — •Philipp Eickholt[1], Sebastian D. Stolwijk[1], Anke B. Schmidt[1], Peter Krüger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms Universität, Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms Universität, Münster, Germany

The unoccupied electronic structure of Tl/Si(111)-(1x1) exhibits a unique spin-orbit-split surface state with rotating polarization vector and giant energy splitting at the $\overline{\mathrm{K}}$ point [1]. Here, we present spin- and angle-resolved inverse-photoemission results on the unoccupied electronic structure of the isoelectronic Tl/Ge(111)-(1x1) surface, which is expected to show similar properties [2]. In fact, along the $\overline{\Gamma\mathrm{K}}$ direction, a similar spin-orbit-split surface state is found with comparable properties as observed on Tl/Si(111). Differences between the two surfaces can be seen along $\overline{\Gamma\mathrm{M}}$, where a Rashba-type spin-split surface state on the Tl/Ge(111) surface lies well within a band gap, while it is degenerate with the bulk bands on the Si substrate. Remarkably, our measurements feature a spin asymmetry directly at the $\overline{\mathrm{M}}$ point where spin degeneracy should prevail.

[1] Sebastian D. Stolwijk et al., Phys. Rev. Lett. **111**, 176402 (2013)
[2] Y. Ohtsubo et al., J.Phys.: Condens. Matter **24**, 092001 (2012)

O 8.10 Mon 12:45 GER 38

Hysteretic melting of a soliton lattice in a commensurate charge modulation — •Tobias Mauerer[1], Pin-Jui Hsu[1], Matthias Vogt[1], J.J. Yang[2], Yoon Seok Oh[3], S-W. Cheong[2,3], Matthias Bode[1], and Weida Wu[3] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Laboratory for Pohang Emergent Materials and Department of Physics,Pohang University of Science and Technology, Pohang 790-784, Republic of Korea — [3]Rutgers Center for Emergent Materials and Department of Physics and Astronomy,Rutgers University, Piscataway, New Jersey 08854, USA

We report on the observation of the irreversible transition of a commensurate charge modulation in $IrTe_2$ from transport and scanning tunneling microscopy (STM) studies. Below the transition ($T_C \approx 275\,K$ on cooling) a $q = 1/5$ charge modulation was observed, which is consistent with previous studies [1,2]. Additional modulations [$q_n = (3n + 2)^{-1}$] appear below a second transition at $T_S \approx 180\,K$ on cooling. The coexistence of various modulations persist up to T_C on warming. The atomic structures of charge modulations and the temperature-dependent STM studies suggest that 1/5 modulation is a periodic soliton lattice which partially melts below T_S on cooling. Our results provide compelling evidence that the ground state of $IrTe_2$ is a commensurate 1/6 charge modulation, which originates from periodic dimerization of Te atoms visualized by atomically resolved STM images.

[1] J. J. Yang *et al.*, Phys. Rev. Lett. **108**, 116402 (2012).
[2] S. Pyon *et al.*, J. Phys. Soc. Jap. **81**, 053701 (2012).