TT 29: Topology- and Symmetry-Protected Materials (Joint session of DS, HL, MA, O and TT organized by O)

Time: Tuesday 10:30–13:30 Location: S051

Invited Talk TT 29.1 Tue 10:30 S051

Toward single atom qubits on a surface: Pump-probe spectroscopy and electrically-driven spin resonance — •William Paul — IBM Research, San Jose CA, USA

We will discuss the characterization of spin dynamics by pump-probe spectroscopy and the use of gigahertz-frequency electric fields to drive spin resonance of a Fe atom on a MgO/Ag(001) surface. Also, the technical challenges in applying a precise voltage to the tip sample junction across a wide radio-frequency bandwidth will be described. The energy relaxation time, T1, of single spins on surfaces can be measured by spin-polarized pump-probe STM (scanning tunneling microscopy) [1]. To date, the relaxation times reported for Fe-Cu dimers on Cu2N insulating films have been of the order ˜100 ns [1]. A three-order-of-magnitude enhancement of lifetime, to ˜200 us, was recently demonstrated for Co on a single-monolayer of MgO [2]. Here, we report on the tailoring of the T1 lifetime of single Fe atoms on single- and multi- layer MgO films grown on Ag(001). Next, we demonstrate electron spin resonance of an individual single Fe atom, driven by a gigahertz-frequency electric field applied across the tip-sample junction, and detected by a spin-polarized tunneling current. The principle parameters of the spin resonance experiment, namely the phase coherence time T2 and the Rabi rate, are characterized for Fe atoms adsorbed to the monolayer MgO film.

[1] Loth et al., Science 329, 1628 (2010) [2] Rau and Baumann et al., Science 344, 988 (2014) [3] Baumann and Paul et al., Science 350, 417 (2015)

TT 29.2 Tue 11:00 S051

Mesoscopic spin coherence through electron focusing in topological insulators — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Long coherence lengths of quasiparticles are an essential ingredient for spintronics applications. Motivated by previous experiments [P. Sessi et al, Nat. Comm. 5, 5349 (2014)] we undertook a combined theoretical and experimental study, using density functional theory and STM, where we found standing wave patterns of mesoscopic dimensions around magnetic defects on the surface of Bi_2Te_3. We identified two necessary conditions for the effect: (i) focusing by the Bi_2Te_3 Fermi surface due to its hexagonal warping and (ii) large scattering strength of the magnetic defects. We modeled different magnetic defects and analyzed the energy dependence of the scattering properties in the energy range where the shape of the constant energy contour changes from circular over hexagonal to snowflake-like. For the calculation of the electronic structure and scattering properties we employed the full-potential relativistic Korringa-Kohn-Rostoker Green-function method [D.S.G. Bauer, Schriften des Forschungszentrums Jülich, Key Tech. 79 (2014); N. H. Long et al., Phys. Rev. B 90, 064406 (2014)].

We enjoy close collaborations with P. Sessi and M. Bode (Würzburg University) and thank for financial support from the DFG (SPP-1666), the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre (RWTH Aachen University).

TT 29.3 Tue 11:15 S051

Generation of transient photocurrents in the topological surface state of Sb_2Te_3 bydirect optical excitation with mid-infrared pulses — •Johannes Reimann, Kenta Kuroda, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

We combine tunable mid-infrared (MIR) pump pulses with time- and angle-resolved two-photon photoemission (2PPE) to study the ultrafast electron dynamics of the topological surface state (TSS) of Sb_2Te_3. It is revealed that MIR pulses permit a direct excitation of the unoccupied TSS owing to an optical coupling across the Dirac point. This is in contrast to the delayed filling observed in previous 2PPE experiments on topological insulators with pump photon energies in the visible range. The novel optical coupling provokes asymmetric transient populations of the TSS at $\pm k_{||}$, which mirrors a macroscopic photoexcited electric surface current. By observing the decay of the asymmetric population, we directly investigate the dynamics of the photocurrent in the time domain. We find a long equilibration time of $\tau_k^e = 2.5$ ps for the population at $\pm k_{||}$ that shows no significant change for different sample temperatures of 80 K and 300 K. Considering a Debye temperature of $\theta_D = 162$ K this result indicates that phonons play only a minor role for the momentum scattering. We suggest that scattering at surface defects is instead the limiting factor for the current lifetime.

TT 29.4 Tue 11:30 S051

Time- and angle-resolved two-photon photoemission from p-doped septuple-layered topological insulators — •Sebastian Otto, Jonas Rietsch, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time- and angle-resolved two-photon photoemission is used to study the electronic structure of septuple-layered antimony telluride crystals of different p-dopings. All surfaces show a topological surface state. The Dirac point is found between $E_F + 0.38$ eV for $GeSb_2Te_4$ and $E_F + 0.25$ eV for $SnBi_{0.2}Sb_{1.8}Te_4$. The topological surface state is populated mainly from the conduction band minimum according to the evolution of its temporal population. Similar to the case of $SnSb_2Te_4$ [1], the electrons in the topological surface state decay rather fast into a partially unoccupied valence band maximum depending on the strength of the p-doping.

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

TT 29.5 Tue 11:45 S051

Controlling the spin-texture of topological insulators with organic molecules — Sebastian Jakobs[1,2], Benjamin Stadtmüller[1], •Dominik Jungkenn[1], Martin Laux[1], Johannes Stöckl[1], Martin Aeschlimann[1], Stefan Mathias[3], and Mirko Cinchetti[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [3]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We present a rational design approach to customize the spin texture of surface states of a topological insulator (TI). This approach relies on the extreme multifunctionality of organic molecules that are used to functionalize the surface of the prototypical TI Bi2Se3. For the rational design we use theoretical calculations to guide the choice and chemical synthesis of appropriate molecules that customize the spin texture of Bi2Se3. The theoretical predictions are then verified in angular-resolved photoemission experiments. We show that the surface can be passivated while the Dirac cone can be shifted at will by tuning the strength of the molecule-TI interaction and Rashba-split quantum-well interface states can be created. These tailored interface properties - passivation, spin-texture tuning and creation of hybrid interface states - open a wide field of opportunities for interface assisted molecular spintronics in spin-textured materials.

TT 29.6 Tue 12:00 S051

Modulating the spin polarization of photoelectrons from a topological insulator — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

It has been predicted that the spin polarization of photoelectrons emitted from a topological insulator is highly tunable so that almost 100 % polarization along any arbitrary direction can be achieved by tuning the polarization of light [1]. There have been a number of experimental confirmations of this photo-induced spin modulation phenomenon [2-6]. Although this photo-induced spin modulation in topological insulators suggests a new kind of spin-polarized electron sources [2], there have been some experimental results that cannot be explained by previous theoretical descriptions [1]. In this presentation, we theoretically investigate photoemission process from topological insulators and interpret the recent experimental observations.

[1] C.-H. Park, S. G. Louie, Phys. Rev. Lett. 109, 097601 (2012).

[2] C. Jozwiak et al., Nat. Phys. 9, 293 (2013).
[3] Z.-H. Zhu et al., Phys. Rev. Lett. 112, 076802 (2014).
[4] Z. Xie et al., Nat. Commun. 5, 3382 (2014).
[5] Y. Cao et al., arXiv:1211.5998v1
[6] J. Sánchez-Barriga et al., Phys. Rev. X 4, 011046 (2014).

TT 29.7 Tue 12:15 S051

Dirac Cone Protected by Non-Symmorphic Symmetry and highly dispersive 3D Dirac crossings in ZrSiS — •Leslie Schoop[1], Mazhar Ali[2], Carola Strasser[1], Viola Duppel[1], Stuart Parkin[2], Bettina Lotsch[1], and Christian Ast[1] — [1]Max Planck Insititut für Festkörperforschung, Stuttgart — [2]Max Planck Institut für Mikrostrukturphysik, Halle

Materials harboring exotic quasiparticles, such as Dirac and Weyl fermions have garnered much attention from the physics and material science communities. Here, we show with angle resolved photoemission studies supported by ab initio calculations that the highly stable, non-toxic and earth-abundant material, ZrSiS, has an electronic band structure that hosts several Dirac cones which form a Fermi surface with a diamond-shaped line of Dirac nodes. We also experimentally show, for the first time, that the square Si lattice in ZrSiS is an excellent template for realizing the new types of 2D Dirac cones protected by non-symmophic symmetry and image an unforseen surface state that arises close to the 2D Dirac cone. Finally, we find that the energy range of the linearly dispersed bands is as high as 2 eV above and below the Fermi level; much larger than of any known Dirac material so far. We will discuss why these characteristics make ZrSiS very promising for future applications.

TT 29.8 Tue 12:30 S051

2D Dirac cones protected by non-symmorphic symmetry in ZrSiS and ZrSiTe — •Andreas Topp[1], Leslie M. Schoop[1], Carola Strasser[1], Bettina V. Lotsch[1,2,3], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — [3]Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-81377 München

Three-dimensional Dirac semimetals which accommodate massless Dirac and Weyl fermions, have recently become of considerable interest because of their exotic physical properties, e.g. an extremly high mobility and magnetoresistance. A new compound, ZrSiS, hosting a square lattice of Si atoms, has been shown to host 3D Dirac cones at the Fermi level with a very large energy range of linear dispersion [1]. Additionally, a new type of Dirac cone protected by non-symmorphic symmetry has been found to exist below the Fermi level which was predicted theoretically to exist in a square lattice [2]. Here, we show by *ab initio* calculations, that in the compound ZrSiTe this cone is moved to the Fermi level. We present the crystal growth results and show preliminary ARPES data concerning the electronic structure of these two compounds.

[1] L. M. Schoop *et al.*, arXiv preprint arXiv:1509.00861 (2015).
[2] S. M. Young, and C. L. Kane, Phys. Rev. Lett. 115, 126803 (2015).

TT 29.9 Tue 12:45 S051

Resonant photoemission of the spin-polarized electronic structure in strongly spin-orbit coupled systems — •Henriette Maass, Hendrik Bentmann, Christoph Seibel, Thiago R. F. Peixoto, and Friedrich Reinert — Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg

Strong spin-orbit coupling leads to a lifting of the spin degeneracy in the electronic structure and the emergence of novel topological phases in non-centrosymmetric environments, such as interfaces or surfaces. Using resonant angle-resolved photoemission experiments (ARPES) we have investigated the spin-polarized electronic structure in the surface alloy $BiAg_2/Ag(111)$ and the topological insulator Bi_2Te_3.

Our data reveals pronounced momentum dependent modulations of the photoemission intensity in the 6p derived surface states of $BiAg_2/Ag(111)$, when the photon energy is tuned across the Bi 5d core level excitation. In particular a complete suppression of spectral weight of spin-up and spin-down valence bands occurs for energies shortly below the Bi $5d_{5/2}$ and the $5d_{3/2}$ core levels, respectively. At the same time a considerable modification of the photoelectron spin-polarization can be observed. We compare these results to the case of the topological insulator Bi_2Te_3, where similar variations in the photoemission intensity occur.

[1] H. Bentmann *et al.*, arXiv 1507.04664

TT 29.10 Tue 13:00 S051

Electronic structure and topology of the natural superlattice phase $\mathbf{Bi_1Te_1} = (\mathbf{Bi_2})_1(\mathbf{Bi_2Te_3})_2$ — •Markus Eschbach[1], Martin Lanius[1], Ewa Mlynczak[1], Jens Kellner[2], Chengwang Niu[1], Peter Schüffelgen[1], Mathias Gehlmann[1], Pika Gospodaric[1], Sven Döring[1], Martina Luysberg[1], Gregor Mussler[1], Gustav Bihlmayer[1], Markus Morgenstern[2], Detlev Grützmacher[1], Lukasz Plucinski[1], 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

We report on experimental and theoretical investigations of thin films of Bi_1Te_1 grown on Si(111), being part of the natural supperlattice phase series $[Bi_2]_x[Bi_2Te_3]_y$ with $x = 1$ and $y = 2$. Contrary to the closely related, prototypical 3D strong topological insulator Bi_2Te_3, its electronic strutcture as well as topological properties have not been adressed so far. In this study, we present detailed characterization of the bulk crystal structure by X-ray diffraction and transmission electron microscopy and the surface chemistry by X-ray photoelectron spectroscopy. The rich surface electronic structure, investigated by spin- and angle-resolved photoemission spectroscopy, reveals surface states that can be easily confused with Dirac cone-like topological surface states. However, we will show by experiment and comprehensive ab inito density functional theory calculations that Bi_1Te_1 is a weak topological insulator.

TT 29.11 Tue 13:15 S051

Probing the electronic structure of the magnetic topological insulator $\mathbf{(BiSbV)_2Te_3}$ with soft X-ray photoelectron spectroscopy — •Thiago Ribeiro Fonseca Peixoto[1,3], Mohammed Al-Baidhani[1,3], Henriette Maass[1,3], Christoph Seibel[1,3], Hendrik Bentmann[1,3], Steffen Schreyeck[2,3], Martin Winnerlein[2,3], Stefan Grauer[2,3], Charles Gould[2,3], Karl Brunner[2,3], Laurens Molenkamp[2,3], and Friedrich Reinert[1,3] — [1]EP VII, Fakultät f. Physik u. Astronomie, Uni-Würzburg — [2]EP III, Fakultät f. Physik u. Astronomie, Uni-Würzburg — [3]Röntgen Center for Complex Materials (RCCM), Uni-Würzburg

By means of X-ray photoemission (XPS) and absorption (XAS) spectroscopy we investigated the electronic structure of $(BiSbV)_2Te_3$ thin films, a three-dimensional magnetic topological insulator, recently reported as an anomalous quantum Hall system [1]. The films were epitaxially grown on a Si(111) crystal and covered by a Se cap to avoid contamination during exposition to air. After thermally desorbing the Se cap, the core-level lines of the constituent elements and the V $L_{2,3}$ absorption edges were measured for different V concentrations (0, 2 and 4 at.%). Our data evidence the incorporation of Se atoms in the film. By means of resonant photoemission we identify the signature of the V 3d states at the Fermi level, which may contribute to the exotic transport properties of the system. We discuss the chemical environment of the V atoms and show that our techniques are well suited for the study of the electronic properties of this novel class of materials.

[1] C.-Z. Chang *et al.*, Nat. Mat. Lett. **14**, 473 (2015).