MA 51: Topological Insulators I (joined session with TT)

Time: Thursday 9:30–12:45 Location: POT 251

Invited Talk MA 51.1 Thu 9:30 POT 251

Sub-nm probing of Topological insulators and Rashba systems — •Markus Morgenstern — II. Institute of Physics and JARA-FIT, RWTH Aachen, D-52074 Aachen, Germany

Spin-orbit interactions in solids are the key for many anticipated new functionalities ranging from the meanwhile traditional Datta-Das transistor to topological quantum computation using Majorana excitations. Local probes can provide crucial information on this interaction down to the nm scale. Within this talk, I will show how scanning tunneling spectroscopy reveals the presence of topologically protected edge states provided by a spin-orbit induced band inversion of heavy metal graphene [1], how the detrimental fluctuations of the spin-orbit interaction can be probed down to the nm length scale [2], and that ferroelectricity induces Rashba-type spin-orbit interaction within the bulk of the simple binary material GeTe [3].

[1] C. Pauly et al., Nat. Phys. 11, 338 (2015); ACS Nano 10, 3995 (2016). [2] J. R. Bindel et al., Nat. Phys. 12, 920 (2016). [3] M. Liebmann et al., Adv. Mat. 20, 560 (2016); H. J. Elmers et al., Phys. Rev. B 94, 201403 (2016).

MA 51.2 Thu 10:00 POT 251

2D Topological Insulators: Trends in Chemical Space — •Carlos Mera Acosta[1,2], Christian Carbogno[1], Adalberto Fazzio[2], Luca M. Ghiringhelli[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Instituto de Física, Universidade de São Paulo, SP, Brazil

2D topological insulators (TI) have attracted considerable scientific interest in recent years [1]. The search for new TIs has often focused on elements with strong spin-orbit coupling (SOC) [2], which can induce the necessary topological transition. In this work, we have computed the topological invariant Z_2 for 200 functionalized honeycomb-lattice systems using our recent Wannier center of charge (WCC) [3] implementation in the FHI-aims electronic structure code. Besides confirming the TI character of well-known materials, e.g., functionalized stanene [1], our study found several other yet unreported TIs. This reveals that also elements with relatively low SOC can form TIs. To analyze the observed trends in chemical space we relate the WCCs to the atomic features of the constituent atoms using a compressed-sensing approach. For this purpose, the LASSO and ℓ_0 minimization of Ref. [4] is extended from learning scalar properties to functions.

This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

[1] Y. Ren, Z. Qiao, and Q. Niu, *RPP* **79**, 6 66501 (2016).
[2] M. Z. Hasan and C. L. Kane, *Rev. Mod. Phys.* **82**, 3045 (2010).
[3] R. Yu, *et al.*, *Phys. Rev. B* **84**, 075119 (2011).
[4] L. M. Ghirighelli, *et al.*, *Phys. Rev. Lett.* **114**, 105503 (2015).

MA 51.3 Thu 10:15 POT 251

Occupied topological surface states in strained α-Sn — Victor Rogalev[1], •Tomáš Rauch[2], Markus Scholz[1], Felix Reis[1], Lenart Dudy[1], Andrzej Fleszar[3], Vladimir Strocov[4], Jürgen Henk[2], Ingrid Mertig[2,5], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany — [3]Institut für Theoretische Physik und Astronomie, Universität Würzburg, 97074 Würzburg, Germany — [4]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [5]Max Planck Institute for Microstructure Physics, 06120 Halle (Saale), Germany

Unstrained α-Sn is a semimetal with a non-trivial band ordering at the Γ point of the bulk Brillouin zone: $E(\Gamma_8^+) > E(\Gamma_7^-) > E(\Gamma_7^+)$. Strain in (001) direction lifts the degeneracy of the Γ_8^+ level at the Fermi energy. We demonstrate that compressive strain turns the system into a strong topological insulator, whereas tensile strain causes a transition into the topological Dirac semimetal phase.

I will present the results of calculations carried out along experimental findings obtained by soft X-ray angle-resolved photoemission. I will show that the existence of a previously unknown surface state located in the occupied projected bulk band structure of α-Sn is unveiled by both experimental and theoretical methods. In addition, its topological origin was confirmed by calculating the topological invariants of the bulk bands.

MA 51.4 Thu 10:30 POT 251

Engineering topological phases in crystalline symmetry-protected monolayers — •Chengwang Niu, Patrick M. Buhl, Gustav Bihlmayer, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The properties that distinguish topological crystalline insulators (TCIs) and topological insulators (TIs) rely on crystalline symmetry and time-reversal symmetry, respectively, which encodes different surface/edge properties. Here, we predict theoretically that TlM, thallium chalcogenide, (M = S and Se) (110) monolayers realize a family of two-dimensional (2D) TCIs characterized by mirror Chern number $\mathcal{C}_M = -2$ with an even number of band inversions. [1] Remarkably, under uniaxial strain (≈ 1%), a topological phase transition between 2D TCI and 2D TI is revealed in TlM. In contrast, for Na_3Bi, the band inversion occur at single k point, thus a coexistence of 2D TI and 2D TCI is obtained. [2] Finally, we show different edge-state behaviors, especially at the time reversal invariant points.

This work was supported by SPP 1666 of the DFG.

[1] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, and Y. Mokrousov, Nano Lett. **15**, 6071 (2015).

[2] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, and Y. Mokrousov, submitted.

MA 51.5 Thu 10:45 POT 251

Anisotropy of Magneto-Transport on the Surface of Topological Insulators — •Alexey Taskin[1], Henry Legg[2], Fan Yang[1], Andrea Bliesener[1], Satoshi Sasaki[3], Yasushi Kanai[3], Kazuhiko Matsumoto[3], Achim Rosch[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne — [2]Institute for Theoretical Physics, University of Cologne — [3]Scientific and Industrial Research, Osaka University

Recent advances in MBE growth and microfabrication technique allow to obtain Topological Insulator (TI) systems where the transport is dominated by the surface. Here we report a magneto-transport study of high-quality bulk-insulating $Bi_{2-x}Sb_xTe_3$ thin films, which were fabricated into devices with electrostatic gates on both bottom and top surfaces. For magnetic fields applied parallel to the surface of a TI, we found a clear anisotropy in magnetoresistance and related planar Hall effect that originates from the fundamental property of the surface Dirac fermions, the locking of their spin and momentum. The key signature of anisotropic magnetoresistance is a strong dependence on the gate voltage with a characteristic two-peak structure near the Dirac point. The observed anisotropy is related to a modification of the topological protection of the Dirac electrons against backscattering from impurities in the in-plane magnetic field and provides an example of a controllable time-reversal breaking on the surface of TIs.

Coffee Break

MA 51.6 Thu 11:30 POT 251

Topological insulator - superconductor hybrid devices — •Peter Schüffelgen, Daniel Rosenbach, Michael Schleenvoigt, Tobias W. Schmitt, Martin Lanius, Christian Weyrich, Tristan Heider, Benjamin Bennemann, Stefan Trellenkamp, Elmar Neumann, Gregor Mussler, Thomas Schäpers, and Detlev Grützmacher — Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany

3D topological insulators (TIs) possess metallic surface states with a spin-locked momentum. Therefore, in proximity to an s-wave superconductor, Majorana zero modes (MZMs) are predicted to occur at the surface of TIs. We found first signatures of 4π-periodic Josephson supercurrents in our topological Josephson junctions. The TI thin film was grown by means of molecular beam epitaxy on a Si(111) substrate and capped in-situ by a thin layer of aluminum to prevent thin film degradation and to preserve the pristine surface states during ex-situ fabrication. To increase the 4π-periodic contribution we fabricated quasi 1D Josephson junctions on pre-patterned silicon substrates. By covering the Si-111 surface partly with a thin layer of Si3N4/SiO2 we made the topological insulator grow only on the silicon surface. In this way we were able to realize 1D trenches by predefining the MESA structure before MBE growth. To further improve the quality of our hybrid devices we developed a process, which allows to deposit superconducting contacts via stencil lithography. Combining this technique with selective area growth allows to fabricate complex devices in-situ.

MA 51.7 Thu 11:45 POT 251

Ultrafast mid-IR pump, THz probe spectroscopy investigating of the topological insulator BSTS — •Matteo Montagnese, Jingy Zhu, Chris Rheinhoffer, Yoichi Ando, and Paul H. M. van Loosdrecht — II. Physikalishes Institut der Universität zu Köln, Zülpicher str 77, D-25127 Köln

We present ultrafast pump-probe measurements on the topological insulator BSTS. We employed a high-intensity tunable mid-IR pulse (2-10 microns) as a pump, generated by difference-frequency mixing in an optical parametric amplifier to excite the BSTS system below the onset of the bulk optical electronic continuum. Upon excitation, the far-IR (0.1-3 THz) response of the system has been probed by a single-cycle coherent THz pulse, generated by optical rectification of a near-IR pulse. The time-resolved transmittance of the THz spectra have been measured employing optical sampling and time-domain techniques. By tuning the pump energy, the impurity states leading to charge puddle formation and the surface state are selectively populated, with the aim of disentangling their respective contributions to the dynamic optical conductivity.

MA 51.8 Thu 12:00 POT 251

Observation of the Quantum Anomalous Hall Effect depending on structural properties of $(VBiSb)_2Te_3$ layers — •Martin Winnerlein, Steffen Schreyeck, Stefan Grauer, Sabine Rosenberger, Kajetan Fijalkowski, Charles Gould, Karl Brunner, and Laurens W. Molenkamp — Physikalisches Institut, Experimentelle Physik III, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The quantum anomalous Hall effect is observed in thin V-doped $(BiSb)_2Te_3$ layers, a magnetic topological insulator. Thin layers revealing quantization are reproducibly deposited by molecular beam epitaxy at growth conditions effecting a compromise between controlled layer properties and high crystal quality. The influence of Sb content, layer thickness, structural quality, used substrates and cap layers is studied.

The Sb content is the main layer parameter to be optimized in order to approach charge neutrality. The Sb content is reliably determined from the in-plane lattice constant measured by X-ray diffraction even in thin layers. Within a narrow range at about 80% Sb content, the Hall resistivity reveals a maximum at 4 K and quantizes at mK temperatures [1]. Under these conditions thin layers grown on Si(111) or InP(111) and with or without a Te cap layer exhibit quantization. The quantization persists independently from the substrate, cap layer, the limited crystal quality and the degradation of the layer. This proves the robustness of the quantum anomalous Hall effect.

[1] S. Grauer *et al.*, Phys. Rev. B **92**, 201304 (2015).

MA 51.9 Thu 12:15 POT 251

Quantum Hall effect in three-dimensional Bi_2Se_3 single crystals — •Olivio Chiatti[1], Marco Busch[1], Sergio Pezzini[2], Steffen Wiedmann[2], Oliver Rader[3], Lada V. Yashina[4], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]High Field Magnet Laboratory, Radboud University Nijmegen, 6525ED Nijmegen, The Netherlands — [3]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [4]Department of Chemistry, Moscow State University, 119991 Moscow, Russia

Topological insulators present surface (or edge) states of helically spin-polarized Dirac fermions, which are readily identified by spectroscopic methods. However, they are not so easily identified in transport, because they can be masked by bulk states. Bi_2Se_3 is one of the prototype topological insulators, but investigating transport by surface states has been hampered by residual bulk charge carriers. We have investigated nominally undoped, high-quality Bi_2Se_3 single crystals, with bulk electron densities of $n \approx 1.8 \cdot 10^{19}$ cm^{-3} and mobilities of up to $\mu \approx 10^3$ cm^2/Vs. Surface states have been confirmed by ARPES measurements [1]. We have measured magnetotransport between $T = 0.3$ K and $T = 72$ K, for tilted magnetic fields up to $B = 33$ T. We observe both Shubnikov-de Haas (SdH) effect and quantum Hall effect (QHE). The SdH oscillations appear dominated by 3D bulk charge carriers. However, the scaling of the QHE with sample thickness can be interpreted as transport over layered 2D states in the bulk.

[1] Chiatti *et al.*, Sci. Rep. **6**, 27483 (2016)

MA 51.10 Thu 12:30 POT 251

The electronic structure of few-quintuple-layer bismuth selenide from first-principles calculations — •Jae Young Kim and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

Topological insulators are materials that behave as insulators in the interior, but have conducting surface states protected by time-reversal symmetry [1]. Bi2Se3, a prototypical example of a three-dimensional topological insulator, is a layered material composed of five-atom layers arranged along the z-direction, known as quintuple layers [2]. In this presentation, we will discuss the results of our first-principles calculations on the electronic properties of few-quintuple-layer Bi2Se3 and their relevance to device applications based on topological insulators.

[1] Hasan, M. Z., & Kane, C. L. (2010). Colloquium: topological insulators. Reviews of Modern Physics, 82(4), 3045.

[2] Zhang, H., Liu, C. X., Qi, X. L., Dai, X., Fang, Z., & Zhang, S. C. (2009). Topological insulators in Bi2Se3, Bi2Te3 and Sb2Te3 with a single Dirac cone on the surface. Nature physics, 5(6), 438-442.