TT 104: Topological Insulators (organized by MA)

Time: Friday 9:30–12:00 Location: HSZ 04

TT 104.1 Fri 9:30 HSZ 04

Experimental characterization and simulation of quasi-particle-interference in the Bi-bilayer topological insulator — •Matteo Michiardi[1], Andreas Eich[2], Gustav Bihlmayer[3], Alex A. Khajetoorians[2], Jens Wiebe[2], Jianli Mi[4], Bo B. Iversen[4], Philip Hofmann[1], and Roland Wiesendanger[2] — [1]Department of physics and astronomy, Aarhus University, Denmark — [2]Institute of Applied Physics, University of Hamburg, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Center for Materials Crystallography, Aarhus University, Denmark

Topological insulators (TI) are a new class of materials that host gapless surface states with spin helicity. While several 3D TIs have been discovered, the interest in 2D TI systems that can host topological edge state is rising. A single bilayer of bismuth is predicted to be such a 2D TI. Here we present an experimental and theoretical study of a Bi-bilayer grown on 3D TI Bi_2Se_3. The use of Bi_2Se_3 as substrate allows the epitaxial growth of the bilayer in the rhombohedral structure, as shown by Scanning Tunnelling Microscopy. We calculate the band structure of the Bi-bilayer/Bi_2Se_3 system by Density Function Theory (DFT) and experimentally study the quasi particle interference (QPI) on the bilayer. In order to clarify the scattering channels responsible for the QPI, we perform simulations based on the Joint Density of States method starting from our DFT calculations. The comparison with the experimental results reveals a good match for a wide range of binding energies for both occupied and unoccupied states.

TT 104.2 Fri 9:45 HSZ 04

Quasiparticle self-consistent *GW* study of bismuth under strain — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

It has been recently claimed on the basis of ARPES measurements that bulk bismuth is a topological semimetal. The discrepancies between this result and previous *ab-initio* calculations were attributed to the failure of density functional theory (DFT) in the prediction of band gaps, because the topological or trivial character of Bi depends only on the "sign" of the very small direct band gap at the L point. We show that bulk Bi is indeed predicted by DFT in the local-density approximation (LDA) to be a trivial semimetal, with a surprisingly overestimated gap at L. We have performed quasiparticle self-consistent *GW* (QS*GW*) calculations for bulk bismuth that support its trivial character. The QS*GW* gap at L as well as the energy overlap between the electron and hole pockets are in much better agreement with experiments than the LDA ones. Thus, the QS*GW* approach appears as the right tool to study the trivial-to-topological transition that Bi experiences under stress, as a result of a change of sign of the gap at L. We have analyzed the effect of strain on the topological properties of bulk Bi. Whereas LDA predicts that an impractical stress is needed for such a transition, QS*GW* shows that bulk Bi becomes a topological semimetal already under very small stress. This work is supported by the Helmholtz Virtual Institute for Topological Insulators (VITI).

TT 104.3 Fri 10:00 HSZ 04

Combined STM/STS- and ARPES-investigation of the quaternary Topological Insulator $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ — •Thomas Bathon[1], Felix Reis[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a combined scanning tunneling microscopy/spectroscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES) characterization of the electronic properties of the quaternary compound $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$. ARPES-data evidence that this compound is still a Topological Insulator (TI) with a single Dirac cone, which is characteristic for the Bi_2X_3-class. The topological properties of the surface state, i.e. forbidden backscattering, have been confirmed by Fourier-transformed differential conductance (dI/dU) maps. Measurements performed both above and below the Fermi level allow us to determine the energy dispersion relation, the carrier velocity, and—by extrapolation to zero momentum—the position of the Dirac point. The observed scattering vectors are not as well-defined as those observed in binary compounds, probably due to substitutional disorder which results in a spatial fluctuation of the chemical potential. Our investigations illustrate how the properties of the well-known TI Bi_2Te_3 can be changed by chemical substitution.

TT 104.4 Fri 10:15 HSZ 04

Surface and bulk contributions to the electronic structure of the topological insulator Sb_2Te_3(0001) — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Jürgen Braun[3], Jan Minár[3], Kenya Shimada[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Department Chemie, Physikalische Chemie, Universität München, Butenandtstraße 5-13, D-81377 München — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Photon energy dependent angle-resolved photoemission measurements were performed to disentangle surface and bulk contributions to the electronic structure of the 3D topological insulator (TI) Sb_2Te_3. We discover a penetration of the topological surface state (TSS) into the bulk valence band regime where it coexists with bulk states without considerable hybridization. Our results indicate an emerging $k_\perp$-dispersion of the TSS at higher binding energies, which we attribute to an increasing bulk character. These observations deviate from previous findings for the isostructural TIs Bi_2Se_3 and Bi_2Te_3. Our results are supported by fully relativistic one-step photoemission calculations. [1] Seibel *et al.* PRB 86, 161105(R) (2012)

15 min. break

TT 104.5 Fri 10:45 HSZ 04

Spin-dependent unoccupied electronic structure of the topological insulator Sb_2Te_3 — •Anna Zumbülte[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Gregor Mussler[3], and Detlev Grützmacher[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Studies on three-dimensional topological insulators focus mainly on the well-known systems of Bi_2Se_3 and Bi_2Te_3 and the related ternary compounds. Theoretical predictions of chalcogenides as topological insulators with a single Dirac cone [1] include an additional compound, Sb_2Te_3. There, due to p-type doping of the available samples, the Dirac point lies above the Fermi level, making it inaccessible to photoemission experiments unless the surface is modified with an adsorbate [2]. Consequently, the electronic structure of this system has been left almost unstudied.

We present spin- and angle-resolved inverse-photoemission measurements of the unoccupied electronic states of Sb_2Te_3. In addition to the Dirac state, further spin-dependent features have been obtained which show a distinct Rashba splitting. The experimental data will be discussed along with bandstructure calculations.

[1] H. Zhang *et al.*, Nat. Phys. **5**, 438 (2009)
[2] C. Seibel *et al.*, Phys. Rev. B **86**, 161105 (2012)

TT 104.6 Fri 11:00 HSZ 04

Comparitive study of the ternary topological insulators Bi_2Se_2Te and Bi_2Te_2Se — •Felix Reis[1], Thomas Bathon[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The 3D topological insulators Bi_2Se_2Te and Bi_2Te_2Se have been investigated by combining the complementary experimental techniques scanning tunneling microscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES). With low temperature STM/STS technique we investigate the structural and electronic properties of both systems. Fourier-transformed quasi-particle interference (QPI)

maps give access to the scattering events within the topological surface state. Taking QPI maps for several energies allows us to obtain information on the position of the Dirac point and the carrier velocity by fitting the linear energy dispersion relation of the Dirac fermions. These results will be compared with the band structure as obtained by ARPES measurements.

TT 104.7 Fri 11:15 HSZ 04

A large-energy-gap oxide topological insulator based on the superconductor BaBiO3 — •Binghai Yan[1,2,3], Martin Jansen[1], and Claudia Felser[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden — [3]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

Topological insulators are a new class of quantum materials that are characterized by robust topological surface states (TSSs) inside the bulk-insulating gap, which hold great potential for applications in quantum information and spintronics as well as thermoelectrics. One major obstacle is the relatively small size of the bulk bandgap, which is typically around 0.3eV for the known topological insulator materials. Here we demonstrate through ab initio calculations that a known superconductor BaBiO3 (BBO) with a Tc of nearly 30 K emerges as a topological insulator in the electron-doped region. BBO exhibits a large topological energy gap of 0.7 eV, inside which a Dirac type of TSSs exists. As the first oxide topological insulator, BBO is naturally stable against surface oxidization and degradation, distinct from chalcogenide topological insulators. An extra advantage of BBO lies in its ability to serve as an interface between TSSs and superconductors to realize Majorana fermions for future applications in quantum computation.

Reference: B. Yan, M. Jansen, C. Feler, Nature Physics 9, 709*711 (2013) (arXiv:1308.2303).

TT 104.8 Fri 11:30 HSZ 04

Topological surface states of HgTe and Heulser compounds — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany.

We studied the topological electronic structures of HgTe and half Heusler compounds (e.g.: XYZ, X = rare earth elements, Y = trasition metal and Z = main group elements) by both *ab initio* calculations. The topological surface structures were investigated by the Wannier function based tight-binding method. The effects of external strains induced from the substrate and surface terminations are taken into account by the atomic positions. Our results agree well with recent photoemission experiments.

TT 104.9 Fri 11:45 HSZ 04

Sputter Deposition of Half-Heusler Topological Insulators — •Benedikt Ernst, Daniel Ebke, Stanislav Chadov, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Heusler compounds have exhibited manifold physical properties in the recent years and attracted a lot of interest in the field of spintronic applications due to their half-metallic properties. Recently, a topological insulating state has been predicted by theory for some of these compounds.

In this work, we have prepared Heusler materials such as LaPdBi and LaPtBi for which a topological insulating behavior was predicted. Co-deposition by DC- and RF magnetron sputtering was used to prepare corresponding thin films. To realize an epitaxial film growth in the crystallographic $C1_b$ structure on MgO-substrates, a buffer layer was applied and optimized. Initial transport properties will be discussed with regard to the film composition and the crystallographic properties.