TT 40: Topological Insulators (jointly with HL, MA)

Time: Wednesday 16:45–19:15 Location: HSZ 04

TT 40.1 Wed 16:45 HSZ 04

Complex spin structure of the topological insulator Bi_2Te_3(0001) — •Jürgen Henk[1], Arthur Ernst[1], Sergey V. Eremeev[2], and Evgueni V. Chulkov[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Donostia International Physics Center, San Sebastian, Spain

Topological insulators — like Bi_2Te_3(0001) — show a unique surface electronic structure. A model Hamiltonian [1] describes well the anisotropic dispersion of the Dirac state, as is evident from agreement with photoemission experiments (e. g. [2]). The spin of the Dirac state shows a circular arrangement in the momentum distribution, even in the presence of warping.

We prove by relativistic first-principles calculations that the spin structure of the Dirac state in Bi_2Te_3(0001) is much more complicated than that derived from model calculations. First, all three spin components at the top Te layer are reversed with respect to those in the subsurface layers, and, second, the circular spin structure is destroyed at the cusps of warped momentum distributions, showing a vortex-like structure. Our findings are explained by hybridization of p orbitals in the topmost quintuple layer and may have implications for spintronic applications.

[1] L. Fu, Phys. Rev. Lett. **103** (2009) 266801.
[2] D. Hsieh et al, Phys. Rev. Lett. **103** (2009) 146401.

TT 40.2 Wed 17:00 HSZ 04

Thermal and structural stability of the topological state on Bi_2Se_3 — •Dandan Guan[1,2], M. Bianchi[1], R. C. Hatch[1], S. Bao[2], J. Mi[3], B. B. Iversen[3], and Ph. Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics, Zhejiang University, Hangzhou, China — [3]Department of Chemistry, Aarhus University, Denmark

Topological insulator surfaces have recently attracted considerable attention, not least because they are predicted to play host to many novel physical phenomena. The topological states are also thought to have possible applications in (spin) transport, since they are not only protected from back-scattering, their very existence can be viewed as a bulk property. This implies that minor surface modifications can change the detailed dispersion of the topological state, but not remove it altogether.

We investigate the thermal and structural stability of the topological state on Bi_2Se_3 using angle resolved photoemission spectroscopy. The electron-phonon coupling strength is obtained through measurements of the temperature-dependent self-energy and the resulting λ value is compared to the bulk and to other surface-localized states. The structural stability is tested by surface modifications through noble gas ion bombardment.

TT 40.3 Wed 17:15 HSZ 04

Does magnetism destroy the Dirac state in a topological insulator? — Arthur Ernst[1], •Jürgen Henk[1], Evgueni V. Chulkov[2], Igor V. Maznichenko[3], and Ingrid Mertig[3] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Donostia International Physics Center, San Sebastian, Spain — [3]Martin Luther University Halle-Wittenberg, Halle, Germany

A striking feature of topological insulators is that the Dirac states are protected by topology. However, how robust are these surface states against perturbations really? Given the prescribed spin structure of the Dirac state, one may ask whether magnetism destroys this state or — at least — modifies its spin-resolved dispersion.

To answer the above question we have investigated theoretically the topological insulator Bi_2Te_3(0001) by means of relativistic *ab initio* calculations. The Bi atoms in the topmost quintuple layer form a substitutional alloy with Mn (i. e. $Bi_{1-c}Mn_c$) that is described within the coherent potential approximation. We find significant modificiations of the Dirac state in dependence of the Mn concentraction c and on the orientation of the Mn magnetic moments.

TT 40.4 Wed 17:30 HSZ 04

Surface electronic structure and surface state topology of Sb(110). — •Marco Bianchi[1], D. Guan[1,2], A. Strozecka[3], C.H. Voetmann[1], J. I. Pasqual[3], S. Bao[2], and Ph. Hofmann[1] — [1]Inst. Fysik og Astronomi Aarhus Universitet, Aarhus, Denmark — [2]Dep. of Physics, Zheijang University, Hangzhou, China — [3]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

Topological insulators are a recently discovered class of materials where the bulk is insulating while fundamental topological considerations require the surfaces to be metallic. The first experimentally confirmed topological insulator was the intermetallic alloy $Bi_{1-x}Sb_x$ ($0.09 < x < 0.18$). This topological insulator phase owes its existence to important changes in the band structure as the two semimetals are alloyed. Theoretical predictions based on the topological character of the bulk electronic structure agree with measurements on the alloy and also predict pure Sb to be a strong topological insulator. On the other hand, the electronic structure of the Bi surfaces, while being very similar to that of the alloy, appears to be consistent with that of a topologically trivial material.

We report on an experimental investigation of the Sb(110) electronic structure combining scanning tunnelling microscopy with angle-resolved photoemission. The topological character of the surface states can be inferred from the number of Fermi level crossings between time-reversal invariant momenta in the surface Brillouin zone. This surface topology is compared to that of Bi(110), Sb(111) and the theoretical predictions.

TT 40.5 Wed 17:45 HSZ 04

Topological insulators in ternary compounds with a honeycomb lattice — •Stanislav Chadov[1], Jürgen Kübler[2], and Claudia Felser[1] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universtität, 55099 Mainz — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, 64289 Darmstadt

Based on electronic structure calculations we propose the certain extension to the class of the topological insulators which provide the convenient material base to realize the phenomenon of quantum spin Hall effect intensively studied nowadays. These new candidates (e. g. LiAuSe, KHgSb) are ternary semiconductors with a weakly coupled honeycomb layers (e. g. Au-Se, Hg-Sb) analogical to a weakly graphite sheets. It makes them very similar to graphene which is a single layer of graphite: their band structures exhibit the so-called linearly dispersive Dirac cone centered at the Fermi energy. However, in contrast to graphene with two Dirac cones at K and K' points, these materials exhibit the surface states formed by only a single Dirac cone at the Γ point, allowing for the non-vanishing quantum spin Hall effect. The additional stuffing" elements (Li, K, etc.) extend the material multifunctionality, i. e. give more possibilities for tuning and coupling of their properties. In contrast to other topologically non-trivial systems, as e. g. recently proposed half-Heuslers, the honeycomb compounds possess the non-zero band gap in the bulk, i. e. provide the "natural" 3D topological materials.

TT 40.6 Wed 18:00 HSZ 04

Thallium-based topological insulators from first principles — •Gustav Bihlmayer[1], Sergey V. Eremeev[2], Stefan Blügel[1], and Eugene V. Chulkov[3] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Institute of Strength Physics and Materials Science, Tomsk, Russia — [3]Donostia International Physics Center (DIPC), San Sebastián, Spain

Currently, there is a substantial interest in topological insulators, which show protected edge-states carrying dissipationless spin currents. Among the new classes of these materials the Tl-based compounds $TlAB_2$ (A=Bi,Sb; B=Se,Te) have attracted considerable interest both on the experimental and theoretical side. We present density functional theory calculations of the bulk materials and their (111) surfaces, displaying protected Dirac-cone shaped surface states together with "trivial" surface states. In contrast to layered materials like Bi_2Te_3, these compounds are of more three-dimensional character. From the bulk calculations we observe a strong sensitivity of the topological properties on the structural details, that have to be described very accurately. In the surface calculations deeply penetrating Dirac-cone states are observed, calling for careful convergence of the calculations with respect to the film thickness. Similar materials, e.g. the sulfides and $InAB_2$ compounds will be discussed for comparison.

TT 40.7 Wed 18:15 HSZ 04

Electronic structure of the topological semiconductors PtYSb, PtLaBi, and PtGdBi explored by hard X-ray photoelectron spectroscopy. — •Siham Ouardi[1], Shekar Shandra[1], Gerhard H. Fecher[1], S. Chadov[1], X. Kozina[1], G. Stryganyuk[1], C. Felser[1], S. Ueda[2], and K. Kobayashi[2] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universtität, 55099 Mainz — [2]National Institute for Materials Science, SPring-8, Hyogo, Japan

One of the recent topics in spintronics is the realization of the so-called topological insulators, that are insulators in the bulk and gapless semiconductors at the surface. Besides the well-known wide range of properties of the Heusler family it was recently shown that many of the heavy Heusler semiconductors with 1:1:1 composition and $C1_b$ structure are zero band-gap insulators and exhibit a inverted band structure. The density of states of several compounds was investigated by bulk sensitive hard X-ray photoelectron spectroscopy. First experimental results on PtYSb, PtLaBi, and PtGdBi give clear evidence for the zero band-gap state. Their structural, spectral and transport characteristics will be compared to calculations.

TT 40.8 Wed 18:30 HSZ 04

Tolerance of topological surface state towards adsorbed magnetic moments: Fe on Bi_2Te_3 — •Markus Scholz[1], Dmitry Marchenko[1], Jaime Sanchez-Barriga[1], Andrei Varykhalov[1], Andrei Volykhov[2], Lada Yashina[2], and Oliver Rader[1] — [1]Helmholtz-Zentrum für Materialien und Energie, Berlin, Deutschland — [2]Moscow State University, Moskau, Russland

Topological surface states on Bi_2Se_3 and Bi_2Te_3 are protected by time reversal symmetry [1]. Magnetic fields break time-reversal symmetry, and they have been used in two-dimensional spin quantum-Hall systems to destroy the topological edge states [2]. Another possibility is to introduce magnetic moments. This has been done by substitution of Mn and Fe into the bulk [3][4]. For Fe a small gap of 44meV was created, however, at very large amounts (12%). In this work, we deposit Fe directly onto the surface where the topological surface state is localized. We show for coverages of 0.25 and 1 ML Fe that the Dirac point remains intact and no gap appears. Core level spectroscopy of Bi and Te states gives insight into the interaction between substrate and adatoms. In addition, extra surface states appear at the Fermi energy which show a large Rashba-type spin-orbit splitting. The orientation of the spin of both, the topological as well as the Rashba-type split surface states is analysed. [1] Kane and Mele, Phy. Rev. Lett 95, 146802 (2005); Liang Fu et al., Phys. Rev. Lett. 98, 106803 (2007) [2] König et al.,Science 318, 5851 (2007) [3] Hsieh et al., Phys. Rev. Lett. 103, 146401 (2009) [4] Chen et al., Science 329, 5992 (2010)

TT 40.9 Wed 18:45 HSZ 04

Rashba-type surface emission observed on W(110) — •Juergen Braun[1], Jan Minar[1], Akio Kimura[2], Koji Miyamoto[2], Markus Donath[3], and Hubert Ebert[1] — [1]Department Chemie, LMU München, Germany — [2]Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan — [3]Physikalisches Institut, Universität Münster, Germany

In this contribution we discuss surface related spectral features of bcc W(110) by means of angle- and spin-resolved photoemission. For more than thirty years Tungsten serves as a prototypical material for studying spin-orbit effects in simple metals. Also, it is used for a quite long time in electron polarimeters [1]. Nevertheless, there still remain some pecularities in its electronic structure concerning surface emission. It is known that a surface resonance exists on W(110) dispersing around $\overline{\Gamma}$ in the vicinity of the Fermi level [2]. But not much is understood concerning surface emission for higher binding energies. From our investigation we found that surface emission dominates the $E(\mathbf{k}_\parallel)$ intensity distribution measured along $\overline{\Gamma N}$. The spin analysis reveals a Rashba-like behavior for features related to the spin-orbit induced symmetry gap existing at $\overline{\Gamma}$. The theoretical analysis has been performed in the framework of the fully relativistic version of the one-step model of photoemission [3].

1. J. Kirschner, Polarized electrons at surfaces, Springer, Berlin (1985). 2. R. H. Gaylord et al., PRL 62, 2036 (1989). 3. H. Ebert et al., The Munich SPR-KKR package, version 5.4, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2010).

TT 40.10 Wed 19:00 HSZ 04

Wave-packet transport in HgTe — •Viktor Krueckl and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Recent experiments have shown the Quantum Spin Hall State in mercury telluride quantum wells and the associated edge channel transport at zero external magnetic field [1]. We employ a four band model to investigate the propagation of such topological edge state wave-packets in the gap, as well as bulk states in the conducting region. Our recently developed algorithm is able to solve the time-dependent scattering problem for arbitrary scattering potentials and gives revealing insight into the occurring edge phenomena. The obtained time evolution of the wavefunction is used to calculate the complete energy dependent scattering matrix for a time-independent Hamiltonian. With this we investigate the transport in different mesoscopic setups and are particularly interested in the scattering of edge states at constrictions.

[1] A. Roth, C. Brüne, H. Buhmann, L. W. Molenkamp, J. Maciejko, X.-L. Qi and S.-C. Zhang, Science **325**, 294 (2009)