O 37: [MA] Joint Session "Topological Insulators II" (jointly with DS, HL, O, TT)

Time: Wednesday 9:30–13:00 Location: EB 301

O 37.1 Wed 9:30 EB 301

Topologically-related properties in presence of disorder. First-principle study — •Stanislav Chadov — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The presence of disorder is often seen as a destructive mechanism which must be reduced by any means. In present study we attempt to make it constructive due to the robustness of the spin current in topological insulators with respect to the time-reversal symmetric perturbations. Based on the first-principle calculations involving the Coherent Potential Approximation (CPA), we inspect the disorder-affected transport properties of the random alloys between topologically non-trivial and trivial materials. The subsequent analysis encounters few interesting aspects: the way how to increase the Hall angle by using random disorder and an indication for the topological Anderson insulator. In addition CPA provides an alternative recipe to validate the non-trivial topological state of the material based on a purely bulk information.

O 37.2 Wed 9:45 EB 301

Probing the topological states of Sb_2Te_3 by spin polarized photoemission spectroscopy — •Christian Pauly[1], Gustav Bihlmayer[2], Marcus Liebmann[1], Dinesh Subramaniam[1], Martin Grob[1], Alexander Georgi[1], Markus Scholz[3], Jaime Sanchez Barriga[3], Stefan Blügel[2], Oliver Rader[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA-FIT, Germany — [3]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany

Using high resolution spin- and angle-resolved photoemission spectroscopy, we map the electronic structure and spin texture of the surface states of the topological insulator Sb_2Te_3. Similar to the well explored Bi_2Te_3 and Bi_2Se_3 which possess TI properties with the most simple electronic structure [1], we directly show that Sb_2Te_3 exhibits Z_2 topological properties with a single spin-Dirac cone at the Γ-point. In addition, a strongly spin-orbit split surface state is observed at lower energy. In Γ-K direction, the band is located within a spin-orbit gap, governing the energy position of the state. In combination with DFT calculation, we provide direct evidence for an argument given by Pendry [2], that there must be at least one surface state inside a SO gap, if the gap is located in the zone. Thus, similar to the topological state, this state is protected by symmetry. [1] H. Zhang et al., Nature Phys. 5, 438 (2009) [2] J. B. Pendry et al., Surf. Sci. 49, 87 (1975)

O 37.3 Wed 10:00 EB 301

Electronic properties and magnetic anisotropy of individual Co adatoms adsorbed on topological insulator surfaces — •T. Eelbo[1], M. Sikora[2], M. Waśniowska[1], M. Dobrzański[2], M. Gyamfi[1], G. Bihlmayer[3], I. Miotkowski[4], A. Kozlowski[2], and R. Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, Hamburg, Germany — [2]Department of Solid State Physics, AGH University of Science and Technology, Aleja Mickiewicza 30, Kraków, Poland — [3]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [4]Department of Physics, Purdue University, West Lafayette, USA

The interaction of magnetic impurities adsorbed on topological insulator surfaces causes changes of the electronic properties of the surfaces or the adatoms themselves. In addition the adatoms can present different magnetic properties due to interaction with the host. For this reason we studied the electronic properties and magnetic anisotropy of individual Co atoms adsorbed on Bi_2Se_3 by means of scanning tunneling microscopy/spectroscopy (STM/STS) and x-ray magnetic circular dichroism (XMCD) at low temperatures. After the deposition onto the cold surface STM measurements reveal two different adsorption sites for Co adatoms. Two resonances in the occupied states for both species of adatoms are found using STS. Moreover, XMCD measurements reveal a magnetic anisotropy with the easy axis being aligned out-of-plane. The experimental findings are compared to results of ab-initio calculations.

O 37.4 Wed 10:15 EB 301

Theoretical study on the reactive chemical doping of the Bi_2Se_3 surface — •Janos Kiss[1,2], Stanislav Chadov[1,2], and Claudia Felser[1,2] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recent experimental results have shown that the surface of Bi_2Se_3 exposed to air will become n-type doped. Furthermore, the surface gradually undergoes an oxidation reaction leading to a degradation of the surface transport properties, where the contribution of the topological surface states are consequently decreasing. This is expected to be caused by Se vacancies. However, the formation mechanism of this vacancies and the interaction of moisture -i.e. water- with Bi_2Se_3 is still not clarified. Therefore, we will present the results of our large scale ab-initio calculations and molecular dynamics simulations in order to investigate the effect of Se vacancies and the reactivity of water upon the electronic and atomic structure of the surface.

O 37.5 Wed 10:30 EB 301

Heusler topological insulators: Electronic structure and transport properties — •C. Shekhar[1], S. Ouardi[2], G. H. Fecher[1,2], A. K. Nayak[1], A. Gloskovskii[2], E. Ikenaga[3], S. Ueda[4], K. Kobayashi[4], and C. Felser[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [3]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan — [4]National Institute for Materials Science, SPring-8, Hyogo, Japan

Topological insulators have a high potential for spintronics devices and quantum computation. Various Heusler compounds crystallize in a fcc structure of the $C1_b$ type and consist of 2 transition metals and a main group element. If the compounds contain heavy metals and a lanthanide element then they exhibit extraordinary physical properties including superconductivity, half-metallic, semiconducting-like behavior, giant magnetoresistivity, heavy fermion state and zero band gap. The density of states of XMZ Heusler compounds (M = Gd, Lu, X= Au, Pt, Pd and Z= Pb, Sb, Bi) were investigated by hard X-ray photoelectron spectroscopy. The comparison of the experimental results to calculations gives evidence for the zero band gap state of the compounds. Further, the temperature dependence of electrical conductivity, magneto resistance, Hall mobility, Seebeck coefficient and thermal conductivity were investigated. The compounds exhibit a high Hall mobility and a linear magnetoresistance (MR). The observed linear MR is a quantum MR and due to the topological insulator state.

O 37.6 Wed 10:45 EB 301

Topological phase transitions in Bi(111) bilayer by breaking time-reversal symmetry — •Hongbin Zhang, Frank Freimuth, Gustav Bihlmayer, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Time-reversal breaking brings forth many novel phenomena in topological insulators [1]. In this work, using the first principles FLAPW method combined with the Wannier functions technique [2], we investigated topological phase transitions with respect to exchange fields of a two-dimensional topological insulator – Bi(111) bilayer [3]. Numerical evaluation of the spin Chern number [4] for different magnitudes of exchange fields reveals that when the time reversal symmetry is broken by a small exchange field, the system keeps the properties of a topological insulator. After a metallic phase in the intermediate region, the quantum anomalous Hall phase with the non-zero Chern number occurs at sufficiently large enough exchange fields. We analyzed the relation between the spin Chern number, the Z_2 number and the Chern number, and also the phase diagram from the viewpoint of the evolution of the electronic structure, edge states and transport properties in this system. We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] X. Qi, *et al.*, Phys. Rev. B. **78**, 195424 (2008).
[2] www.flapw.de; F. Freimuth, *et al.*, Phys. Rev. B. **78**, 035120 (2008).
[3] M. Wada, *et al.*, Phys. Rev. B **83**, 121310(R) (2011).
[4] E. Prodan, *et al.*, Phys. Rev. B **80**, 125327 (2009).

O 37.7 Wed 11:00 EB 301

Predicting surface states from the bulk embedding self-energy — •Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Institute for Advanced Simulation & Peter Grünberg Institut, Forschungszentrum Jülich und JARA, 52425 Jülich, Germany

The protected states localized at surfaces and interfaces of topological insulators are a consequence of the electronic structure of the bulk. Their peculiar features like the typical spin-structure makes them an interesting field of basic research with possible applications in spintronics.

We demonstrate how these states can be efficiently simulated by means of the embedding self-energy as obtained in the Green function embedding technique[1]. The embedding self-energy, which can be understood as a generalized logarithmic derivative, is a property of the bulk crystal only and contains all information required to analyze the consequences of the bulk topology on the surface bandstructure. Using the FLAPW implementation of the embedding method as provided in the FLEUR-code[2], we show how the surface states of prototypical topological insulators like Bi_2Se_3 can be studied efficiently with an easy and direct access to effects for example due to electric fields applied to the surface.

[1] D. Wortmann, H. Ishida, S. Blügel. Phys. Rev. B **66**, 075113(02)
[2] http://www.flapw.de

15 min. break

O 37.8 Wed 11:30 EB 301

Influence of magnetic impurities on doping and scattering properties of topological surface states: Fe on Bi_2X_3 (X=Te, Se) — •Markus R. Scholz[1], J. Sánchez-Barriga[1], D. Marchenko[1], A. Varykhalov[1], E. Rienks[1], A. Volykhov[2], L. V. Yashina[2], and O. Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Moscow State University

We study the effect of Fe impurities deposited on the surface of the topological insulators Bi_2Se_3 and Bi_2Te_3 by means of photoelectron spectroscopy. The topological surface state reveals surface electron doping when the Fe is deposited at room temperature and hole doping when deposited at low temperture ($\sim$ 10 K). We show that in both cases the topological surface state remains intact and gapless. We analyze the line broadening for pure Bi_2X_3 (X=Se, Te) and after deposition of Fe. We observe that the constant broadening in the bulk band gap range increases by a factor of 2 upon deposition of Fe. Because we deposit the Fe without electron doping, this result is not due to a gain in warping as was recently suggested. We discuss the results based on different types of scattering mechanisms.

O 37.9 Wed 11:45 EB 301

Origin of the strong circular dichroism of the topological surface state of Bi_2Te_3 — •Jaime Sánchez-Barriga[1], M. R. Scholz[1], D. Marchenko[1], A. Varykhalov[1], O. Rader[1], A. Volykhov[2], L. V. Yashina[2], J. Braun[3], J. Minár[3], and H. Ebert[3] — [1]Helmholtz-Zentrum Berlin — [2]Moscow State University — [3]Ludwig-Maximilians-Universität München

We have recently reported a strong circular dichroism effect in angle-resolved photoemission of the spin polarized topological surface state of Bi_2Te_3 [1]. The effect has been observed recently also for Bi_2Se_3 and the origin is controversial [2-4]. An initial-state model has been employed to determine the spin orientation directly [3]. We present a series of photoemission measurements and density functional calculations coupled to one-step photoemission theory. Both experiment and theory reveal that the dichroism effect changes sign as a function of photon energy which excludes the initial-state model.

[1] M. R. Scholz, J. Sánchez-Barriga, D. Marchenko, A. Varykhalov, A. Volykhov, L. V. Yashina, O. Rader, submitted to Phys. Rev. Lett. (2010), arXiv:1108.1053
[2] S. R. Park et al., arXiv:1103.0805
[3] Y. H. Wang, D. Hsieh, D. Pilon, L. Fu, D. R. Gardner,Y. S. Lee, N. Gedik, arXiv:1101.5636
[4] Y. Ishida et al., Phys. Rev. Lett. 107, 077601 (2011)

O 37.10 Wed 12:00 EB 301

Prediction of topological insulators in TlBiSe2 family of chalcogenides — •binghai yan — BCCMS, University of Bremen, Bremen

In this work, we predicted several new topological insulator materials in thallium (Tl) based ternary chalcogenides from first-principles calculations, including TlBiQ2 and TlSbQ2 (Q=Te, Se and S). TlBiSe2 and TlSbSe2 are found to be strong TIs with a large energy gap (~ 0.2 eV), while TlBiTe2 is a topological semimetal. A simple Dirac-type dispersion of topological surface states is observed, similar to the Bi2Se3 type of materials. On the other hand, TlBiS2, TlSbTe2 and TlSbS2 are small gap insulators near the topological trivial-nontrivial transition boundary. Particularly TlBiTe2 can be a good candidate in the seeking of Majorana fermions for its co-existing superconductivity property. The topological feature of TlBiSe2 and TlBiTe2 has already been confirmed by recent experiments. References: 1. B.H. Yan, C.X. Liu, H.J. Zhang, C.Y. Yam, X.L. Qi, Th. Frauenheim and S.C. Zhang, Europhys. Lett. 90, 37002 (2010). 2. Y. L. Chen, Z. K. Liu, J. G. Analytis, J.-H. Chu, H. J. Zhang, B. H. Yan, S.-K. Mo, R. G. Moore, D. H. Lu, I. R. Fisher, S. C. Zhang, Z. Hussain, and Z.-X. Shen, Phys. Rev. Lett. 105, 266401(2011).

O 37.11 Wed 12:15 EB 301

A recipe for new Topological Insulators based on bonds, bands, symmetry andheavy atoms — •L. Müchler[1], B. Yan[2,3], S. Chadov[1,4], F. Casper[1], S-C. Zhang[2], and C. Felser[1,4] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Department of Physics, McCullough Building,Stanford University,Stanford, CA 94305-4045, USA — [3]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

In this work we will present a recipe to find new Topological Insulators (TIs) based on bonds, bands, symmetry and heavy atoms. A big issue concerning the compounds known up to now is the control of the bulk carrier density to produce truly insulating samples in the bulk. Using concepts from chemistry and supported by density-functional calculations, we want to motivate an extended search for new compounds with tunable bulk properties.

O 37.12 Wed 12:30 EB 301

Graphene nanoribbons with Au induced spin-orbit effects: a DFT study — •Gustav Bihlmayer and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Historically, the prediction of a topological protection of the edge state of a zig-zag graphene nanoribbon (ZGNR) was at the beginning of the field of topological insulators. Unfortunately, a realization of this system is prevented by (i) the extremely small spin-orbit coupling (SOC) in graphene and (ii) the tendency towards formation of antiferromagnetically coupled edge states in ZGNRs.

New experimental and theoretical results show that SOC effects can be enhanced by substrates and/or adatoms with a large atomic number, so that up to 100 meV spin-splitting can be realized in the graphene. Additionally, hybridization with the substrate changes also the localization of the edge state and its tendency towards antiferromagnetic ordering. Density functional theory calculations of Au supported graphene (with and without adatoms) and ZGNRs will illustrate these effects and point the way towards a realization of a ZNGR with a topologically protected edge state.

O 37.13 Wed 12:45 EB 301

Collision dominated scattering in 3D topological insulators — •Peter Lemmens[1], Vladimir Gnezdilov[2], Dirk Wulferding[1], Yurii Pashkevich[3], Ekaterina Pomjakushina[4], Kazimierz Conder[4], and Helmuth Berger[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]ILTPE NAS, Ukraine — [3]DonFTI, Donetsk, Ukraine — [4]PSI, Villigen, Switzerland — [5]EPFL, Lausanne, Switzerland

Despite topological protection in 3D topological insulators there exist scattering processes induced by a resonant excitation from a bulk valence band to Dirac states. This signal in Raman scattering has a Lorentzian lineshape and spin-helical symmetry with a scattering rate of 40 cm^{-1}. A comparison of different compounds (Bi_2Se_3, Bi_2Te_3), substitution experiments as well as first results on BiTeI with giant Rashba spin splitting are presented. Work supported by DFG and NTH.