MA 43: Topological Insulators I (jointly with DS, HL, O, TT)

Time: Wednesday 15:00–18:00 Location: HSZ 401

MA 43.1 Wed 15:00 HSZ 401

Mn-doped topological insulators Bi_2Te_3 and Bi_2Se_3: an ab initio study of magnetism and transport properties — •Karel Carva[1], Pavel Baláž[1], Jakub Šebesta[1], Josef Kudrnovský[2], František Máca[2], and Václav Drchal[2] — [1]Charles University, DCMP, Ke Karlovu 5, CZ-12116 Prague, Czech Republic — [2]Institute of Physics, ASCR,Na Slovance 2, CZ-18221 Prague, Czech Republic

For the interpretation of experiments studying the Bi_2Te_3 and Bi_2Se_3 family of topological insulators it is necessary to include the native defects into the picture. Using similar methods one can study also the magnetic doping, which has attracted a lot of interest recently [1]. We calculate on an ab initio level the electronic structure of Bi_2Te_3 and Bi_2Se_3 doped by Mn at different possible positions and also in the presence of native antisites and vacancies. This provides for the first time a comprehensive map of possible behavior affecting strongly the bulk resistivity, carrier concentration and magnetism. It allows us to tune these properties, and also help to uncover the location of Mn atoms, since the substitutional or interstitial Mn placement exhibits strikingly different properties. Calculations indicate that the presence of interstitials may help to understand experimental observations[2].

Exchange interactions between Mn magnetic moments in bulk Mn-doped Bi_2Te_3 / Bi_2Se_3 have been calculated using ab initio methods. These results allow us to study the Curie temperatures by means of atomistic Monte Carlo simulations.

[1] Y. S. Hor et al., Phys. Rev. B 81, 195203 (2010)
[2] K. Carva et al., Phys. Rev. B 93, 214409 (2016)

MA 43.2 Wed 15:15 HSZ 401

Unraveling the Spin Structure of Unoccupied States in Bi_2Se_3 — •Christian Langenkämper[1], Anna Zumbülte[1], Jürgen Braun[2], Tobias Förster[3], Anke B. Schmidt[1], Jianli Mi[4], Bo Iversen[4], Philip Hofmann[5], Jan Minár[2,6], Hubert Ebert[2], Peter Krüger[3], Michael Rohlfing[3], and Markus Donath[1] — [1]Physikalisches Institut, WWU Münster, Germany — [2]Department of Chemistry, LMU München, Germany — [3]Institut für Festkörpertheorie, WWU Münster, Germany — [4]Center for Materials Crystallography, Department of Chemistry, Aarhus University, Denmark — [5]Department of Physics and Astronnomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — [6]New Technologies Research Centre, University of West Bohemia Pilzen, Czech Republic

The control of spin currents in topological insulators using optical transitions opens new perspectives in (opto-)spintronics. To understand these processes involving topological surface states, a profound knowledge about the dispersion and the spin polarization of both the occupied and the unoccupied electronic states is crucial. We present a joint experimental and theoretical study on the unoccupied electronic states of Bi_2Se_3. We discuss spin- and angle-resolved inverse photoemission results in comparison with calculations for both the intrinsic band structure and, within the one-step model of (inverse) photoemission, the expected spectral intensities. This allows us to unravel the intrinsic spin texture of the unoccupied bands at the surface of Bi_2Se_3.

MA 43.3 Wed 15:30 HSZ 401

Enhanced Mobility of Spin-Helical Dirac Fermions in Disordered 3D Topological Insulators — Joseph Dufouleur[1], Louis Veyrat[1], Bastien Dassonneville[1], Christian Nowka[1], Silke Hampel[1], Pavel Leksin[1], Barbara Eichler[1], Oliver G. Schmidt[1], Bernd Büchner[1], and •Romain Giraud[1,2] — [1]IFW, Dresden, Germany — [2]INAC-SPINTEC, Grenoble, France

We reveal the enhanced transport length of 2D spin-helical Dirac fermions in highly-disordered 3D topological insulators, due to anisotropic scattering, by electrical transport measurements of Bi_2Se_3 nanostructures [1]. By comparing the quantum mobility, related to the electronic mean-free path, to the mobility obtained from transconductance measurements, related to the transport length (backscattering), we evidence the long-range nature of the scattering potential for surface Dirac fermions and some limitation due to a residual bulk/surface coupling. In wide nanostructures, it is shown that the long phase coherence length results from the enhanced diffusion constant, in very good agreement with results obtained from previous studies of the weak anti-localization [2]. Our work suggests that the spin-flip length ($l_{sf} \approx l_{tr}$) could reach the micron size in materials with a reduced bulk doping, which reveals the true potential for building functionalized spintronic and ballistic electronic devices out of disordered 3D topological insulators.

[1] J. Dufouleur et al., Nano Lett. 16, 6733 (2016)
[2] Z. Li et al., Phys. Rev. B 91, 041401 (2015)

MA 43.4 Wed 15:45 HSZ 401

Spin-dependent very-low-energy electron diffraction at Bi_2Se_3 — •Andre Reimann[1], Christian Langenkämper[1], Anna Blob[1], Jürgen Braun[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Germany

The topological insulator Bi_2Se_3 exhibits prominent spin effects in both the occupied and unoccupied electronic bandstructure due to strong spin-orbit coupling. This promises large effects also for spin-dependent electron reflection.

We present a combined experimental and theoretical study of the spin-dependent electron reflection of Bi_2Se_3 along the $\overline{\Gamma}\,\overline{K}$ and the $\overline{\Gamma}\,\overline{M}$ direction. Experimentally we performed spin-dependent very-low-energy electron diffraction (VLEED) experiments over a wide range of energies and angles of incidence. Theoretically we used ab-initio calculations by means of the SPKKR layer code.

For both directions, we derived maps for the reflectivity and the Sherman function. We found high spin asymmetries up to 37%, which are caused by the large spin-orbit coupling of Bi_2Se_3. These features show a strong energy and angle dependence. Futhermore, we identified the VLEED finestructures, which contain information about the surface barrier.

MA 43.5 Wed 16:00 HSZ 401

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jürgen Braun[1], Hubert Ebert[1], Jaime Sanchez-Barriga[3], Oliver Rader[3], Jan Honolka[4], and Andreas Ney[5] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep. — [3]Helmholz Zentrum, Berlin — [4]ASCR, Institute of Physics, Prague — [5]Johannes Kepler University Linz, Austria

Band gap opening of topological surface states due to magnetic doping is the subject of a long standing and ongoing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. We will present several examples for detailed theoretical studies on various bulk as well as surface doped topological insulators performed by means of the SPR-KKR band structure method. Our results will be discussed in direct comparison with corresponding ARPES [1], XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, 7, 10559 (2016)
[2] A. Ney et al., in preparation
[3] J. Honolka et al., PhysRevB 94, 161114 (2016)

15 min. break.

MA 43.6 Wed 16:30 HSZ 401

Lifetime and surface to bulk scattering of the topological surface state in 3D topological Insulators — •Philipp Rüssmann, Phivos Mavropoulos, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Doping of topological insulators, such as Bi_2Se_3 or Bi_2Te_3, may result in a shift of the Fermi level to a position where the Topological Surface States (TSS) and the bulk states coexist. Then, the TSS lifetime τ_s due to impurity scattering is decomposed in surface-to-surface and surface-to-bulk contributions with scattering rates τ_{ss}^{-1} and τ_{sb}^{-1}, respectively, where $\tau_s^{-1} = \tau_{ss}^{-1} + \tau_{sb}^{-1}$. We investigate this decomposition in Bi_2Se_3 and Bi_2Te_3 by means of density-functional calculations.

In a detailed analysis we find that conduction and valence band play a different role in the surface to bulk state scattering. Especially for the important case of n-doping, the conduction band contribution is

very small compared to the surface-state contribution. As a consequence, the surface electrons remain topologically protected in spite of coexisting bulk bands.

For the calculation of electronic structure and scattering properties we employed the full potential relativistic Korringa-Kohn-Rostoker Green-function method. We acknowledge financial support from the DFG (SPP-1666), from the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre at the RWTH Aachen University.

MA 43.7 Wed 16:45 HSZ 401

Surfaces and interfaces of topological insulators from relativistic many-body calculations. — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

We present a description of surfaces of topological insulators (TIs) as well as interfaces between different TIs and between TIs and trivial materials. We focus on materials of the Bi_2Se_3 family. We use the all-electron FLAPW formalism and the relativistic many-body *GW* method [1]. Including many-body effects in the calculation and incorporating the spin-orbit coupling into the self-energy are critical to obtain reliable results for these TIs [1-5]. For the description of surface and interface states, we use a basis of Wannier functions to construct the slabs and heterostructures Hamiltonians. This approach allows us to study very large systems with a high accuracy. We discuss the differences between surface and interface states and the interaction ("crosstalk") between energetically non-degenerate Dirac cones at the interface and surfaces of the heterostructure.

[1] Aguilera *et al.*, Phys. Rev. B **88**, 165136 (2013). [2] Aguilera *et al.*, Phys. Rev. B **91**, 125129 (2015). [3] Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013). [4] Nechaev *et al.*, Phys. Rev. B **87**, 121111(R) (2013). [5] Michiardi *et al.*, Phys. Rev. B **90**, 075105 (2014).

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MA 43.8 Wed 17:00 HSZ 401

Topological thin films of Bi and InBi coexisting on InAs(111) — •L Nicolai[1,2,7], K Hricovini[1,2], J-M Mariot[1,3], M C Richter[1,2], O Heckmann[1,2], U Djukic[1], T Balasubramanian[4], M Leandersson[4], J Sadowski[4], J Denlinger[5], I Vobornik[6], J Braun[7], H Ebert[7], and J Minar[7,8] — [1]LPMS, UCP, Cergy, France — [2]DSM-IRAMIS, Spec, Cea-Saclay, France — [3]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [4]MAX-lab, Lund Univ., Sweden — [5]ALS, Berkeley, USA — [6]EST, Trieste, Italy — [7]LMU Munich, Germany — [8]Univ. of West Bohemia, Plzeň, Czech Rep.

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states. [1] Wada et *al.*, Phys. Rev. B 83,121310 (2011) [2] Liu et *al.*, Phys. Rev. Lett. 107, 136805 (2011) [3] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996)

MA 43.9 Wed 17:15 HSZ 401

Instability of the topologically protected surface state in Bi_2Se_3 upon deposition of gold — •Andrey Polyakov[1], Holger L. Meyerheim[1], Christian Tusche[2], Daryl E. Crozier[3], and Arthur Ernst[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany, Germany — [3]Department of Physics, Simon Fraser University Burnaby, BC Canada, V5A 1S6

We present an experimental and theoretical analysis of the stability of the Topological surface state (TSS) in Bi_2Se_3 upon sub-monolayer deposition of Au. Extended x-ray absorption fine structure experiments provide clear evidence that Au -when deposited on the (0001) surface kept at 160 K- substitutes Bi atoms within the first quintuple layer. This goes in parallel with the dramatic weakening of the spectral density of the TSS as observed by angular resolved photoemission. In accordance with first-principles calculations, Au in Bi substitutional sites within the first QL creates a d-type resonant state near E_F, which hybridizes with the TI bands and substantially modifies its surface electronic structure. According to the model of Black-Schaffer et al. [1] a bulk-surface interaction is a prerequisite for the gap opening, since the TSS is not protected by scattering processes involving bulk three-dimensional states. References: [1] A. M. Black-Schaffer and A. V. Balatsky, Phys. Rev. B 86, 115433 (2012). Acknowledgements: Work supported by SPP 1666. Work at the APS is supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

MA 43.10 Wed 17:30 HSZ 401

Magnetic exchange on the surface of topological insulators — •Alessandro Barla[1], Sanjoy K. Mahatha[1], Paolo Sessi[2], Kai Fauth[2], Thomas Bathon[2], Matthias Bode[2], Miguel Angel Valbuena[3], Sylvie Godey[3], Aitor Mugarza[3], Pierluigi Gargiani[4], Philipp Rüssmann[5], Phivos Mavropoulos[5], Gustav Bihlmayer[5], Stefan Blügel[5], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, CNR, I-34149 Trieste, Italy — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, D-97074 Würzburg, Germany — [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), E-08193 Cerdanyola del Vallès, Spain — [4]ALBA Synchrotron Light Source, E-08290 Cerdanyola del Vallès, Spain — [5]PGI-1 and IAS-1, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Three-dimensional topological insulators have conducting surface states in the bulk band gap, protected by time-reversal symmetry, which locks spin with momentum. It was shown, however, that surface magnetic doping can break time-reversal symmetry and induces backscattering of Dirac states [1]. We present the results of our investigations of the magnetic properties of individual atoms of 3d transition metals (Mn, Fe, Co) deposited on the surface of the topological insulator Bi_2Te_3. All studied adatoms present an out-of-plane magnetic anisotropy associated with sizeable orbital moments and we find evidence of surface-mediated magnetic exchange interactions which are of opposite sign for Mn and Co.

[1] P. Sessi et al., Nat. Commun. 5, 5349 (2014).

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