TT 63: Topological Insulators: Theory (jointly with HL, DS, MA, O)

Time: Wednesday 9:30–11:30 Location: ER 270

TT 63.1 Wed 9:30 ER 270

Weyl and Dirac semimetals: A platform for new interface phenomena — •Adolfo G. Grushin[1], Jorn W. F. Venderbos[2], and Jens H. Bardarson[3] — [1]Max Planck Institute for the physics of Complex Systems, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, MA, USA — [3]Max Planck Institute for the physics of Complex Systems, Dresden, Germany

The Weyl semimetal (WSM) state is sometimes loosely referred to as the three-dimensional cousin of graphene since its low energy theory is described by an even number of copies of the Weyl Hamiltonian. Closely related to WSM, the Dirac semimetals hosts the Weyl nodes at the same point in the Brillouin Zone and it is realised in Cd_3As_2 and Na_3Bi compounds. In this talk I will explore the rich surface state physics that these states can host and how can it be probed, including coexistence of Dirac and Fermi arc states at the topological insulator-weyl semimetal interfaces as well as signatures of the chiral anomaly.

TT 63.2 Wed 9:45 ER 270

Spin chirality tuning and Weyl semimetal in strained $HgS_{1-x}Te_x$ — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

We have theoretically investigated the phase diagram of $HgS_{1-x}Te_x$. The parameters which have been varied are the concentration x and the in-plane strain, which could be applied by an appropriate substrate in an experiment. In the topological phase diagram we found a normal metallic phase, two topological insulator phases with different spin chiralities of the surface states and a Weyl semi-metal phase. The phases have been probed by calculating topological invariants and the dispersion of the surface states for both crystal terminations of the (001) surface by an *ab-initio* based tight-binding model.

TT 63.3 Wed 10:00 ER 270

Topological phases in (interfacial) phase-change materials — •Peter Schmitz, Wei Zhang, and Riccardo Mazzarello — Institute for Theoretical Solid State Physics, RWTH Aachen University

We investigate the topological, spectral and structural properties of $[Sb_2Te_3]_x[GeTe]_y$ (GST) compounds, some of which are interfacial phase change materials (IPCMs), as a function of strain and stacking sequence by performing a DFT study of bulk and slab models and discuss the relevance of a 3D (topological) Dirac semimetal phase ((T)DSM), eg. to GST225.

IPCMs can perform fast reversible transitions, induced by electric fields or heat, between crystalline states of different stacking. Since they also possess strong spin-orbit coupling and a strong topological insulator (STI) + normal insulator(NI) layering, they are a promising platform to investigate nontrivial interface states and direct applications to data storage in terms of switching topological phases. Until now they were shown to exhibit STIs and *unstable* DSM-like critical states corresponding to STI/NI transitions [1]. Then recently [2] a *robust* TDSM phase was predicted for crystals having certain rotational symmetries: The STI/NI transition point can be extended to a line and 2 Dirac points appear in the bulk spectrum.

Analyzing whether such phases can be obtained in GST compounds is also interesting since the problem of a TDSM in a multilayer structure has not yet been discussed.

[1] J. Tominaga et al, Adv. Mat. Inter. 1 (2014);
[2] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)

TT 63.4 Wed 10:15 ER 270

Effect of Bi bilayers on the topological states of Bi_2Se_3: A first-principles study — Kirsten Govaerts[1], Kyungwha Park[2], Christophe De Beule[1], Dirk Lamoen[1], and •Bart Partoens[1] — [1]CMT-group and EMAT, University of Antwerp, Belgium — [2]Virginia Tech, Department of Physics, USA

Bi_2Se_3 and vice versa, has not been explored much. Bi bilayers are often present between the quintuple layers of Bi_2Se_3, since $(Bi_2)_n(Bi_2Se_3)_m$ form stable ground-state structures. Moreover, Bi_2Se_3 is a good substrate for growing ultrathin Bi bilayers. By first-principles techniques, we first show that there is no preferable surface termination by either Bi or Se. Next, we investigate the electronic structure of Bi bilayers on top of, or inside a Bi_2Se_3 slab. If the Bi bilayers are on top, we observe a charge transfer to the quintuple layers that increases the binding energy of the surface Dirac cones. The extra states, originating from the Bi bilayers, were declared to form a topological Dirac cone, but here we show that these are ordinary Rashba-split states. This result, together with the appearance of a new Dirac cone that is localized slightly deeper, might necessitate the reinterpretation of several experimental results. When the Bi bilayers are located inside the Bi_2Se_3 slab, they tend to split the slab into two topological insulators with clear surface states. Interface states can also be observed, but an energy gap persists because of strong coupling between the neighboring quintuple layers and the Bi bilayers.

TT 63.5 Wed 10:30 ER 270

Topological states in α-Sn and HgTe quantum wells: a comparison of ab-initio results — •Sebastian Küfner and Friedhelm Bechstedt — Friedrich Schiller Universität Jena

Quantum well (QW) structures based on HgTe are theroretically predicted and experimentally verified to exhibit the quantum-spin Hall phase. Despite the similarities of the bulk band structures, studies of α-Sn QW structures are missing. We compare the properties of QW structures made by the different zero-gap semiconductors α-Sn and HgTe, but both sandwiched in nearly lattice-matched CdTe barriers by means of first-principles calculations including quasiparticle corrections and spin-orbit interaction. The two well materials possess different space groups O_h^7 (diamond structure) and T_d^2 (zinc-blende structure). The spin-orbit interaction, in particular that in the p-derived valence states, is different due to the contribution of both atoms in the unit cell (α-Sn) and mainly the anion (HgTe) to the states at the top of the valence bands, and the different local electrostatic properties due to the different bonding character in the QW layers and their interfaces with the CdTe barrier material. We investigate the similarities and differences of the two embedded zero-gap semiconductors on the formation of quantum-well, edge and interface states in detail.

TT 63.6 Wed 10:45 ER 270

Quasiparticle band structure of the topological insulator Bi_2Se_3 — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi_2Se_3 is a prototype topological insulator. Its simple surface band structure with only one Dirac point makes it an ideal system for exploring the properties of topological surface states. Up to now, the vast majority of theoretical investigations of the electronic structure of Bi_2Se_3 has utilized DFT calculations. In Bi_2Se_3 and related compounds, however, many body perturbation theory in the GW approximation yields both quantitative and qualitative quasiparticle corrections of the DFT bulk band structures [1].

Here we discuss results for bulk Bi_2Se_3 from GW calculations employing a localized basis as well as from a perturbative LDA+GdW approach [2]. The latter provides a numerically very efficient method for the calculation of quasiparticle corrections with only slightly reduced precision compared to GW. The applicability of the LDA+GdW formalism to the Bi_2Se_3 surface with the Dirac state will also be addressed.

[1] I. Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013)
[2] M. Rohlfing, Phys. Rev. B **82**, 205127 (2010)

TT 63.7 Wed 11:00 ER 270

Calculation of topological invariants from a maximally localized Wannier functions derived model Hamiltonian — •Patrick M. Buhl, Chengwang Niu, Yuriy Mokrousov, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Using density-functional methods it is possible to provide an accurate description of topological phases in complex materials. We demonstrate how topological characterization can be performed in a unified manner based on Wannier functions generated from the full-potential linearized augmented plane-wave method as implemented in the FLEUR

code [1]. Taking as examples bcc Fe, Na_3Bi and PbTe we compute various topological invariants and identify topologically non-trivial points in the electronic structure of these materials in bulk and their close relation to the surface electronic structure. In particular, we focus on the Weyl semimetallic phase as a transitional phase between various topological phases in the same material and on the role of the Weyl points in the electronic structure for topological properties. Financial support by the HGF-YIG Programme VH-NG-513 and SPP 1666 of the DFG is gratefully acknowledged.

[1] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008)

TT 63.8 Wed 11:15 ER 270

Functionalized Bismuth Films: Giant Gap Quantum Spin Hall and Valley-Polarized Quantum Anomalous Hall States — •Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The search for new large band gap quantum spin Hall (QSH) and quantum anomalous Hall (QAH) insulators is critical for their realistic applications at room temperature [1,2]. Here we predict, based on first principles calculations, that the band gap of QSH and QAH states can be as large as 1.01 eV and 0.35 eV in an H-decorated Bi(111) film [3]. The origin of this giant band gap lies both in the large spin-orbit interaction of Bi and the H-mediated exceptional electronic and structural properties. Moreover, we find that the QAH state also possesses the properties of quantum valley Hall state, thus intrinsically realising the so-called valley-polarized QAH effect. We further investigate the realization of large gap QSH and QAH states in an H-decorated Bi($\bar{1}$10) film and X-decorated (X=F, Cl, Br, and I) Bi(111) films.

This work was supported by the Priority Program 1666 of the DFG and project VH-NG-513 of the HGF.

[1]M. Hasan and C. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

[2]X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).

[3]Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov, submitted.