MA 26: Topological insulators: Theory (with HL/O/TT)

Time: Wednesday 9:30–11:15 Location: POT 151

MA 26.1 Wed 9:30 POT 151

Stabilizing Chern and fractional Chern insulators — •Adolfo G. Grushin, Johannes Motruk, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Dresden

The experimental realization of Chern insulators (CI) and fractional Chern insulators (FCI), zero field lattice analogues of the integer and fractional Hall effects respectively, is still a major open problem in condensed matter. For the former, it was proposed that short range interactions at the mean-field level can drive a trivial insulator into a CI. For the latter, the effect of band dispersion and sizes of the single-particle gaps with respect to the interaction strength have been argued to be important to stabilize an FCI state. In this talk we will examine the robustness and fate of these statements both with exact diagonalization and infinite density matrix renormalization group (iDMRG).

MA 26.2 Wed 9:45 POT 151

Point contacts and localization in generic helical liquids — •Christoph P. Orth, Grégory Strübi, and Thomas L. Schmidt — University of Basel, Switzerland

We consider two helical liquids on opposite edges of a two-dimensional topological insulator, which are connected by one or several local tunnel junctions. In the presence of spatially inhomogeneous Rashba spin-orbit coupling, the spin of the helical edge states is momentum dependent, and this spin texture can be different on opposite edges. We demonstrate that this has a strong impact on the electron transport between the edges. In particular, in the case of many random tunnel contacts, the localization length depends strongly on the spin textures of the edge states.

MA 26.3 Wed 10:00 POT 151

***ab-initio* investigation of topological states and symmetry inversion in HgTe-CdTe Quantum wells** — •Sebastian Kuefner, Juergen Furthmueller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Topological insulators (TIs) recently attracted a high level of attention in solid state physics due to their unique physical properties. Generally, a TI is a material that is insulating in the bulk but exhibits metallic surface or edge states. These states are topologically protected which means that they are independent of surface orientation and passivation. The edge states usually have linear band dispersion forming Dirac cones.

The electromagnetic properties of the edge states might be used for the realisation of topological superconducting phases. In two dimensions the edge states build the quantum spin Hall state (QSH). In 2006, Bernevig et al. predicted the occurence of the QSH in HgTe-CdTe superlattices theoretically by an **kp**-approch which was later verified by König et al. experimentally.

However, these results have not yet been discussed in the framework of a reasonable electronic structure theory based on *ab-initio* methods but account for quasiparticle effects and spin-orbit coupling. Using density-functional theory together with the Tran-Blaha approximation we discuss the occurence of topological quantum-well states and investigate the topological transition in atomic structures.

MA 26.4 Wed 10:15 POT 151

Nontrivial Interface States Confined Between Two Topological Insulators — •Tomáš Rauch[1], Markus Flieger[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

By *ab initio*-based tight-binding calculations, we show that nontrivial electronic states exist at an interface of a $\mathcal{Z}_2$ topological insulator and a topological crystalline insulator. At the exemplary (111) interface between Bi_2Te_3 and SnTe, the two Dirac surface states at the Brillouin zone center $\overline{\Gamma}$ annihilate upon approaching the semi-infinite subsystems but one topologically protected Dirac surface state remains at each time-reversal invariant momentum $\overline{\mathrm{M}}$. This leads to a highly conducting spin-momentum-locked channel at the interface but insulating bulk regions. For the Sb_2Te_3/Bi_2Te_3 interface we find complete annihilation of Dirac states because both subsystems belong to the same topology class.

MA 26.5 Wed 10:30 POT 151

Natural three-dimensional topological insulators in Tl_4PbTe_3 and Tl_4SnTe_3 — •Chengwang Niu[1,2], Ying Dai[1], Baibiao Huang[1], Gustav Bihlmayer[2], Yuriy Mokrousov[2], Daniel Wortmann[2], and Stefan Blügel[2] — [1]School of Physics, Shandong University, Jinan, China — [2]Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently discovered three-dimensional topological insulators have attracted much interest due to their exceptional properties of possessing insulating bulk but time-reversal symmetry protected metallic surfaces with Dirac-like band structure [1,2]. The search for new topological insulators is critical for both fundamental and practical interests. Based on first-principles calculations, we reveal that both Tl_4PbTe_3 and Tl_4SnTe_3 are strong topological insulators with different band inversion behaviors at Γ point [3]. The mechanisms of band inversion in Tl_4PbTe_3 and Tl_4SnTe_3, as well as in Bi_2Se_3 and Sb_2Se_3, are investigated and classified. The Z_2 topological invariants and topological surface states are investigated to confirm the topologically non-trivial phase. Our calculations further indicate that the electron- or hole-type Dirac fermion can be effectively engineered by hole doping, which is necessary for device applications of topological insulators.

[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] C. Niu et al., in preparation.

MA 26.6 Wed 10:45 POT 151

Electronic properties of the topological crystalline insulator SnTe and its (001) and (111) surfaces: an ab-initio study — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The insulator SnTe belongs to the recently discovered class of materials in which a crystalline symmetry ensures the existence of topologically protected surface states. We report on the properties of these states at the (001) and (111) surfaces. To this end, we have employed density-functional theory.

The bulk band structure of SnTe is characterized by inversion at the four equivalent L points giving rise to a mirror Chern number $n_m = -2$. The (001) surface exhibits two mirror planes and shows four Dirac cones at non-time-reversal-invariant points along the $\pm\bar{\Gamma}\bar{\mathrm{X}}$ and $\pm\bar{\Gamma}\bar{\mathrm{X}}'$ lines, respectively. Here we explore the influence of lattice deformations on the stability of the surface states. Our results reveal that distortions of the topmost layers which break a mirror symmetry locally at the surface do *not* lead to an opening of the surface band gap. We find that only *bulk* lattice deformations, e.g. rhombohedrial distortions, that break one or both mirror symmetries also in the bulk part of the system give rise to a surface band gap. Our calculations show that the Sn terminated (111) surface exhibits Dirac cones centered at $\bar{\Gamma}$ and $\bar{\mathrm{M}}$. In particular at the $\bar{\mathrm{M}}$ point, these topologically protected states are distinctly extended into the bulk. Interestingly, we observe for the Te terminated (111) surface a gap-closing Dirac state only at the $\bar{\Gamma}$ point

MA 26.7 Wed 11:00 POT 151

Adsorbate- and vacancy-induced band bending in Bi_2Se_3: ab-initio calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi_2Se_3 is one of the first topological insulators ever discovered. It has been widely studied both experimentally und theoretically, due to its simple electronic structure with only one Dirac point at $\bar{\Gamma}$. In experiments, a downward band bending and an ageing effect are frequently observed. This has been attributed to an intrinsic n-doping and to coverage with adsorbates. Models for the band bending mostly focussed on the intrinsic doping.

Using DFT calculations, we show that a long-ranged potential also occurs for an adsorbate-covered surface, even without intrinsic doping. As a prototype adsorbate, we have investigated potassium at various coverages. The resulting changes in the charge density, the

potential, and the band structure can be attributed to two distinct origins: short-ranged adsorbate-specific changes and the formation of a long-ranged potential (which is independent of the specific adatom). We will explain how the band bending is related to the layered structure of Bi_2Se_3. Similar effects result from our calculations for different types of adsorbates as well as for selenium vacancies in the surface layer.