MA 5: Topological Insulators 2 (jointly with DS,HL,O,TT)

Time: Monday 15:00–18:00 Location: H10

Invited Talk MA 5.1 Mon 15:00 H10

The THz response of topological insulator surface states — •N. Peter Armitage — The Institute of Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

Topological insulators (TIs) are newly discovered states of matter characterized by an *inverted* band structure driven by strong spin-orbit coupling. One of their most touted properties is the existence of robust "topologically protected" surface states. I will discuss what topological protection means for transport experiments and how it can be probed using the technique of time-domain THz spectroscopy applied to thin films of Bi_2Se_3. By measuring the low frequency optical response, we can follow their transport lifetimes as we drive these materials through instabilities either by doping through a quantum phase transition into a topologically trivial regime or by reducing the film thickness. I'll also discuss our work on the magnetic field dependence of the Kerr rotation in Bi_2Se_3, where we find an unprecedentedly large value of the angle of rotation of reflected light, which is due to the cyclotron resonance of the 2D Dirac fermions.

15 min. break

MA 5.2 Mon 15:45 H10

Peierls dimerization at the edge of 2D topological insulators? — •Gustav Bihlmayer[1], Hyun-Jung Kim[2], Jun-Hyung Cho[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics and Research Institute for Natural Sciences, Hanyang University, Seoul, Republic of Korea

Edge states of two-dimensional topological insulators (2D-TIs) attracted considerable interest as they support dissipationless spin-currents. Recently, it was proposed that the zigzag-edge of a Bi(111) bilayer, identified as a 2D-TI [1,2], is unstable with respect to a Peierls dimerization [3], a phenomenon that occurs quite general in one-dimensional structures. This proposal was based on an *ab initio* investigation without taking spin-orbit coupling (SOC) into account. We investigate the effect of SOC on the atomic structure of zigzag Bi(111) and Sb(111) nanoribbons. Although we find that edge-reconstructions can influence the number of conductive channels, we conclude that the topological protection of the states in the Bi ribbon actually prevents the Peierls mechanism to get effective, since the opening of a Peierls gap at the zone boundary is forbidden by time-reversal symmetry. We compare the situation to the Sb structure, but also in the topologically trivial case of the Sb(111) bilayer ribbon we find a suppression of the dimerization due to SOC effects.

[1] S. Murakami, Phys. Rev. Lett. 97, 236805 (2006) [2] M. Wada et al., Phys. Rev. B 83, 121310(R) (2011) [3] L. Zhu et al., J. Phys. Chem. C 114, 19289 (2010)

MA 5.3 Mon 16:00 H10

Engineering quantum anomalous Hall (QAH) phases with orbital and spin degrees of freedom — •Hongbin Zhang, Frank Freimuth, Gustav Bihlmayer, Marjana Ležaić, Stefan Blügel, and Yuriy Mokrovsov — Peter Grünberg Institut and Institute for Advanced Simulation, FZJ and JARA, 52425 Jülich, Germany

Combining tight-binding models and first-principles calculations, we demonstrate that under external exchange fields, non-zero Chern numbers and nontrivial QAH effects can be induced by on-site spin-orbit coupling (SOC) in buckled honeycomb lattices with *sp* orbitals. In the Haldane model [1], the occurrence of the QAH effect is attributed to complex valued next-nearest-neighbor hopping matrix elements. Detailed analysis of a generic tight binding model reveals that there exist different mechanisms giving rise to complex hoppings, utilising both orbital and spin degrees of freedom of electrons on a lattice. Furthermore, it is shown that in Bi- or Sb(111) bilayers [2], different topological phases exist as function of the magnitude of SOC and external exchange fields. These phases are characterised using Chern and spin Chern numbers [3] in combination with transverse charge and spin conductivities. At last, we show that introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is altered due to partially filled *d* states around the Fermi energy. – Support by Helmholtz Young Investigators Group Programmes VH-NG-409 and -513 is acknowledged.

[1] F.D.M. Haldane, PRL **61**, 2015 (1988). [2] H. Zhang, *et al.*, PRB **86**, 035104 (2012). [3] E. Prodan, PRB **83**, 195119 (2011).

MA 5.4 Mon 16:15 H10

Prediction of weak topological insulators in layered semiconductors — •Binghai Yan[1,2], Lukas Müchler[1,2], and Claudia Felser[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden — [2]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

We report the discovery of weak topological insulators by ab initio calculations in a honeycomb lattice. We propose a structure with an odd number of layers in the primitive unit cell as a prerequisite for forming weak topological insulators. Here, the single-layered KHgSb is the most suitable candidate for its large bulk energy gap of 0.24 eV. Its side surface hosts metallic surface states, forming two anisotropic Dirac cones. Although the stacking of even-layered structures leads to trivial insulators, the structures can host a quantum spin Hall layer with a large bulk gap, if an additional single layer exists as a stacking fault in the crystal. The reported honeycomb compounds can serve as prototypes to aid in the finding of new weak topological insulators in layered small-gap semiconductors.

MA 5.5 Mon 16:30 H10

Dirac States in a Novel Topological Insulator: Epitaxial alpha-Tin Layers on Indium Antimonide — •J. Schäfer[1], A. Barfuss[1], G. Bihlmayer[2], D. Wortmann[2], L. Dudy[1], P. Höpfner[1], A. Bostwick[3], E. Rotenberg[3], and R. Claessen[1] — [1]Phys. Inst., Universität Würzburg, D — [2]Peter Grünberg Inst. and Inst. Adv. Sim., FZ Jülich, D — [3]Lawrence Berkeley Nat. Lab., USA

This study addresses a new material realization of a topological insulator (TI) thus far only proposed theoretically, which is formed by α-Sn in the diamond lattice on InSb substrates. The epitaxial growth opens various pathways to access and manipulate the topological surface state (TSS). This includes the evolution of the Dirac bands as a function of thickness, or surface coating layers which alter the spin-orbit interaction. Interestingly, the TI band properties are closely related to that of strained HgTe, for which the Quantum Spin Hall effect was demonstrated.

Here we report on the electronic structure of α-Sn(001) based on angle-resolved photoemission (ARPES), complemented by density functional theory (DFT). We observe the formation of a clearly pronounced Dirac cone. The Fermi level in ARPES is located close to the Dirac point. Its position can be controlled by dopants, which allows to adjust the Fermi level crossings of the TSS. The Dirac cone is discernible down to bulk band energies, and its constant energy surfaces seemingly reflect the lattice symmetry. The experimental findings are consistent with DFT calculations including spin-orbit interaction, which document the formation of a TSS.

MA 5.6 Mon 16:45 H10

Observation of terahertz photocurrents in the topological insulator Bi_2Se_3 — •Lukas Braun[1], Luca Perfetti[2], Martin Wolf[1], and Tobias Kampfrath[1] — [1]Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau cedex, France

Recent experiments have indicated that optical excitation of topological insulators (TIs) with circularly polarized light can induce spin-polarized electron currents along the TI surface. The direction of this photocurrent can be controlled by varying the circular polarization of the driving light from right- to left-handed. So far, only DC photocurrents have been detected [J. W. McIver *et al.* Nature Nanotechnology **7**, 96 (2012)]. Since electrons moving through a solid typically undergo scattering on sub-picosecond time scales, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution.

Here, we drive ultrashort current bursts in n-doped Bi_2Se_3 by excitation with a laser pulse (10fs, 800nm, 10nJ). The photocurrent gives rise to the emission of a terahertz (THz) electromagnetic pulse whose transient electric field $E(t)$ is detected by means of electro-optic sampling with a time resolution of 10fs. We observe extremely broadband THz emission covering the range from 10 to 30THz, and the THz intensity is found to depend strongly on the helicity of the pump pulses. A method is presented that allows us to extract the transient current $j(t)$ from the measured $E(t)$. We finally discuss the origin of $j(t)$ and implications for the dynamics of photoexcited TI electrons.

MA 5.7 Mon 17:00 H10

Static screening properties of topologically protected surface states — •Daniel Wortmann, Gustav Bihlmayer, Yuriy Mokrousov, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The electrons occupying surface states of topological insulators (TI) provide charges that can screen electric fields applied perpendicular to the surface. Being a very basic phenomenon, its realistic description is rather difficult: model approaches fail to provide quantitative results while DFT calculations of insulating slabs with external electric fields suffer from difficulties arising from the incomplete screening of the field inside the slab.

We demonstrate that the embedded Green function method [1,2] can be utilized to investigate the effects of an applied field on the surface states. Our approach describes the formation of surface states in terms of their scattering properties at the semi-infinite bulk states by means of a generalized logarithmic derivative. Besides discussing the underlying idea of this elegant theoretical tool and its application to prototypical topological insulators, we present a comparison of the expected screening effects seen in a topological insulator with those in a topological material.

[1] see http://www.flapw.de for details of the code

[2] D. Wortmann, H. Ishida, S. Blügel, Phys. Rev. B **65**, 165103 ('02)

MA 5.8 Mon 17:15 H10

Topological phases of spin chains — Kasper Duivenvoorden and •Thomas Quella — Universität zu Köln, Institut für Theoretische Physik, Köln, Deutschland

The Haldane phase of one-dimensional $S = 1$ spin chains with $SU(2)$ symmetry is one of the first topological states of matter. In particular, it features a bulk-boundary correspondence, with $S = 1/2$ degrees of freedom emerging at the boundaries of the system. Moreover, it exhibits a diluted anti-ferromagnetic order which can be measured using a non-local string order parameter. With the prospect of being able to simulate spin chains with $SU(N)$ symmetry in the laboratory using ultracold earth-alkaline atoms it is a natural and interesting question whether similar topological phases also exist beyond $N = 2$.

In a recent paper we have shown that this is indeed the case. More precisely, spin chains with $SU(N)$ symmetry allow for up to N different topological phases, $N - 1$ of which are topologically non-trivial. These phases exhibit topological order that is reflected in a specific entanglement pattern resulting from the matrix product state representation of the corresponding ground state wave function. It may be detected using a non-local string order parameter which characterizes each of the N phases unambiguously. Analytical and numerical results confirm that our order parameter may be used to extract a quantized topological invariant.

MA 5.9 Mon 17:30 H10

Strongly-correlated topological semiconductors — •Stanislav Chadov[1], Claudia Felser[1], Leon Petit[2], Hubert Ebert[3], and Jan Minár[3] — [1]MPI-CPFS Dresden — [2]STFC Daresbury Laboratory, UK — [3]LMU München

Using the fully-relativistic Green's function formalism we analyze the electronic structure topology in series of the heavy rock-salt type semiconductors PuX, SmX (X=Te, Se, S). Due to the partial filling of their f-shells, these materials exhibit strong dynamical correlations which destroy the Bloch-like eigenstates. Thus, the usual analysis based on the symmetry of the eigenstates cannot be applied. Here we recall the adiabatic approach, which allows to analyze the topology based on a purely bulk information disregarding the Bloch or localized character of the electronic states. The dynamical correlations were treated within the DMFT scheme implemented in the framework of the SPR-KKR Green's function method.

MA 5.10 Mon 17:45 H10

Correlation between linear Magnetoresistance and Mobility of Heusler Topological Insulators — •C. Shekhar, A. K. Nayak, S. Ouardi, G. H. Fecher, and C. Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Topological insulators (TIs) are a class of quantum materials and belong to a new state of matter with topologically protected gapless Dirac fermionic states. Among the TIs series Heusler compounds are promising candidates for the nanoelectronic devices. If these compounds contain heavy metals (Au, Pb, Pd, Pt, Sb and Bi) and a lanthanide element then they exhibit extraordinary physical properties including *zero band gap*. Generally, gapless compounds show high mobility, where no threshold energy is required to conduct carriers from occupied states to empty states. Very recently, the exciting discovery of graphene is an example of high-mobility compounds due to its linear dispersion of the bands, where charge carriers behave like massless particles. However, the Heusler TIs having *zero band gap* are also expected to show high mobility. The Heusler TIs also exhibit nonsaturating and positive magnetoresistance, that shows systematic variations with temperature. The best fitting of observed MR is found with the combination of linear and quadratic field dependence and may be written in form of a quadratic equation: $\mathrm{MR} = a|B| + (b/2)B^2$, where B is applied field. It is clear that this MR originates from the contribution of both linear and parabolic terms. The parabolic term is well known and comes from the Lorentz force, while the origin of the linear MR is intriguing.