DS 38: Topological Insulators (Joint session of DS, HL, MA, O and TT, organized by MA)

Time: Wednesday 15:00–17:45 Location: H32

DS 38.1 Wed 15:00 H32

Bulk and surface properties of topological insulators from *GW* calculations. — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

Many-body calculations within the *GW* approximation are attracting much attention in the study of topological insulators (TIs). They have shown to be critical both in the one-shot approach [1] (e.g. for the Bi_2Se_3 family) and in a quasiparticle self-consistent (QS) *GW* method [2] (e.g. for Bi). In both cases, the spin-orbit coupling has to be incorporated directly into the *GW* self-energy [3]. Within the all-electron FLAPW formalism, we have performed DFT, one-shot *GW*, and QS*GW* calculations for well-known TIs. These calculations are very demanding for low-dimensional systems. Therefore, we construct a tight-binding Hamiltonian for the description of topological surface states in a slab geometry. The corresponding parameters are deduced from *GW* calculations of the bulk. With this approach, we discuss the effects of quasiparticle corrections on the surface states of TIs and on the interaction between bulk and surface states. We show that the *GW* bulk and surface band structure agrees better to results from photoemission experiments than the DFT one. [1] Phys. Rev. B 87, 121111(R) (2013). [2] *Ibid* 91, 125129 (2015). [3] *Ibid* 88, 165136 (2013).

We acknowledge the Virtual Institute for Topological Insulators of the Helmholtz Association.

DS 38.2 Wed 15:15 H32

Magnetic Properties of Mn-doped Bi_2Se_3 and Bi_2Te_3: Ab Initio and Atomistic Simulations — •Pavel Baláž[1], Karel Carva[1], Róbert Tarasenko[1], Vladimír Tkáč[1], Jan Honolka[2], and Josef Kudrnovský[2] — [1]DCMP, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Institute of Physics, ASCR, Na Slovance 2, CZ-18221 Prague 8, Czech Republic

Ferromagnetic Curie temperature and other magnetic magnetic properties of bulk Mn-doped Bi_2Se_3 and Bi_2Te_3 3D topological insulators are systematically studied by means of atomistic Monte Carlo simulations. Exchange interactions between the Mn magnetic moments have been calculated using ab initio methods. Tight-binding linear muffin-tin orbital method has been employed, together with the coherent potential approximation to describe the high degree of disorder in the system. Spin-orbit interaction is included in the ground state calculation. In the studied materials Mn atoms might either replace a Bi atom (substitutional position) or fill an empty position in van Der Waals gap between the atomic layers (substitutional position). It has been shown that exchange interaction between Mn magnetic moments might lead to a ferromagnetic phase transition. The Curie temperature is shown to be significantly dependent on the concentration of Mn atoms in substitutional and interstitial positions. Theoretical results were compared to recent experimental studies [1].

[1] R. Tarasenko et al., to be published in Physica B: Phys. Cond. Mat., DOI: 10.1016/j.physb.2015.11.022

DS 38.3 Wed 15:30 H32

Transport measurements on ferromagnet / Half Heusler TI bilayer structures — •Benedikt Ernst[1], Robin Klett[2], Jan Haskenhoff[2], James Taylor[3], Yong Pu[3], Günter Reiss[2], Stuard S. P. Parkin[3], and Claudia Felser[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — [3]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle

Heusler compounds exhibit a manifold of physical properties and attracted in the recent past a lot of interest in the field of spintronic applications due to their half-metallic properties.

In the present work bilayer systems of ferromagnetic materials and half Heusler topological insulators (TI) are studied. The systems were deposited using DC- and RF magnetron co-sputtering. The samples were characterized by X-ray diffraction and electron microscopy techniques. On fabricated devices, the transport properties and spin properties were studied by different measurement techniques including ST-FMR and spin injection experiments.

Additional measurements of the unidirectional spin Hall magnetoresistance were realized. In this effect, we measure a change in the magnetoresistance depending on the direction of the magnetization, which is proportional to the spin Hall angle. We varied the combination of different ferromagnetic materials with different Tis of the YPtBi, YPdBi, LaPtBi and LaPdBi system, and the thicknesses of the layers, to investigate the effects on the transport properties.

DS 38.4 Wed 15:45 H32

Surface preparation and momentum microscopy of the „topological Kondo insulator“ SmB_6 — •Christian Tusche[1,2], Martin Ellguth[1], Fumitoshi Iga[3], and Shigemasa Suga[2,4] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]College of Science, Ibaraki University, Japan — [4]Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan

The strongly correlated rare-earth compound SmB_6 is believed to be a topological Kondo insulator, where a topologically non-trivial surface state lives in the hybridization gap at low temperatures. While most experimental studies rely on cleaved surfaces, high resolution- and spin resolved photoemission experiments [1] usually suffer from the short live time of the reactive surface at low temperatures.

Here we present the reproducible surface preparation of large high quality SmB_6 single crystals by in-situ Ar-ion sputtering and controlled annealing. In particular, Sm-rich or B-rich surface terminations are obtained by low (≈1080°C) or high (>1200°C) temperature annealing. Using a momentum microscope [2], wide wave vector regions are studied by photoemission with He-I ($h\nu$=21.2 eV) and laser ($h\nu$=6.0 eV) excitations, on the Sm-terminated surface. The results reveal localized f-electron resonances at E_F and strong hybridization, paving the way to measure detailed Fermi surface and valence band spin textures.

[1] Suga et al., J., Phys. Soc. Japan 83, 014705 (2014)

[2] C. Tusche, A. Krasyuk, J. Kirschner, Ultramicroscopy (2015)

DS 38.5 Wed 16:00 H32

Spin control in the topological surface state of SnTe — •Nicolas Klier[1], Sam Shallcross[1], Sangeeta Sharma[2], and Oleg Pankratov[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The interface of SnTe with a vacuum results in a topological Dirac surface state [1,2]. Based on an effective Hamiltonian derived from tight-binding we investigate the properties of this surface state both with and without an in-plane electric current. The RKKY interaction is found to be strongly non-collinear due to the spin texture of the Dirac state. In the presence of an in-plane current we find (i) a polarization of the surface state and (ii) that the RKKY interaction is strongly modified by the presence of a current leading to a possible "topological spin torque effect".

[1] B.A. Volkov, and O.A. Pankratov, Zh.Eksp. Theor. Fiz. 75, 1362, 1978.

[2] B.A. Volkov, and O.A. Pankratov, JETP Lett.42, 178, 1985.

15 min. break

DS 38.6 Wed 16:30 H32

Adiabatic Pumping of Chern-Simons Axion Coupling — •Maryam Taherinejad[1] and David Vanderbilt[2] — [1]Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-0849, USA

The Chern-Simons axion (CSA) coupling θ makes a contribution of topological origin to the magnetoelectric response of insulating materials. Here we study the adiabatic pumping of the CSA coupling along a parametric loop characterized by a non-zero second Chern number $C^{(2)}$ from the viewpoint of the hybrid Wannier representation. The hybrid Wannier charge centers (WCCs), when plotted over the 2D projected Brillouin zone, were previously shown to give an insightful visualization of the topological character of a 3D insulator. By defining Berry connections and curvatures on these WCC sheets, we derive a new formula for θ, emphasizing that it is naturally decomposed into a topological Berry-curvature dipole term and a nontopological correction term. By explicit calculations on a model tight-binding Hamiltonian, we show how the Berry curvature on the WCC sheets is transported by a lattice vector via a series of Dirac sheet-touching events, resulting in the pumping of e^2/h units of CSA coupling during one closed cycle. The new formulation may provide a particularly efficient means of computing the CSA coupling θ in practice, since there is no need to establish a smooth gauge in the 3D Brillouin zone.

DS 38.7 Wed 16:45 H32

Accessing the transport limits of topological states — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Topological insulators host on their surface spin-momentum locked Dirac states. Beyond their fundamental interest, these materials raised great expectations to create new functionalities in spintronics and magneto-electrics. Their success depends on our understanding of their response to Coulomb perturbations such as electric fields, which can be effectively used to gate their surface. These phenomena have so far been primarily explored by spatially averaging techniques.

Here, by using scanning tunneling microscopy and spectroscopy, we visualize the response of topological states to local charges and electric fields at the nanoscale. We demonstrate that, contrary to the general believe, local electric fields can not be effectively screened by topological states, but penetrate into the bulk indicating a behavior which is far from being metallic. The analysis of our data allows to detect the existence of a finite conductivity which, because of the local character of our measurements, can be safely quantified without being affected by sample inhomogeinities. Finally, we will show how, by taking advantage of this intrinsic limitation, a new approach to tune both charge and spin transport in this fascinating class of materials can be explored.

DS 38.8 Wed 17:00 H32

Interplay between warping and magnetic effects in Fe monolayer on Sb2Te3 — •Farideh Hajiheidari[1], Wei Zhang[1,2], and Riccardo Mazzarello[1,3] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Center for Advancing Materials Performance from the Nanoscale, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, PR China — [3]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Three-dimensional topological insulators (TIs) realize an unconventional electronic phase originating from time-reversal symmetry and strong spin-orbit interaction (SOI). These materials are bulk insulators but possess conducting surface states in the bulk band gap. The surface states are topologically protected against non-magnetic disorder. However, impurities which break time-reversal symmetry induce a band gap in the system. This is of critical importance for potential device applications involving spin-based transport. In this work, we present a density-functional-theory study of the magnetic properties of a Fe monolayer on the (111) surface of the topological insulator Sb2Te3. We optimize the geometry of the system and determine the band structure and the easy axis of magnetization for the Fe atoms. We show that the easy axis is in-plane. In spite of this, the presence of the monolayer leads due to the opening of a gap of the order of meV, due to the interplay between magnetism and warping effects. Finally, we discuss the relevance of our findings to recent experiments about magnetic adatoms and monolayers deposited on TIs.

DS 38.9 Wed 17:15 H32

Towards topological tunnel devices - A versatile method for processing tunnel junctions from high quality single crystals — •Robin Klett[1,2], Karsten Rott[1,2], Daniel Ebke[3], Chandra Shekhar[3], Joachim Schönle[4], Wolfgang Wernsdorfer[4], Stuart Parkin[5], Claudia Felser[1,2], and Günter Reiss[1,2] — [1]Physics Department, Bielefeld University, Germany — [2]Center for Spinelectronic Materials and Devices, Universitätsstraße 25, 33605 Bielefeld, Germany — [3]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [4]CNRS, Institut NEEL and Univ. Grenoble Alpes, F-38000 Grenoble, France — [5]Max Planck Institute for Microstructure Physics, 06120 Halle/Saale, Germany

We present a new and versatile concept for devices based on topological materials. To maintain their topological character high quality samples with clean interfaces to adjacent functional device components are mandatory. This requirement forms a bottleneck of current research, because very often the established thin film deposition fails to produce such high quality samples and bare surfaces of single crystals lack the necessary flatness. We demonstrate a novel, all-in-ultrahigh-vacuum process that enables to realize, e.g. tunnel junctions, Andreev contacts or SQUID rings from single crystalline bulk material. The validity of the technique is verified and illustrated with tunnel junctions made from cleaved single crystals of the half-Heusler topological superconductor candidate YPtBi.

DS 38.10 Wed 17:30 H32

Effective geometric phases and topological transitions in SO(3) and SU(2) rotations — •Henri Saarikoski[1], J. Enrique Vázquez-Lozano[2], José Pablo Baltanás[2], Junsaku Nitta[3], and Diego Frustaglia[2] — [1]RIKEN Center for Emergent Matter Science, Japan — [2]Departamento de Física Aplicada II, Universidad de Sevilla, Spain — [3]Department of Materials Science, Tohoku University, Japan

We address the development of geometric phases in classical and quantum magnetic moments (spin-1/2) precessing in an external magnetic field. We show that nonadiabatic dynamics lead to a topological phase transition determined by a change in the driving field topology. The transition is associated with an *effective* geometric phase which is identified from the paths of the magnetic moments in a spherical geometry. The topological transition presents close similarities between SO(3) and SU(2) cases but features differences in e.g. the limiting values of the geometric phases [1]. We discuss possible experiments where the effective geometric phase would be observable [2].

[1] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, J. Nitta, and D. Frustaglia, arXiv:1511.08315 (2015). [2] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, F. Nagasawa, J. Nitta, and D. Frustaglia, Phys. Rev. B 91, 241406(R) (2015).