TT 104: Topological Insulators II (jointly with MA, DS, HL, O)

Time: Thursday 15:00–17:45 Location: EB 202

TT 104.1 Thu 15:00 EB 202

Topological surface states of Heusler-type topological insulators — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute for Physics of the Complex Systems, Dresden, Germany

Some promising half-Heusler compounds, RPtBi (R = La, Lu, Y), are demonstrated experimentally to be superconductors and are predicted to be topological insulators. The topological feature of bulk is band inversion and the s orbital of Pt atom is the main clue. However, their topological surface states (TSSs) remain unclear. In this work, we use *ab initio* method to investigate the TSSs. In experiment, they are found at the Γ point inside the valence bands. Spin texture is also calculated to confirm the topologically nontrivial surface states. External strain can push the TSSs from the valence bands up into gap.

TT 104.2 Thu 15:15 EB 202

Topological surface states on NaBaBi with two opposite spin textures — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany.

By breaking the inversion symmetry of the 3D Dirac metal Na_3Bi, we realize topological insulator (TI) phases in a known compound NaBaBi using $ab-initio$ calculations. Two distinct TI phases emerge: one phase is due to the band inversion between $Bi-p$ and $Na-s$ bands, and the other phase (under pressure) is induced by the inverted $Bi-p$ and $Ba-d$ bands. Both phases exhibit Dirac-cone-type surface states, but opposite spin textures. In the upper cone, a left-hand spin texture exists for the s-p inverted phase (similar to a common TI, e.g. Bi_2Se_3) while a right-hand spin texture appears for the $p-d$ inverted phase. NaBaBi presents a prototype model for TIs that exhibit different spin textures in the same material.

TT 104.3 Thu 15:30 EB 202

Indirect exchange interaction through topological surface states in crystalline topological insulators of a SnTe class — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

As predicted theoretically [1,2] and confirmed experimentally [2,3] the interface of SnTe and vacuum (i.e. the material's surface) hosts topologically stable Dirac states. We investigate the properties of this state within a **k.p** model that includes a full account of the bulk band structure [4]. An essential advantage of an analytical band model [4] is that it allows to unequivocally trace the two key degrees of freedom that this system possesses: spin and pseudospin. The indirect exchange interaction between magnetic impurities is a perfect probe for the surface Dirac states, especially for their spin structure. We revealed explicitly the dependence of this interaction on the properties of the bulk band states, in particular on the spin orbit coupling strength and on the crystal field splitting parameters. Depending on these parameters, the interaction may be either of Ising type or of a novel anisotropic XY type with the spin direction aligned with the connection vector between the two impurities.

[1] B.A. Volkov, and O.A. Pankratov, *J*ETP Lett. **42**, 178, 1985.
[2] T.H. Hsieh *et al.*, *N*ature Comm. **3**, 982, 2012.
[3] Y. Tanaka *et al.*, *N*ature Phys. **8**, 800, 2012.
[4] B.A. Volkov, and O.A. Pankratov, *Z*h.Eksp. Theor. Fiz. **75**, 1362, 1978.

TT 104.4 Thu 15:45 EB 202

Edge states in topological magnon insulators — Alexander Mook[1], •Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle (Saale), Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

For magnons, the Dzyaloshinskii-Moriya interaction accounts for spin-orbit interaction and causes a nontrivial topology that allows for topological magnon insulators. In this theoretical investigation [1] we present the bulk-boundary correspondence for magnonic kagome lattices by studying the edge magnons calculated by a Green function renormalization technique. Our analysis explains the sign of the transverse thermal conductivity of the magnon Hall effect in terms of topological edge modes and their propagation direction. The hybridization of topologically trivial with nontrivial edge modes enlarges the period in reciprocal space of the latter, which is explained by the topology of the involved modes.

[1] Phys. Rev. B **90** (2014) 024412.

TT 104.5 Thu 16:00 EB 202

Magnon waveguides from topological magnon insulators — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle

Topological magnon insulators exhibit a nontrivial topology due to the Dzyaloshinskii-Moriya interaction. They host topologically nontrivial edge magnons and, consequently, energy as well as spin currents along their edges [1,2].

Bringing two topological magnon insulators into contact results in topologically protected unidirectional interface magnons. As these interface modes decay toward both bulk regions, their currents are confined to a few nanometer wide strip around the interface. Owing to the topological nature of the edge states, the edge currents follow any geometry.

We address theoretically the formation of interface edge magnons and their currents. On top of this, we propose recipes to compose magnon waveguides with nano-scale confinement.

[1] L. Zhang et al., PRB **87**, 144101 (2013).
[2] A. Mook et al., PRB **90**, 024412 (2014).

TT 104.6 Thu 16:15 EB 202

Probing the Electronic Properties of Individual MnPc Molecules Coupled to Topological States — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik 2, Universitaet Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Hybrid organic-inorganic interfaces have been widely reported to host emergent properties that go beyond those of their single constituents. Coupling molecules to the recently discovered topological insulators, which possess linearly dispersing and spin-momentum-locked Dirac fermions, may offer a promising platform towards new functionalities.

Here, we report a scanning tunneling microscopy and spectroscopy study of the prototypical interface between MnPc molecules and a Bi_2Te_3 surface. MnPc is found to bind stably to the substrate through its central Mn atom. The adsorption process is only accompanied by a minor charge transfer across the interface, resulting in a moderately n-doped Bi_2Te_3 surface. More remarkably, topological states remain completely unaffected by the presence of the molecules, as evidenced by the absence of scattering patterns around adsorption sites. Interestingly, we show that, while the HOMO and LUMO orbitals closely resemble those of MnPc in the gas phase, a new hybrid state emerges through interaction with the substrate.

TT 104.7 Thu 16:30 EB 202

first principle study of structural, electronic and magnetic properties of graphene nanoribbons deposited on the topological insulator Sb2Te3 — wei zhang[1,2], •farideh hajiheidari[1], yan li[1,3], manuel j. schmidt[1], and riccardo mazzarello[1,4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [3]IEK-6, Forschungszentrum Jülich, D-52425 Jülich, Germany — [4]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Magnetic perturbations are known to affect the surface properties of a topological insulator (TI) dramatically. According to mean-field calculations, zigzag graphene nanoribbons (zGNRs) possess spin-polarized edge states. Hence, zGNRs deposited on a TI could be a promising candidate for an experimental investigation of proximity effects between a magnetic system and a TI. In this work, we carry out a first-principles investigation based on density functional theory of zGNRs on the Sb2Te3 (001) surface. We use gradient-corrected density func-

tionals in combination with semi-empirical van der Waals corrections. Both H-free and H-terminated zGNRs are considered. In the case of H-free zGNRs, the strong interaction between the edge atoms and the TI surface is shown to lead to the bending of the zGNRs , however, the edge magnetism is preserved. Moreover, the magnetic anisotropy axis is perpendicular to the surface of the substrate. In the H-terminated case, on the other hand, the interaction is less significant and edge magnetism is fully preserved.

TT 104.8 Thu 16:45 EB 202

WSe_2 Synthesis, Characterization and Properties — •Catherine R Rajamathi, Binghai Yan, Marcus Schmidt, Kumari Gaurav Rana, Chandra Shekhar, Siham Ouardi, Guido Kreiner, and Claudia Felser — Max-Planck Institute for Chemical Physics of Solids, Dresden

Layered transition metal dichalcogenides (TMDs) are widely studied systems as they are chemically versatile and technologically enthralling. The facile tunability of their electronic structure by varying certain parameters - carrier type (n- or p-type), composition, structure or sample size expand their applications from catalysis to topological insulators. Single crystals were synthesized from its polycrystalline components using $SeCl_4$ as the transport agent. Mono- or few-layered tungsten selenide obtained by the scotch-tape technique discussed in this talk are direct-gap semiconductors. FET devices fabricated from a few-layered sample of WSe_2 show ambipolar transistor behavior. In addition, hybrid materials such as $WSe_{2-x}Te_x$ may be promising due to high magnetoresistance and surface states on WTe_2 single crystals.

TT 104.9 Thu 17:00 EB 202

Classification of spin liquids on the square lattice with strong spin-orbit coupling — •Johannes Reuther[1,2], Shu-Ping Lee[3], and Jason Alicea[3] — [1]Freie Universität Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]California Institute of Technology

The investigation of spin liquids is a fascinating field in condensed matter physics that is increasingly motivated by experiments. Exhaustive classifications of spin liquids have been carried out in several systems, particularly when full SU(2) spin-rotation symmetry is present. Systematic studies that explore strongly spin-orbit-coupled magnetic compounds (for which there are many experimental examples) are, however, relatively scarce. We report on a classification of Z_2 spin liquids on the square lattice when SU(2) spin symmetry is maximally lifted. Using projective symmetry group methods, we find that, surprisingly, the lifting of spin symmetry yields vastly more spin liquid states compared to SU(2)-invariant systems. A generic feature of the SU(2)-broken case is that the spinons naturally undergo $p + ip$ pairing; consequently, many of these Z_2 spin liquids feature a topologically nontrivial spinon band structure supporting gapless Majorana edge states. These boundary modes are often protected by a combination of time reversal and lattice symmetries and hence resemble recently proposed topological crystalline superconductors.

TT 104.10 Thu 17:15 EB 202

Fate of the 1/3 magnetization plateau in quantum triangular antiferromagnets with various anisotropies — •Fedor Simkovic[1], Natasha Perkins[2], and Andrey Chubukov[2] — [1]King's College, London, England — [2]University of Minnesota, Minneapolis, United States

The triangular Heisenberg lattice is investigated by means of semiclassical 1/S expansion. Although classically the up-up-down phase with 1/3 magnetisation exists only at one magnitude of the field, it is stabilised by quantum fluctuations and forms a magnetisation plateau around this point. We investigate into three types of anisotropies for the triangular lattice, and access the stability of the aforementioned phase towards the limits of decoupled chains, the square, honeycomb, Kagome, rhombille and scaled triangular lattices.

TT 104.11 Thu 17:30 EB 202

Matrix product operators: Local equivalences and topological order in 2D — •Oliver Buerschaper — Freie Universität Berlin

Projected entangled pair states (PEPS), which naturally generalize matrix product states (MPS) to higher dimensions, describe the low energy properties of local quantum Hamiltonians with an energy gap very well. For this reason they are increasingly used as a valuable tool in both analytical and numerical studies of strongly correlated 2D quantum systems. Some of the most interesting such systems exhibit topological order, i.e. patterns of long-range entanglement which cannot be detected by any local order parameter. At the same time, excitations in these systems typically exhibit fractional statistics and may be used, for instance, as a resource for topological quantum computation.

For both fundamental and practical reasons, it is thus of the utmost importance to understand and classify PEPS in 2D, especially those with topological order. Recently it was found that symmetries defined in terms of certain matrix product operators (MPO) provide a mechanism for the emergence of topological order in PEPS. Furthermore, the kind of topological order was seen to depend on the algebraic properties of the given MPO symmetry. Here we show that many, seemingly distinct MPO symmetries are, in fact, locally equivalent and characterize PEPS with the *same* kind of topological order. We discuss interesting ramifications for the classification of 2D quantum systems.