TT 68: Topological Insulators and Weyl Semimetals (joint session MA/TT)

Time: Wednesday 15:00–18:15 Location: EB 407

TT 68.1 Wed 15:00 EB 407

Topological Phase Transitions from Relativistic Many-Body Calculations — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

We discuss topological phase transitions (TPTs) on the basis of relativistic *GW* and quasiparticle self-consistent *GW* (QS*GW*) calculations where the spin-orbit coupling is incorporated directly into the self-energy. TPTs can be caused by the variation of the thickness of a sample, the spin-orbit strength, alloying, strain, etc. The well known underestimation of band gaps in standard DFT translates into an overestimation of the inverted band gaps that are responsible for the topological character of materials. This results in standard DFT being unable to provide correctly the critical points of TPTs. As practical examples, we concentrate on semimetals Bi and Sb. In addition to the TPT that bismuth undergoes under strain [1], we discuss that a thickness-mediated TPT can also occur. This sheds light on the discrepancies about the topological or trivial character of bulk-like samples of Bi. Finally, we simulate $Bi_{1-x}Sb_x$ alloys varying the Sb concentration in order to find the critical concentration for which the system becomes a topological insulator.

[1] I. Aguilera *et al.*, Phys. Rev. B **91**, 125129 (2015).

Financial support from the Virtual Institute for Topological Insulators of the Helmholtz Association.

TT 68.2 Wed 15:15 EB 407

High throughput screening of two dimensional topoloigical insulators — •Xinru Li[1], Zeying Zhang[1,2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China

Topological insulators (TIs), with insulating band gaps and nontrivial edge states, have been widely investigated not only for its fundamental importance but also owing to its potential technological applications. The two-dimensional (2D) TIs are particularly interesting, as they can get easily implemented into devices. There have been many 2D TIs predicted theoretically or synthesized experimentally. However previous efforts have relied mostly on time-consuming trial-and-error procedures. Here, starting from a 2D materials database with 826 slab systems predicted to be stable, we performed high-throughput screening over all materials at the first principles level. For nonmagnetic 2D materials with small ($<$ 0.1 eV)band gaps, maximally localized Wannier functions are constructed in an automated way in order to characterize the topological character by examining the surface states. Combined with explicit evaluation of the topological invariants, we have successfully identified one novel 2D TI, whose topological properties will be discussed in detail.

TT 68.3 Wed 15:30 EB 407

Classification of topological antiferromagnets for spintronics — •Libor Šmejkal[1,2], Jairo Sinova[1,2], and Tomáš Jungwirth[2] — [1]INSPIRE group, Uni Mainz, Germany — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Rep.

Our recent prediction of the interplay between topological Dirac quasiparticles and spin orbit torques in antiferromagnets has opened new possibilities of studying topological spintronics [1]. In this talk we will classify topological antiferromagnets based on minimal models, present new material candidates and novel magneto-transport effects, e.g. tunable topological anisotropic magnetoresistance or quantum anomalous Hall effect. The presence of topological quasiparticles can lead to a large signal/noise ratios and novel functionalities in read-out signals in spintronics devices [2]. For example, based on ab initio theory, we have predicted a large anisotropic magnetoresistance reaching 6% in Mn2Au antiferromagnet which was recently observed in current induced torques experiments [3]. We will also demonstrate that antiferromagnets are natural candidates for combining magnetic order with topological Dirac quasiparticles owing to their unique effective time-reversal symmetries, which are not present in ferromagnets [1,2].

[1] L. Šmejkal, J. Železný, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. 118 , 106402 (2017) [2] L. Šmejkal, Y. Mokrousov, B. Yan, and A. H. MacDonald, arXiv:1706.00670 [3] S. Yu. Bodnar, L. Šmejkal, M. Jourdan, et al. arXiv:1706.02482

TT 68.4 Wed 15:45 EB 407

Edelstein effect in Weyl semimetals — •Annika Johansson[1,2], Jürgen Henk[2], and Ingrid Mertig[2,1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Using semiclassical Boltzmann transport theory, we predict a current-induced spin polarization in Weyl semimetals, similar to the Edelstein effect of surface states in Rashba systems or in topological insulators [1]. The theory is applied to the Weyl semimetal TaAs simulated by an effective two-band model [2,3], for which we estimate the magnitude of the effect. The main contribution comes from the topological surface states, i. e. the Fermi arcs, which provide an enormous current-induced spin polarization.

[1] V. M. Edelstein, Solid State Commun., **73**, 233 (1990) [2] S. Murakami and S.-i. Kuga, Phys. Rev. B **78**, 165313 (2008) [3] R. Okugawa and S. Murakami, Phys. Rev. B **89**, 235315 (2014)

TT 68.5 Wed 16:00 EB 407

Ferro- and ferrimagnetic coupling in $Cr/Bi_2Se_3(0001)$ — •Andrey Polyakov[1], Katayoon Mohseni[1], E. Daryl Crozier[2], Manuel Valvidares[3], Victor N. Antonov[1], Lev V. Bekenov[1], Arthur Ernst[4], Holger L. Meyerheim[1], and Evgueni V. Chulkov[5] — [1]MPI für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Department of Physics, SFU Burnaby, BC Canada, V5A 1S6 — [3]Alba Synchrotron, 08290 Cerdanyola del Valles Barcelona, Spain — [4]Institut für Theoretische Physik, Johannes Kepler Universität, A 4040 Linz, Austria — [5]DIPC, 20018 San Sebastian/Donostia, Basque Country, Spain

Using surface x-ray diffraction, x-ray absorption fine structure and x-ray magnetic circular dichroism experiments in combination with ab-initio calculations we have studied the atomic and magnetic structure of ultra-thin Cr films deposited in the 0.2 to 2.5 monolayer thickness regime on $Bi_2Se_3(0001)$. We find a complex pattern of different adsorption sites (substitutional, van-der Waals gap, and surface double layer formation) involving ferro- and ferri-magnetic exchange. Magnetic moments are close to $4\mu_B$ related to Cr^{2+}. Our study sheds new light on the understanding of magnetic doped topological insulators. Acknowledgements: Supported by SPP 1666. Work at the APS is supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

TT 68.6 Wed 16:15 EB 407

Circular-polarized-light induced spin characterization of Dirac-cone surface state at W(110) — •Koji Miyamoto[1], Henry Wortelen[2], Taichi Okuda[1], Jürgen Henk[3], and Markus Donath[2] — [1]HSRC, Japan — [2]WWU Münster, Germany — [3]MLU, Germany

Recently, for the topological surface state (TSS) of Bi_2Se_3, several groups have observed an interesting phenomenon by spin- and angle-resolved photoemission (SARPE): the observed spin features of the photoelectrons are strongly dependent on the light polarization [1]. This effect is currently highly debated in the field of optospintronics. So far, the observations of the effect are limited to surfaces with C_{3v} symmetry.

The surface of W(110) shows a spin-polarized Dirac-cone-like state within a spin-orbit-induced gap, which is reminiscent of a TSS [2]. Here, in contrast to so-far studied topological insulators, the surface structure has C_{2v} symmetry.

We studied spin feature of the Dirac-cone-like surface state along $\overline{\Gamma H}$ at W(110) by using SARPE with left and right circular polarized light. It is found that the observed spin textures is caused by spin dependent matrix element influenced by C_{2v} symmetry. This finding opens a new way to manipulate the spin polarization of photoelectron in systems with C_{2v} symmetry.

*[1] C. Jozwiak *et al.*, Nat., Phys. **9**, 293 (2013).
*[2] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012).

TT 68.7 Wed 16:30 EB 407

Magnetization-direction tunable nodal-line and Weyl phases — •Zeying Zhang[1,2], Qiang Gao[2], ChengCheng Liu[1], Yugui

Yao[1], and Hongbin Zhang[2] — [1]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China — [2]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Emergent phenomena in materials with nontrivial topological nature have attracted intensive attention recently, as observed in both 2D and 3D topological insulators. From the symmetry point of view, nodal-line and Weyl semimetals are of particular interest, and they host intriguing properties such as negative magneto-resistance. In this work, we investigate a symmetry based three-band tight-binding model, after consider spin-orbit coupling (SOC) and different magnetization-directions, it is confirmed that the number of Weyl points and nodal line can be tuned by the magnetization direction. It is observed that the mirror symmetry plays a crucial role in protecting the degeneracy of nodal-lines. We propose a new class of materials C_4CrX_3 (X=Ge and Si) which host such a nontrivial semi-metallic phase. The systems have neither spatial inversion nor time reversal symmetries, but surprisingly it is observed that both Weyl points and nodal-lines exist in the ferromagnetic ground state. The degeneracy of nodal-lines can be controlled by the magnetization direction after considering SOC, confirmed by first-principles calculations.

15 min. break.

TT 68.8 Wed 17:00 EB 407

Topological jumps in a finite-size Dzyaloshinskii-Moriya antiferromagnetic chain — •Jaroslav Chovan[1,2] and Dominik Legut[1] — [1]IT4Innovations National Supercomputing Center VSB - Technical University Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]Department of Physics, Matej Bel University, Banska Bystrica, Slovakia

Recently, experiments with thin films of chiral ferromagnets MnSi and $CrNbS_6$ observed sudden jumps in magnetoresistence and/or magnetization induced by a magnetic field applied perpendicularly to the chiral axis. Subsequent theory traced the origin of these jumps to a field-induced transitions between topological sectors with different number of magnetic solitons and established the importance of boundary conditions. Here, we explore the topic in the context of a two-sublattice antiferromagnet. We thus carry out a detailed calculation of magnetic properties of a finite Heisenberg antiferromagnetic chain with Dzyaloshinskii-Moriya interactions in the presence of external magnetic field. By comparing the energies of magnetic solitons from different topological sectors, we calculate the ground state dependence on the chain size N and the field H. We construct a phase diagram and analyze the topological jumps between the individual sectors in detail and discuss ambiguity in counting the number of magnetic solitons for even-number spin chain. Our results may guide future experiments.

This work was supported by Czech Science Foundation grant No. 17-27790S, project No. CZ.02.1.01/0.0/0.0/16_013/0001791, and Slovak Grant VEGA No. 1/0269/17.

TT 68.9 Wed 17:15 EB 407

Impact of in-gap states on the magnetic stability/excitations of dopants in topological insulators — •Juba Bouaziz, Julen Ibanez-Azpiroz, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Doping topological insulators with magnetic impurities breaks time reversal symmetry, leading to the prediction of a gap opening at the Dirac point when the magnetic moments are along the *c*-axis [1]. This could potentially functionalize the topological surface states by enabling control of the quantum anomalous Hall effect and dissipationless transport. Several investigations obtained conflicting results, generating a lot of controversy on this point. Since the orientation of the magnetic moments depends on their magnetic anisotropy energy, we use first-principles calculations to investigate isolated $3d$ and $4d$ transition metal impurities on the surfaces and in the bulk of Bi_2Te_3 and Bi_2Se_3. We explore the impact of impurity-induced in-gap states on the orientation of the magnetic moments, their dynamical spin-excitations and on the zero-point spin-fluctuations affecting the magnetic stability [2]. We propose to use scanning tunneling spectroscopy in the inelastic mode or in the electron spin resonance mode to verify our predictions. – Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

[1] Y. L. Chen et *al.*, Science. **329**, 659 (2010).
[2] J. I. Azpiroz et *al.*, Nano Lett. **16**, 4305 (2016).

TT 68.10 Wed 17:30 EB 407

Prediction of a magnetic Weyl semimetal with strong anomalous Hall and Nernst effect in the Heusler compensated ferrimagnet Ti_2MnAl — •Jonathan Noky[1], Wujun Shi[1,2], Lukas Müchler[3], Kaustuv Manna[1], Yang Zhang[1,4], Klaus Köpernik[4], Roberto Car[3], Jeroen van den Brink[4], Claudia Felser[1], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]School of Physical Science and Technology, ShanghaiTech University, Shanghai 200031, China — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — [4]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

We predict the inverse Heusler compound Ti_2MnAl, which is a compensated ferrimagnet with a Curie temperature of over 650 K, to be a magnetic Weyl semimetal. Despite the vanishing net magnetic moment, we calculate a large intrinsic anomalous Hall (AHE) and anomalous Nernst (ANE) effect. These effects stem directly from the Berry curvature distribution of the Weyl points, which are only 14 meV away from the Fermi level and isolated from trivial bands. Since spin-rotation symmetry is broken by the magnetic structure, the Weyl points are stable also without spin-orbit coupling. Additionally, because Weyl points of opposite topological charge show a large spatial separation, this system exhibits huge Fermi arcs.

Ti_2MnAl and, to a lesser extend, also Ti_2MnGa and Ti_2MnIn are first examples of systems with Weyl points, large AHE, and large ANE in spite of a vanishing net magnetic moment.

TT 68.11 Wed 17:45 EB 407

Magnetic Weyl Semimetal in Quasi Two-dimensional Half Metallic $Co_3Sn_2S_2$ and $Co_3Sn_2Se_2$ — •Qiunan Xu[1], Enke Liu[1], Lukas Muechler[2], Claudia Felser[1], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden 01187 , Germany — [2]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

A Weyl semimetal can exist in a time reversal or inversion symmetry breaking system. Since the Berry curvature is odd under time reversal, the Berry curvature from Weyl points are expected to generate a large anomalous Hall effect in time reversal symmetry breaking Weyl semimetals. Since the Weyl points are far away from Fermi energy for most of the candidate magnetic Weyl semimetals, Weyl points related physics was observed in them so far. In this work, we find a Weyl semimetal phase in half metallic ferromagnet $Co_3Sn_2S_2$ with Weyl points only 60 meV away from the Fermi level, which derive from nodal lines that are gapped by spin-orbit coupling. Therefore, the Weyl-related physics should be easy to detected by both surface ARPES and bulk transport measurements. Due to the Berry curvature deriving from the gapped nodal lines and Weyl points, its anomalous Hall conductivity can reach up to 1200 S/cm. Substituting S by Se, $Co_3Sn_2Se_2$ shows very similar property. Moreover, since $Co_3Sn_2S_2$ and $Co_3Sn_2Se_2$ are both easily grown quasi two-dimensional compounds, they provide an ideal platform for the study of magnetic Weyl physics and its future application in topological material based spintronic devices.

TT 68.12 Wed 18:00 EB 407

Core-Shell Nanowires of 3D Topological Insulators — •Kevin Geishendorf, Tommi Tynell, Kornelius Nielsch, and Andy Thomas — Institute for Metallic Materials, IFW Dresden

Topological insulators (TI) are promising candidates for next generation electronic/spintronic devices. The gapless surface states (SS) in TI exhibit a very high mobility and strongly suppressed backscattering due to spin-momentum locking. However, to exploit those advantageous one has to decrease the finit bulk conductance present in most TI systems.

One approach to achieve this reduction is to utilize band bending which occurs at the interface between two materials with different Fermi levels. The band bending leads to a charge depletion/ or accumulation near the interface. It therefore provides a tool to shift the fermi energy closer to the Dirac point.

In this work we have grown core-shell nanowires using Vapor-Liquid-Solid (VLS) growth and Atomic Layer Deposition (ALD). As core material Bi_2Se_3 and as shell materials Al_2O_3 and Sb_2Te_3 were employed. The uniformity, crystallinity and composition of those core-shell nanowire was investigated using TEM, nanodiffraction and EDX. Furthermore, devices for transport experiments were built using optical lithography and lift-off techniques. With those devices cryogenic magneto transport measurements have been performed revealing quantum interference effects such as weak-antilocalization and universal conductance fluctuations.