MA 4: Topological insulators and spin-dependent transport phenomena

Time: Monday 9:30–13:15 Location: H52

MA 4.1 Mon 9:30 H52

Properties of Majorana Fermions in a Planar Josephson Junction — •Aidan Wastiaux and Falko Pientka — Max-Planck Institute for the Physics of Complex Systems, Dresden

As topologically protected quasi-particles, Majorana fermions are of great interest for the future of quantum information. The most promising experimental platform for Majorana states is based on heterostructures of superconductors and semiconductor nanowires in a magnetic field. In Ref. [1], an alternative platform based on a 2D Josephson junction in a 2d semiconductor with spin-orbit coupling has been proposed. The topological phase can be controlled by an in-plane magnetic field and the phase difference across the junction. Motivated by recent experimental progress [2], we investigate properties of the topological phase and Majorana states in this platform.

MA 4.2 Mon 9:45 H52

Laser induced DC photocurrents in 3D topological insulators Hall bar and nanowire devices — •Nina Meyer[1], Thomas Schumann[1], Eva Schmoranzerová[2], Kevin Geishendorf[3], Gregor Mussler[4], Jakob Walowski[1], Petr Nemec[2], Andy Thomas[3], Kornelius Nielsch[3], Detlev Grützmacher[4], and Markus Münzenberg[1] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [4]Inst. for Semiconductor Nanoelectronics, PGI-9, Forschungszentrum Jülich, Germany

It has been demonstrated experimentally that spin-polarized currents can be generated by illuminating a topological insulator (TI) with circularly polarized light [1]. In this talk, we will sum up our results for (Bi, Sb)$_2$Te$_3$ thin films Hall bar structures and Bi$_2$Se$_3$ core-shell nanowires. During the photocurrent measurements, the laser light polarisation is changed at every laser spot position. Due to the polarisation dependence, the different contribution to the photocurrent are separated and displayed as spatially resolved 2D maps. For the Hall bar structure a lateral accumulation of spin polarization at the TIs edges due to the spin Nernst effect is found [2]. For the nanowires, the interaction between nanowire and Au contact due to the Schotky effect and a constant spin polarized current far off the contacts is found.

[1] J.W. McIver et al., Nature Nanotechnology 7, 96-100 (2012)
[2] T. Schumann et al., arXiv:1810.12799 (submitted)

MA 4.3 Mon 10:00 H52

Characterization of topological band structure features away from the Fermi level via the anomalous Nernst effect — •Jonathan Noky, Johannes Gooth, Claudia Felser, and Yan Sun — Max Planck Institute for Chemical Physics of Solids, Dresden, Deutschland

Resolving the structure of energy bands in transport experiments is a major challenge in condensed matter physics and material science. Sometimes, however, when traditional electrical measurements only provide very small signals, it has been proven beneficial to employ thermoelectric measurements which are sensitive to the first derivative of the electrical property with respect to energy, rather than to its value itself. Due to the large interest in topological effects these days, it is important to identify a similar concept for detecting the Berry curvature (BC) in a band structure. The BC can be created by different mechanisms like Weyl points or the gapping of nodal lines due to symmetry breaking. Nowadays, the common way to access the BC directly via measurements is the anomalous Hall effect, but the corresponding signal can be too small to be detected when the topological features of the band structure lie too far off the Fermi level.

We investigate the strong BC due to nodal line gappings in regular Heusler compounds for different positions of the Fermi level. From this we derive a way to resolve topological band structure features which are elusive to see in anomalous Hall measurements utilizing the anomalous Nernst effect.

MA 4.4 Mon 10:15 H52

The Z_2 topology of bismuth — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The Z_2 topology of bulk and thin films of pure bismuth has been a matter of debate in the last few years. Whereas all first-principles calculations with different levels of sophistication predict a trivial Z_2 invariant, a couple of photoemission experiments display surface states that look non-trivial. The discrepancies between theory and experiment were originally attributed to the failure of density functional theory (DFT) in the prediction of band gaps, because the topological or trivial character of Bi depends only on the "sign" of the tiny ($\sim$15 meV) direct band gap at the L point. In [1] we showed that quasiparticle self-consistent GW (QSGW) calculations support the trivial character. These are, to date, the most accurate calculations for bulk Bi in the literature. However, this did not explain the discrepancy with experiments. In this talk, I will explain, based on QSGW calculations, why the apparent contradiction between theory and experiment is, as a matter of fact, no contradiction, and that the "topologically-looking" experimental surface states are actually compatible with a trivial Z_2 invariant. We note that we focus on the Z_2 topological character only and not on the high-order topology, recently predicted for Bi.

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

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

MA 4.5 Mon 10:30 H52

Transport and scanning tunneling microscopy study on layered Dirac material EuMnBi2 — •Xinglu Que[1,2], Qingyu He[1,2], Claus Mühle[1], Jürgen Nuss[1], Lihui Zhou[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Japan

The interplay of correlation and topology could give rise to novel properties. In this presentation we report our investigation of a layered magnetic Dirac material EuMnBi2, by using transport and STM. EuMnBi2 exhibits rich magnetic textures, by controlling which distinct electronic structures are accessible. Antiferromagnetically ordered Eu ions decouple the Bi layers which host Dirac fermions, leading to the emergence of multilayer Quantum Hall effect as revealed by our transport data. The application of an external magnetic field drives the material into different states. The STM reveals well defined steps after low temperature cleavage. Local spectroscopy finds features derived from Bi, in good agreement with band structure calculations.

MA 4.6 Mon 10:45 H52

First-principles study of electrical transport with phonons and magnons — •David Wagenknecht[1,2], Dominik Legut[2], Karel Carva[1], and Ilja Turek[1] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Czechia — [2]IT4Innovations & Nanotechnology Centre, VŠB-Technical University of Ostrava, Czechia

We will present first-principles calculations of magnetic materials with a combined influence of chemical disorder (impurities) and finite-temperature effects (phonons and spin fluctuations). The alloy analogy model (AAM) within the fully relativistic tight-binding linear muffin-tin orbital (TB-LMTO) method and the coherent potential approximation (CPA) was successfully used to describe transition metals and simple alloys [1, 2], an effect of spin disorder in the Earth's core [3], and spin-resolved conductivities in half-metallic half-Heusler NiMnSb [4]. Special attention will be paid to a comparison of phenomenological methods (Debye theory or fitting experimental data) and proper ab initio calculations. For systems, where the former ones may be used, computational effort may be greatly reduced. Our efficient AAM within TB-LMTO method with the CPA can describe even complex structures such as multi-sublattice magnetic materials where the properly described disorder is essential for, e.g., a spin polarization of the electrical current.

[1] D. Wagenknecht et al. T-MAG 53 11 (2017); [2] D. Wagenknecht et al. Proc. SPIE 10357, 103572W (2017); [3] V. Drchal et al. PRB 96, 024432 (2017); [4] D. Wagenknecht et al. JMMM 747, 517-521 (2019)

MA 4.7 Mon 11:00 H52

Spin Hall magnetoresistance in metals on antiferromagnetic α-Cr$_2$O$_3$ — •Tobias Kosub[1], Asser Elsayed[1], Richard Schlitz[2], Jürgen Fassbender[1], Sebastian Gönnenwein[2], and

Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]TU Dresden, Dresden, Germany

Spin Hall magnetoresistance (SMR) is a crucial phenomenon for insulator spintronics as it enables regular metals to be used to drive and sense magnetic effects in the insulators. While the effect has been thoroughly studied for ferrimagnetic insulators [1], antiferromagnetic [2] and paramagnetic insulators are interesting materials for future spintronics applications.

We present a thorough study of both longitudinal and transverse magnetotransport signatures of the spin Hall magnetoresistance, for various metals on Cr_2O_3. We monitor the system above and beyond the Nèel temperature - in the antiferromagnetic and paramagnetic phases. The magnetotransport effects are generally larger in the paramagnetic phase, highlighting the potential importance of paramagnets for spintronic applications.

Several inconsistencies with established SMR theory are reported and we offer different explanations taking into account the paramagnetic nature of the material.

[1] H. Nakayama et al., *Phys. Phys. Lett.* **110**, 206601 (2013)
[2] R. Schlitz et al., *Appl. Phys. Lett.* **112**, 132401 (2018).

15 min. break

MA 4.8 Mon 11:30 H52

Magnonic Weyl states in Cu_2OSeO_3 — •L. Zhang[1], Y. A Onykiienko[2], P.M. Buhl[1], Y. V Tymoshenko[2], P. Čermák[3,4], A. Schneidewind[3], S. Blügel[1], D.S. Inosov[2], and Y. Mokrousov[1,5] — [1]PGI and IAS, FZ Jülich and JARA, 52425 Jülich, Germany — [2]IFMP, TU Dresden, D-01069 Dresden, Germany — [3]JCNS, FZ Jülich GmbH, Outstation at Heinz MLZ, Lichtenbergstraße 1, D-85747 Garching, Germany — [4]Charles University, Faculty of Mathematics and Physics, Ke Karlovu 5, 121 16, Praha, Czech Republic — [5]Institute of Physics, JGU Mainz, 55099 Mainz, Germany

The multiferroic ferrimagnet Cu_2OSeO_3 with a chiral crystal structure has recently attracted significant attention due to the emergence of a skyrmion order in this material [1]. Here the topological properties of its magnon excitations were investigated by linear spin-wave theory and inelastic neutron scattering. Considering only the Heisenberg exchange interactions, two Weyl points are observed at high symmetry points with topological charges ± 2. Each Weyl point splits into two as the symmetry of the system is further reduced, if in addition the nearest neighbor Dzyaloshinsky-Moriya interaction is taken into consideration, which is decisive for obtaining an accurate fit to the experiment results. The predicted topological properties are verified by surface state and Chern number analysis. In addition, we predict that a sizeable thermal Hall conductivity can be associated with the emergence of the Weyl points, the position of which can be tuned by changing the crystal symmetry of the material. [1] Portnichenko, P. Y. et al., Nat. Commun. 7, 10725 (2016)

MA 4.9 Mon 11:45 H52

Symmetry aspects of spin-filtering in molecular junctions: hybridization and quantum interference effects — •Dongzhe Li[1] and Alexander Smogunov[2] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Service de Physique de l'Etat Condensé, CEA, CNRS, Université Paris-Saclay, CEA Saclay, Gif-sur-Yvette F-91191, France

Control and manipulation of electric current and especially its degree of spin polarization across single molecules is currently of great interest in the field of molecular spintronics. Using state-of-the-art *ab initio* transport calculations, we explore one of possible strategies based on the modification of nanojunction symmetry which can be realized, for example, by a mechanical strain. Such modification can activate new molecular orbitals which were inactive before due to their orbital mismatch with electrode's conduction states. This can result in several important consequences such as: i) a significant suppression of the majority spin conductance was found in low symmetry configurations due to quantum interference effects seen as Fano-like features in electron transmission functions and ii) strongly enhanced conductance of minority spin due to increased molecule-metal hybridization when the symmetry is lowered. We illustrate the idea on two basic molecular junctions: Ni/Benzene/Ni (perpendicular vs tilted orientations) and Ni/Si chain/Ni (zigzag vs linear chains). We believe that our results may offer new potential route for creating molecular devices with a large on/off spin polarization via quantum interference effects.

MA 4.10 Mon 12:00 H52

Reconfigurable spin tunnel diode based on stacked two-dimensional materials — •Ersoy Sasioglu[1], Stefan Blügel[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale) Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Tunnel diodes and transistors are considered as one of the most promising candidates for the future high-speed, low-power nanoelectronic devices due to their predicted ultra-high frequency operation in the THz range. Recently we proposed a reconfigurable spin tunnel diode and transistor concept using spin gapless semiconductors (SGSs) and half metallic magnets (HMMs) [1]. The two-terminal spin tunnel diode is comprised of a SGS electrode and a HMM electrode separated by a thin insulating tunnel barrier and allows electrical current to pass either in one direction or in other direction depending of the relative orientation of the magnetization direction of the electrodes. Two-dimensional stacked van der Waals materials, which form high-quality heterointerfaces due to absence of dangling bonds, offer a unique platform for realization of such a spin diode concept. By employing the nonequilibrium Green's function method combined with density functional theory we demonstrate the reconfigurable rectification characteristics of the spin tunnel diode based on two-dimensional stacked transition-metal dichalcogenides and dihalides. Funding by the European Union (EFRE) is greatly acknowledged.

[1] Ersoy Şaşıoğlu and Stefan Blügel, (2017), PCT Patent No. WO 2017076763(A1).

MA 4.11 Mon 12:15 H52

Nonmagnet-Barrier Interface Drives Tunnelling Anisotropic Magnetoresistance — •Philipp Risius, Carsten Mahr, Michael Czerner, and Christian Heiliger — Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Gießen

Tunnel junctions with a single ferromagnetic layer (semi-magnetic tunnel junction, SMTJ) may show magnetoresistance if spin-orbit interaction (SOI) is present in the ferromagnetic layer. This effect is called tunneling anisotropic magnetoresistance (TAMR). SMTJs employing a thin iron layer, magnesium oxide as tunnel barrier, and vanadium as leads (V|Fe|MgO|V) show TAMR and an appreciable spin-orbit torque at room temperature [1]. We investigate the origins of TAMR by calculating the transport across SMTJs from first principles, and investigate the effect of disorder at the Fe|V interface. For this, we utilized a fully relativistic Korringa-Kohn-Rostoker non-equilibrium Green's function method including the coherent potential approximation and vertex corrections [2]. We recovered the k-resolved transmission and temperature-dependent TAMR ratio. Crucially, we show that the effect depends on a subtle interplay of the interfaces on both sides of the tunnel barrier, and that the magnitude of SOI at the ferromagnet-insulator interface can even be secondary to the choice of materials.

[1] S. Miwa, J. Fujimoto, P. Risius et al., *Phys. Rev. X* **7**(3), 031018 (2017).
[2] C. Franz, M. Czerner and C. Heiliger, *J. Phys. Condens. Matter* **25**, 425301 (2013).

MA 4.12 Mon 12:30 H52

Current induced Néel-order switching in antiferromagnetic CuMnAs deposited by magnetron sputtering — •Tristan Matalla-Wagner, Matthias Rath, Jan-Michael Schmalhorst, Günter Reiss, and Markus Meinert — Center for Spinelectronic Materials and Devices, Bielefeld University, Germany

Antiferromagnets which fulfill certain symmetry properties allow for an intrinsic relativistic Néel-order spin-orbit torque (NSOT) driven by an electrical current [1]. The antiferromagnetically coupled sublattices of tetragonal CuMnAs are inversion partners and, thus, can experience a NSOT which can reorient the Néel-vector $\boldsymbol{L}$ perpendicular to the applied charge current [2]. Therefore, this material is suitable to manufacture novel antiferromagnetic memory devices that are extraordinarily robust against external influences [3]. Here, we report on our experiments on the electrical switching of the Néel-order using short current pulses in highly oriented films of CuMnAs, deposited using dc-magnetron sputtering. The dependence of the switching efficiency on the sample temperature, current density and pulse width is examined. Our findings corroborate the hypothesis of a thermally activated switching of $\boldsymbol{L}$ in sputtered CuMnAs, similar to the switching of sputtered Mn_2Au [4].

[1] J. Železný *et al.*, Phys. Rev. Lett. **113**, 157201 (2014)
[2] P. Wadley *et al.*, Science **351**, 587 (2016)

[3] T. Jungwirth *et al.*, Nat. Nanotechn. **11**, 231 (2016)
[4] M. Meinert *et al.*, Phys. Rev. Applied **9**, 064040 (2018)

MA 4.13 Mon 12:45 H52

Multifunctional Antiperovskites driven by Strong Magnetostructural Coupling — •Harish Kumar Singh, Ilias Samathrakis, Nuno Fortunato, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, Otto-Berndt-Straße 3, 64287 Darmstadt, Germany

Magnetic antiperovskites (APVs) show various stable magnetic ordering and among which noncollinear antiferromagnetic (AFM) states display many intriguing magnetic properties such as barocaloric, piezomagnetic, etc. In this work, we performed density functional theory calculations to evaluate the magnetic ground state, magnetocystalline anisotropy energy, piezomagnetic effect (PME), and intrinsic anomalous Hall conductivity (IAHC) of 57 APVs with chemical formula M_3XZ (M= Cr, Mn, Fe, Co and Ni, Z= C and N). It is found that 20 compounds have noncollinear AFM state. By imposing 1% tensile and compressive biaxial strain, large piezomagnetic and piezospintronic effects are observed. For instance with 1% strain, the IAHC of Cr_3PtN increased by 251 S/cm and Cr_3IrN shows a strong PME with net magnetization of 0.21 μB/f.u. Detailed analysis on the electronic structure and lattice properties reveal that the underlying driving force can be attributed to strong magnetostructural coupling.

MA 4.14 Mon 13:00 H52

Origin of anomalous Hall effect in magnetic antiperovskites — •Ilias Samathrakis, Harish Kumar Singh, and Hongbin Zhang — Theory of Magnetic Materials, TU Darmstadt, Darmstadt, Germany

Antiferromagnet materials have recently become a hot research topic for spintronic applications. Being a special class of antiferromagnets, noncollinear magnets have also attracted a lot interest. In this work, we investigated how to induce finite anomalous Hall conductivity in antiperovskite Mn_3GaN and Mn_3NiN by tuning the magnetization direction between the Γ_{5g} and Γ_{4g} configurations, as well as by applying biaxial strain. The origin of the resulting anomalous Hall conductivity is elucidated by analyzing the electronic structure in detail. It is observed that the spatial position and the energy splitting of the Weyl points give rise to the non-vanishing conductivity values.