

TT 69: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Thursday 10:30–13:15

Location: H24

Topical Talk TT 69.1 Thu 10:30 H24
Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — ●IVO SOUZA — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies (“Weyl points”) in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a “gyrotropic magnetic effect” (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk TT 69.2 Thu 11:00 H24
Dirac Fermions in Antiferromagnetic Semimetal — ●PEIZHE TANG, QUAN ZHOU, GANG XU, and SHOU-CHENG ZHANG — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

TT 69.3 Thu 11:30 H24
Spin Hall effect in non-collinear antiferromagnets Mn3X (X=Sn, Ge, Ga) — ●YANG ZHANG^{1,3}, YAN SUN¹, CLAUDIA FELSER¹, and BINGHAI YAN^{1,2} — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ³Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in non-collinear antiferromagnetic (AFM) compounds Mn3X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [~ 1000 ($*/e$)*(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for the room-temperature spintronic applications.

TT 69.4 Thu 11:45 H24
Electronic reconstruction and anomalous Hall conductivity in 3d-oxide honeycomb lattices within the corundum structure — ●SANTU BAIDYA and ROSSITZA PENTCHEVA — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of 3d transition metal oxide honeycomb lay-

ers confined in the corundum structure (α -Al₂O₃) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. (M₂O₃)/(Al₂O₃)₅, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound M₂O₃, strong deviations from the bulk behavior are observed in the case of Ti₂O₃ and Mn₂O₃ bilayers. Our results indicate a formation of a quasi two-dimensional electron gas with a vertical confinement of ~ 5 Å for Ti₂O₃ and ~ 8.5 Å for Mn₂O₃. As a function of lateral strain (Ti₂O₃)/(Al₂O₃)₅ undergoes a metal-to-insulator transition associated with a switching of orbital polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in (M₂O₃)/(Al₂O₃)₅ (M=Ti, Mn).

TT 69.5 Thu 12:00 H24
Anomalous hall effect in triangular antiferromagnetic ordered structure — ●HAO YANG¹, SUN YAN², FELSER CLAUDIA², PARKIN STUART¹, and BINGHAI YAN² — ¹Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — ²Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn3X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

TT 69.6 Thu 12:15 H24
Anomalous Hall conductivity and orbital magnetization as local quantities — ●ANTIMO MARRAZZO¹ and RAFFAELE RESTA² — ¹THEOS, EPF Lausanne, Switzerland — ²Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist’s viewpoint—closely related: both have an expression as \mathbf{k} -space integrals of the appropriate geometrical quantity. The \mathbf{k} space is an artificial construct: all bulk properties are embedded in the ground state density matrix in \mathbf{r} space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in \mathbf{r} space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the “nearsightedness” of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic \mathbf{B} field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

TT 69.7 Thu 12:30 H24
Laser induced DC photocurrents in a Topological Insulator thin film — ●THOMAS SCHUMANN¹, NINA MEYER¹, GREGOR MUSSLER⁴, EVA SCHMORANZEROVÁ², DAGMAR BUTKOVICOVÁ², HELENA REICHLOVÁ³, LUKAS BRAUN⁵, CHRISTIAN FRANZ⁶, MICHAEL CZERNER⁶, PERTR NĚMEC², DETLEV GRÜTZMACHER⁴, TOBIAS KAMPFRATH⁵, CHRISTIAN HEILIGER⁶, and MARKUS MÜNZENBERG¹ — ¹IfP, EMA University Greifswald, Germany — ²MFF, Charles Uni-

versity, Prague, Czech Republic — ³FZU, Prague, Czech Republic — ⁴PGI-9, Jülich, Germany — ⁵FHI Berlin, Germany — ⁶University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent. We report our recent results on laser induced photocurrents in a ternary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver,D.Hsieh,H.Steinberg,P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

TT 69.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — ●CHRISTIAN TUTSCHKU¹, ROLF W. REINTHALER¹, CHAO LEI², ALLAN H. MACDONALD², and EWELINA M. HANKIEWICZ¹ — ¹Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — ²Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical

means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

[1] A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001)

[2] D. A. Ivanov, PRL **86**, 268 (2001)

[3] J. Alicea et al., Nature Physics **7**, 412 (2011)

TT 69.9 Thu 13:00 H24

Unpaired Majorana modes in Josephson junctions arrays with gapless bulk excitations — ●MANUEL PINO GARCIA — Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 Frelinghuysen rd, Piscataway, 08854 New Jersey, USA

The search for Majorana bound states in solid-state physics has been limited to materials which display a gap in their bulk spectrum. We will show that such unpaired states appear in certain quasi-one-dimensional Josephson junctions arrays with gapless bulk excitations. The bulk modes mediate a coupling between Majorana bound states via the Ruderman-Kittel-Yosida-Kasuya mechanism. As a consequence, the lowest energy doublet acquires a finite energy difference. For realistic set of parameters this energy splitting remains much smaller than the energy of the bulk eigenstates even for short chains of length $L \sim 10$. In this talk, we first explain the JJA system and how to model it with an Ising-like Hamiltonian. Then, a qualitative argument is employed to obtain the low-energy effective theory using unpaired Majorana modes. We will show numerical results which confirm the validity of this effective theory and discuss problems that may arise in the experimental realization of our proposal.