DS 23: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I (Joint session of DS and O, organized by O)

Time: Tuesday 14:00–16:00 Location: H24

Topical Talk DS 23.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — •Shuichi Murakami — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z2 topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

DS 23.2 Tue 14:30 H24

Topological orbital magnetic moments — •Manuel dos Santos Dias, Juba Bouaziz, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic spin textures, even without SOI, justifying the 'topological' label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

DS 23.3 Tue 14:45 H24

The orbital Rashba effect — •Dongwook Go[1,2], Patrick Buhl[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Hyun-Woo Lee[2], and Stefan Blügel[1] — [1]Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\text{orb-R}}(\mathbf{k}) = \alpha_{\text{orb-R}}\mathbf{L}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$, where $\mathbf{L}$ is the orbital moment derived from atomic orbitals and $\alpha_{\text{orb-R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the **k**-space. The mechanism behind the emergence of the $H_{\text{orb-R}}(\mathbf{k})$ can be understood as the **k**-dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag *s*-orbital and a Bi *p*-orbital leads to the orbital Rasbha effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

DS 23.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — •Juba Bouaziz, Manuel dos Santos Dias, Phivos Mavropoulos, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinksii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].

[1] J. Bouaziz *et al.* in preparation.
[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

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DS 23.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — •Imara L. Fernandes, Benedikt Schweflinghaus, Juba Bouaziz, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).

[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79** (2014).
[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).
[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

DS 23.6 Tue 15:30 H24

Topological magnons: Any chance to find them? — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., $Lu_2V_2O_7$, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe_3Sn_2 as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang et al., PRB **87**, 144101 (2013); [2] A. Mook et al., Phys. Rev. B **89**, 134409 (2014); *eidem*, Phys. Rev. B **90**, 024412 (2014); *eidem*, Phys. Rev. B **91**, 224411 (2015); *eidem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell et al., Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose et al., Science **329**, 297 (2010).

DS 23.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory

— •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).