MA 10: Topological Insulators (joint session MA/TT)

Time: Monday 15:00–17:15 Location: HSZ 403

MA 10.1 Mon 15:00 HSZ 403

Benchmark study of symmetry-adapted ML-DFT models for magnetically doped topological insulators — •Johannes Wasmer[1], Rubel Mozumder[1], Philipp Rüssmann[1,2], Ira Assent[1,3], and Stefan Blügel[1] — [1]Forschungszentrum Jülich, Germany — [2]University of Würzburg, Germany — [3]Aarhus University, Denmark

We present a benchmark study of surrogate models for impurities embedded into crystalline solids. Using the Korringa-Kohn-Rostoker Green Function method [1], we have built databases of several thousand calculations of single impurities (monomers) embedded into different elemental crystals, as well as magnetic transition metal impurity dimers embedded in the topological insulator Bi_2Te_3. We predict the converged monomer impurity electron potential and the isotropic exchange interaction of the impurity dimer in the classical Heisenberg model. From these surrogates, we intend to build transferable models for larger systems in the future, which will accelerate the convergence of our DFT codes. The study compares various recent E(3)-equivariant models such as ACE and MACE [2] in terms of performance and reproducible end-to-end workflows.

[1] P. Rüßmann et al., npj Comput Mater 7, 13 (2021)
[2] I. Batatia et al., arXiv:2206.07697 (2022)

MA 10.2 Mon 15:15 HSZ 403

High thorughput magnetic topological materials search II — •Iñigo Robredo[1,2], Yuanfeng Xu[3,4], Andrei Bernevig[2,3], Claudia Felser[1], Nicolas Regnault[3,6], Luis Elcoro[5], and Maia G. Vergniory[1,2] — [1]MPI CPFS Dresden — [2]DIPC — [3]Princeton University — [4]Zhejiang University — [5]Basque Country University — [6]Sorbonne Université

The development of topological quantum chemistry has proven to be a game changing tool for predicting topological phases in realistic materials, both non-magnetic and magnetic. Building on the work of previous studies, in this work we expand the family of magnetic insulators and semimetals with non-trivial topological properties. We analyzed 408 magnetic structures from the Bilbao Crystallographic Server magnetic database, whose crystal and magnetic structures have been experimentally reported. To take into account the localized nature of magnetic elements, we perform electronic structure calculations and topological diagnosis as a function of the Hubabrd U parameter. This results in a topological phase iagram for each material as a function of the Hubbard interaction potential. We provide full details of the materials, which can be readily grown to explore their new topological phenomena.

MA 10.3 Mon 15:30 HSZ 403

Manipulating topological feature of massive Dirac particle with scalar potential — •Sumit Ghosh[1,2], Yuriy Mokrousov[1,2], and Stefan Blügel[1] — [1]PGI-1, Forschungszentrum Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Germany

Topology is one of the central aspect of modern spintronics. Different physical observables as well as transport properties that originates from the nontrivial topology of the system shows significant robustness against different external perturbation. Manipulating the topology of a system on the other hand is a highly non-trivial task since it requires tuning the internal degrees of freedom. In this presentation we are going to present an intrinsic mechanism to manipulate the topological feature and associated transport properties by using scalar potential. We systematically demonstrate how a scalar potential can invert the mass term of a massive Dirac particle which subsequently leads to the change of the topological index. We further demonstrate how this mechanism can be exploited to control the formation of edge states which can control the transport properties. This study thus provides a better understanding of the origin of the topological properties as well as a simple way to manipulate them. [https://arxiv.org/abs/2204.06412]

MA 10.4 Mon 15:45 HSZ 403

Mapping out the topological phase diagram of FeSn — Soumya Sankar[1], Ruizi Liu[2], Xuejian Gao[1], Qifang Li[3,4], JiaChang Zheng[1], Caiyun Chen[1], Chengping Zhang[1], Kun Qiang[2], Zi Yang Meng[3,4], Kam Tuen Law[1], Qiming Shao[1,2], and •Berthold Jäck[1] — [1]HKUST, Clear Water Bay, Kowloon, Hong Kong SAR — [2]HKUST, Department of Computer Science and Electrical Enginerring, Clear Water Bay, Kowloon, Hong Kong SAR — [3]Hong Kong University, Department of Physics, Pokfulam Road, Hong Kong SAR — [4]University of Tokyo, Department of Physics, Hongo, Bunkyo City, Tokyo

Metallic kagome magnets exhibit a flat band and a Dirac point in their electronic structure and long-range magnetic order. The combination of these properties creates favourable conditions to search for strongly correlated and topological electronic states. The near-ideal kagome band structure of the inter metallic kagome series X1Y1 offers opportunities to study the interplay between strong electronic correlations, topology, and magnetism.

We have used molecular beam epitaxy and electronic transport measurements to study the interplay of magnetism and band topology in thin films of antiferromagnetic FeSn. We will present results from a magnetic field and temperature dependent study of the anomalous Hall effect. Combining these measurements with magnetic Monte-Carlo simulations and theoretical model calculations, we map out the topological phase diagram of FeSn over a large temperature range.

We acknowledge support by the GRC, and the Croucher Foundation.

15 min. break

MA 10.5 Mon 16:15 HSZ 403

Investigation of the magnetic topological insulator family (MnPn2Te4) (Pn2Te3) n, (Pn=Bi, Sb) by μSR and NMR — •Manaswini Sahoo[1,2], Anna Isaeva[1], Bernd Büchner[1], and Roberto De Renzi[2] — [1]Leibniz IFW Dresden, Dresden, Germany — [2]University of Parma,Parma, Italy

Time-reversal symmetry breaking in a topological insulator (TI) opens a surface gap and distinguishes chiral quantum states that could eventually be exploited in electrically controlled spintronic devices. The recent discovery of layered van der Waals materials opens a new approach to achieve this.(MnBi2Te4) (Bi2Te3) n is one of the first such examples, where the increasing number n of TI layers controls the magnetic dimensionality of the material. These compounds do display the quantum anomalous Hall effect, where spontaneous magnetization and spin-orbit coupling lead to a topologically non-trivial electronic structure. In the case of (MnBi2Te4) (Bi2Te3) n, Zero Field μSR shows more than one internal field at the muon site with the majority one decreasing in value when n is increased. The muon spin precessions display very fast relaxations of static inhomogeneous nature. Whereas in the sister compound MnSb2Te4, Zero Field μSR shows a broader distribution of magnetic field at the muon due to larger intermixing between Mn/Sb in the sample. Importantly, the weak Transverse Field shows a sharp magnetic transition at the same Tc, with a clear relaxation peak due to critical fluctuations, taking place in the whole volume of the material. This local information from μSR together with NMR is crucial to correctly interpret macroscopic magnetization data.

MA 10.6 Mon 16:30 HSZ 403

Magnetic dilution effect and topological phase transitions in antiferromagnet $Mn_{1-x}Pb_xBi_2Te_4$ — •Yueh-Ting Yao[1], Tiema Qian[2], Tay-Rong Chang[1,3,4], and Ni Ni[2] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Department of Physics and Astronomy and California NanoSystems Institute, University of California, Los Angeles, California 90095, USA — [3]Center for Quantum Frontiers of Research and Technology (QFort), Tainan 701, Taiwan — [4]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan

The interplay between magnetism and topology have taken the central stage of modern condensed matter physics in the past three years. The fine control of magnetism and topology in a magnetic topological insulator is crucial for realizing various novel magnetic topological phases, such as axion insulator, magnetic Weyl semimetals, etc. In this work, we investigate the evolution of magnetism and band topology in $Mn_{1-x}Pb_xBi_2Te_4$ via angle resolved photoemission spectroscopy (ARPES), first-principles calculations, and electronic transports. We present the comprehensive phase diagram by controlling Pb content and magnetism in this alloy system. Moreover, we provide the first topological crystalline insulator with non-trivial glide mirror Chern number in MnBi2Te4-family materials, which is protected by nonsymmorphic symmetry arise from antiferromagnetic (AFM) configuration. Our work provides a fruitful platform with continuously tunable magnetism and topology for investigating emergent phenomena and pave a way towards potential new applications of nanoelectronics.

MA 10.7 Mon 16:45 HSZ 403

Thermal Hall Effect of Magnon-Phonon Hybrid Quasiparticles in a Fluctuating Heisenberg-Kitaev Antiferromagnet — •Robin R. Neumann[1], Alexander Mook[2], Jürgen Henk[1], and Ingrid Mertig[1] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Johannes Gutenberg University, Mainz, Germany

Magnons, the quantized excitations of localized spins, and phonons, the quantized excitations of the lattice, are two types of quasiparticles that are responsible for heat transport in magnetic insulators. However, phonons by themselves do not contribute to the *transverse* heat current induced by a temperature gradient, i.e., the thermal Hall effect (THE). Magnons, on the other hand, may exhibit a Berry curvature, a magnetic field in reciprocal space, that leads to an intrinsic THE.

In this talk, I address the THE in a Heisenberg-Kitaev antiferromagnet subjected to a magnetic field. The applied field drives the system from a zigzag antiferromagnetic to a spin-flop state. The magnon-driven THE indicates the magnetic phase transition by a sign change at the critical field. Furthermore, when the magnetoelastic interaction is considered, the phonon and magnon bands hybridize and additional Berry curvature at the avoided crossings emerge. Depending on the strength of the spin-phonon coupling, this may lead to an overall reversal of the THE while the field-induced sign change at the critical field remains mostly robust. These results showcase that magnon-phonon hybridization can be pivotal for the interpretation of transport experiments.

MA 10.8 Mon 17:00 HSZ 403

Limitations of the Bulk-Boundary Correspondence in Topological Magnon Insulators due to Magnon-Magnon Interactions — •Jonas Habel[1], Johannes Knolle[1], Alexander Mook[2], and Josef Willsher[1] — [1]Technical University of Munich, Germany (Theory of Quantum Matter and Nanophysics) — [2]Johannes Gutenberg University Mainz, Germany

Magnon excitations in ordered quantum magnets can exhibit topological band structures characterized by non-zero Chern numbers. Such magnonic Chern insulators are widely believed to host protected chiral edge modes due to the bulk-boundary correspondence, in analogy to electronic Chern insulators. However, in contrast to electrons, magnons are bosons and can thus be subject to exotic number-nonconserving many-body interactions, enabling potentially strong spontaneous decays at zero temperature.

To assess their effect on the chiral edge magnons, we study a topological honeycomb-lattice ferromagnet with Dzyaloshinskii-Moriya interactions using many-body perturbation theory. We discover that non-harmonic terms of the spin-wave expansion may lead to severe lifetime reduction of edge modes and their delocalisation into the bulk. For sufficiently strong interactions, the spectral weight of the chiral edge magnons vanishes entirely. These findings indicate that topological magnon bands within the harmonic framework do not necessarily give rise to protected edge modes in the full spin theory, suggesting limitations of the bulk-boundary correspondence in this case.