

## MA 15: Topological Insulators and Weyl Semimetals (joint session MA/TT)

Time: Tuesday 9:30–13:00

Location: H 2013

MA 15.1 Tue 9:30 H 2013

**behavior of Dirac fermion in non-symmorphic CeTX<sub>2</sub> systems** — ●SAWANI DATTA<sup>1,4</sup>, KHADIZA ALI<sup>2</sup>, RAHUL VERMA<sup>1</sup>, DENIS VYALIKH<sup>3</sup>, BAHADUR SINGH<sup>1</sup>, A THAMIZHAVEL<sup>1</sup>, SAROJ P DASH<sup>2</sup>, and KALOBARAN MAITI<sup>1</sup> — <sup>1</sup>Tata Institute of Fundamental Research, Mumbai, India — <sup>2</sup>Chalmers University of Technology, Gotheborg, Sweden. — <sup>3</sup>DIPC, Donostia, San Sebastian, Spain — <sup>4</sup>Max Plank Institute for Solid State Research, Stuttgart, Germany

We have studied the behavior of Dirac fermions in the presence of strong electron correlation in nonsymmorphic Kondo lattice systems, CeTX<sub>2</sub> (T=Cu/Ag, X=As/Sb) employing high-resolution angle-resolved photoemission spectroscopy [1]. Experiments reveal crossings of highly dispersive linear bands at the Brillouin zone boundary protected by non-symmorphic symmetry [2]. In addition, anisotropic Dirac cones are observed constituted by the square net Sb(As) 5p(4p) states forming a diamond-shaped nodal line. The Dirac bands are linear in a wide energy range with an unusually high slope and exhibit distinct Dirac points in these highly spin-orbit coupled systems. Along with these bulk crossings, CeCuAs<sub>2</sub> also exhibits a surface Dirac crossing at the  $\Gamma$ -point. These results seed the emergence of an area of robust topological fermions even in the presence of strong correlation. [1] S. Datta et al. arXiv:2311.05278 [2] L. M. Schoop et al., Nat. Commun. 7, 11696 (2016).

MA 15.2 Tue 9:45 H 2013

**Isotropic 3D topological phases with broken time reversal symmetry** — HELENE SPRING<sup>1</sup>, ANTON R. AKHMEROV<sup>1</sup>, and ●DANIEL VARJAS<sup>2,3,4</sup> — <sup>1</sup>Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 4056, 2600 GA Delft, The Netherlands — <sup>2</sup>Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm, Sweden — <sup>3</sup>Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — <sup>4</sup>IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstr. 20, 01069 Dresden, Germany

Axial vectors, such as current or magnetization, are commonly used order parameters in time-reversal symmetry breaking systems. These vectors also break isotropy in three dimensional systems, lowering the spatial symmetry. We demonstrate that it is possible to construct a fully isotropic and inversion-symmetric three-dimensional medium where time-reversal symmetry is systematically broken. We propose an amorphous system with scalar time-reversal symmetry breaking, implemented by hopping through chiral magnetic clusters along the bonds. The average spatial symmetries alone protect a statistical topological insulator phase in this system. We demonstrate the topological nature of our model by constructing a bulk integer topological invariant, which guarantees gapless surface spectrum on any surface with several overlapping Dirac nodes, analogous to crystalline mirror Chern insulators. We also show the expected transport properties of a three-dimensional statistical topological insulator, which remains critical on the surface for odd values of the invariant.

MA 15.3 Tue 10:00 H 2013

**Behavior of Dirac Fermions in Kondo lattice systems** — ●KALOBARAN MAITI — Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India

We studied the behavior of Dirac fermions in novel Kondo lattice system employing ARPES. We show that a binary system, SmBi show signature of multiple gapped and un-gapped Dirac cones in the band structure. Employing ultra-high-resolution ARPES, we discover destruction of a surface Fermi surface across the Neel temperature while the behavior of Dirac cones survive across the magnetic transition. ARPES data of a non-symmorphic Kondo lattice system, CeAgSb<sub>2</sub> exhibit distinct Dirac cones as well as diamond-shaped nodal lines; the slope of these linear bands is unusually high, larger than that in graphene and maintains its high value in a wide energy range indicating robust high velocity of these relativistic particles. The slope becomes smaller in the vicinity of strongly correlated Ce 4f bands forming a kink; a unique case due to correlation induced effects.

References: 1. Sawani Datta et al., arXiv:2311.05278 2. A.P. Sakhya et al. Phys. Rev. Mater. 2021, 5, 054201. 3. A.P. Sakhya et al. Phys. Rev. B 2022, 106, 085132.

MA 15.4 Tue 10:15 H 2013

**Strain control on band topology and surface states in antiferromagnetic EuCd<sub>2</sub>As<sub>2</sub>** — ●NAYRA ALVAREZ<sup>1</sup>, RODRIGO JAESCHKE<sup>1</sup>, VENKATA KRISHNA<sup>1</sup>, ADRIAN VALADKHANI<sup>2</sup>, ROSER VALENTI<sup>2</sup>, LIBOR SMEJKAL<sup>1</sup>, and JAIRO SINOVA<sup>1,3</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg Universität — <sup>2</sup>Institut für Theoretische Physik, Goethe-Universität Frankfurt — <sup>3</sup>Inst. of Physics Academy of Sciences of the Czech Republic

Topological semimetal antiferromagnets provide a rich source of exotic topological states which can be controlled by manipulating the orientation of the Neel vector, or by modulating the lattice parameters through strain. We investigate via ab initio density functional theory calculations, the effects of shear strain on the bulk and surface states in two antiferromagnetic EuCd<sub>2</sub>As<sub>2</sub> phases with out-of-plane and in-plane spin configurations. We demonstrate the control of the band topology and how they can lead to hinge modes as well, which may prove useful to realize the long-sought after axion states and to stimulate further research in the field of strain effects on Dirac semimetals[1].

[1] Pari, Nayra A. Álvarez, et al. "Strain control of band topology and surface states in antiferromagnetic EuCd<sub>2</sub>As<sub>2</sub>." arXiv preprint arXiv:2310.19186 (2023)

MA 15.5 Tue 10:30 H 2013

**Nonlocal Spin Dynamics Arising From Induced Interactions at the Interface of a Topological Insulator and a Ferromagnet** — ●CHRISTIAN S. JOHNSEN and ASLE SUDBØ — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

In recent years, topologically stable magnetic textures called skyrmions have received much attention for their potential uses in information technology. One such use is making skyrmions the information carriers in low-dissipation information storage devices because skyrmions can be moved using exceedingly small currents. One proposed setup is to move them using a low-dissipation current on the surface of a topological insulator. In this work, an effective field theory for the spins in such a heterostructure is derived. The theory shows time-dependent induced spin-spin interactions such as DMI and the presence of non-negligible retardation effects which alter the system's spin dynamics. In particular, we derive an inertial term and various dissipative terms in the Landau-Lifshitz-Gilbert equation.

MA 15.6 Tue 10:45 H 2013

**Surface reconstruction effects in thin films of Antiferromagnetic Topological Insulator MnBi<sub>2</sub>Te<sub>4</sub>** — ●SHAHID SATTAR and CARLO MARIA CANALI — Department of Physics and Electrical Engineering, Linnaeus University, Kalmar SE-39231, Sweden

Intrinsic magnetic topological insulator MnBi<sub>2</sub>Te<sub>4</sub> (MBT) characterized by a non-zero topological  $Z_2$  index has recently gained significant interest and attention. Experiments on thin films of MBT have confirmed the presence of the anomalous quantum Hall and axion insulating phases in odd and even septuple-layer films respectively. In this work, we investigate surface reconstruction effects on topological characteristics in thin films of MBT using first-principles calculations and an effective  $\mathbf{k} \cdot \mathbf{p}$  model Hamiltonian. We discuss the implications of surface reconstruction on both the Chern and axion insulating phases and discuss the presence of Rashba surface states for the latter. Our results provide a theoretical framework needed to elucidate the nature of surface reconstruction in magnetic TI thin films, which can be useful for their experimental realization.

MA 15.7 Tue 11:00 H 2013

**The MT Protected Topological States and Local Symmetry in 2D Antiferromagnetic SrMn<sub>2</sub>Bi<sub>2</sub>** — ●HAO WANG<sup>1</sup>, CHENGWANG NIU<sup>2</sup>, LIBOR SMEJKAL<sup>3,4</sup>, and YURIY MOKROUSOV<sup>1,3</sup> — <sup>1</sup>Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — <sup>2</sup>School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China — <sup>3</sup>Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — <sup>4</sup>Institute of Physics Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Praha 6, Czech Republic

Antiferromagnetic topological insulators (AFMTIs) represent a novel

class of topological states for spintronics. Understanding symmetry protection and exploring AFMTIs with desirable properties are crucial. In this study, through first-principles calculations and symmetry analysis, we investigate the topological properties of monolayer SrMn<sub>2</sub>Bi<sub>2</sub>, demonstrating sensitivity to magnetic configurations. In the out-of-plane AFM ground state, we observe a gapless helical edge state protected by the mirror plane combined with time-reversal symmetry. In the FM state, this system resides in a quantum anomalous Hall phase, and topology trivial for in-plane magnetization. We show that the topological properties can be efficiently manipulated by strain. Additionally, constructing proper Wannier functions obeying symmetry constraints is crucial to avoid spurious states in surface spectra. Our work provides an ideal candidate for AFMTIs and guides the symmetry analysis of magnetic topological materials using Wannier functions.

### 15 min. break

MA 15.8 Tue 11:30 H 2013

**Electrical Activity of Topological Chiral Edge Magnons** — ●ROBIN R. NEUMANN<sup>1</sup>, ALEXANDER MOOK<sup>2</sup>, JÜRGEN HENK<sup>1</sup>, and INGRID MERTIG<sup>1</sup> — <sup>1</sup>Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — <sup>2</sup>Johannes Gutenberg University, Mainz, Germany

Magnons, the bosonic quasiparticles of spin waves, have been predicted to feature similar topological phases as electrons. In particular, the topological band structure of the quantum Hall systems has its magnonic analogue in the topological magnon insulator (TMI), which hosts topologically protected chiral edge excitations. Beyond theoretical studies, however, there exist no direct experimental evidence of their existence as the lack of charge renders them invisible to most surface-sensitive probes.

In this talk I demonstrate how magnetoelectric coupling imparts an electric dipole moment to the chiral magnons that manifests in equilibrium and nonequilibrium. Considering a two-dimensional ferromagnetic TMI, an electric edge polarization perpendicular to the sample's edges is driven by thermal fluctuations of the collinear magnetic ground state in equilibrium. On the other hand, the TMI features a unique in-gap resonance in its electrical absorption spectrum that stems from the chiral magnons showcasing their electrical activity. These results suggest THz spectroscopy as promising probe for topological magnons.

MA 15.9 Tue 11:45 H 2013

**Interplay of magnetism and band topology in Eu<sub>1-x</sub>Ca<sub>x</sub>Mg<sub>2</sub>Bi<sub>2</sub> (x=0, 0.5, 0.67) from first principles study** — ●AMARJYOTI CHOUDHURY, NARAYAN MOHANTA, and TULIKA MAITRA — IIT Roorkee, India

The recent discovery of time-reversal symmetry-breaking magnetic Weyl semimetals (WSMs) has sparked extensive research in quantum topological materials. We systematically studied magnetic orders, electronic structure, and the interplay between magnetic order and band topology in EuMg<sub>2</sub>Bi<sub>2</sub> (EMB) and its Ca-doped variant using density functional theory (DFT). Our investigation reveals various magnetic order-driven topological phases, such as a topological insulator in the A-type antiferromagnetic (A-AFM) phase with Eu moments along the *b*, a Dirac semimetal in the A-AFM phase with Eu moments along the *c* direction, and a Weyl semimetal in the ferromagnetic (FM) phase with Eu moments along the *c* direction. These phases are energetically close and tunable by external factors like magnetic field or chemical substitution. In the FM state of EuMg<sub>2</sub>Bi<sub>2</sub>, we identify an ideal Weyl semimetal with a single pair of Weyl points (WPs) close to the Fermi level along  $\Gamma$ -A direction. Doping with 50% and 67% Ca at Eu sites moves the WPs even closer to the Fermi level, making it highly desirable for applications. Additionally, the separation between WPs decreases in doped compounds, impacting anomalous Hall conductivity (AHC). Our first-principles calculation of AHC shows high peak values at these WPs, decreasing with Ca doping, indicating Ca as a potential external handle to tune AHC in this system.

MA 15.10 Tue 12:00 H 2013

**Chiral spin textures in the B20 material family** — ●IÑIGO ROBREDO<sup>1</sup>, JONAS KRIEGER<sup>2</sup>, NIELS SCHRÖTER<sup>2</sup>, MAIA VERGNIORY<sup>1</sup>, and CLAUDIA FELSER<sup>1</sup> — <sup>1</sup>MPI CPfS — <sup>2</sup>MPI Microstructure Physics

The spin texture of electronic bands has been studied for decades in magnetic materials due to its promising applications in the field of spintronics, which aims to exploit the spin degree of freedom. Recently, it has been shown that non-magnetic materials can present exotic spin

textures, which makes them promising for microelectronics applications due to the lack of stray fields. In order to present non-trivial spin degeneracies, these systems break crystalline rotoinversion symmetries, and are thus structurally chiral. In this work we revisit the chiral toy model in space group 198 introduced in Ref [1] as a proxy for materials in the B20 family and study the spin textures as a function of spin-orbit coupling strength. We study the spin texture of the surface Fermi arcs, which has also attracted attention recently [2], and show that the spin-momentum locking varies along the surface BZ.

[1] Mao Lin, Iñigo Robredo, Niels B. M. Schröter, Claudia Felser, Maia G. Vergniory, and Barry Bradlyn Phys. Rev. B 106, 245101 [2] Jonas A. Krieger, Samuel Stolz, Inigo Robredo, et al, arXiv:2210.08221

MA 15.11 Tue 12:15 H 2013

**Nonlinear optical diode effect in a magnetic Weyl semimetal** — ●CHRISTIAN TZSCHASCHEL<sup>1,2</sup>, JIAN-XIANG QIU<sup>2</sup>, XUE-JIAN GAO<sup>3</sup>, HOU-CHEN LI<sup>2</sup>, CHUNYU GUO<sup>4</sup>, HUNG-YU YANG<sup>5</sup>, CHENG-PING ZHANG<sup>3</sup>, YING-MING XIE<sup>3</sup>, YU-FEI LIU<sup>2</sup>, ANYUAN GAO<sup>2</sup>, DAMIEN BÉRUBE<sup>2</sup>, THAO DINH<sup>2</sup>, SHENG-CHIN HO<sup>2</sup>, YUQIANG FANG<sup>6,7</sup>, FUQIANG HUANG<sup>6,7</sup>, JOHANNA NORDLANDER<sup>2</sup>, QIONG MA<sup>5</sup>, FAZEL TAFTI<sup>5</sup>, PHILIP J.W. MOLL<sup>4</sup>, KAM TUEN LAW<sup>3</sup>, and SUYANG XU<sup>2</sup> — <sup>1</sup>Max Born Institute, Berlin, Germany — <sup>2</sup>Harvard University, Cambridge, USA — <sup>3</sup>Hong Kong University of Science and Technology, Hong Kong, China — <sup>4</sup>Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — <sup>5</sup>Boston College, Chestnut Hill, USA — <sup>6</sup>Shanghai Institute of Ceramics, Chinese Academy of Science, Shanghai, China — <sup>7</sup>College of Chemistry and Molecular Engineering Peking University, Beijing, China

We report the observation of a nonlinear optical diode effect (NODE) in the magnetic Weyl semimetal CeAlSi, where the magnetic state of CeAlSi introduces a pronounced directionality in the nonlinear optical second-harmonic generation (SHG). By physically reversing the beam path, we observe a strong directional contrast over a wide bandwidth exceeding 250 meV. Supported by first-principles calculations, we establish the linearly dispersive bands emerging from Weyl nodes as the origin of the extreme bandwidth. We further demonstrate current-induced magnetization switching and thus electrical control of the NODE in a spintronic device structure. Our results advance ongoing research to identify novel phenomena in magnetic quantum materials.

MA 15.12 Tue 12:30 H 2013

**Origin of incommensurate magnetic order in rare-earth magnetic Weyl semimetals** — ●JUBA BOUAZIZ<sup>1</sup>, GUSTAV BIHLMAYER<sup>1</sup>, CHRISTOPHER E. PATRICK<sup>2</sup>, JULIE B. STAUNTON<sup>3</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich JARA, D-52425 Jülich, Germany — <sup>2</sup>Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom — <sup>3</sup>Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

We investigate rare-earth magnetic Weyl semimetals through first-principles simulations, analyzing the connection between incommensurate magnetic order and the presence of Weyl nodes in the electronic band structure. Focusing on PrAlSi, NdAlSi, and SmAlSi, we demonstrate that the reported helical ordering does not originate from the nesting of topological features at the Fermi Surface or the Dzyaloshinskii-Moriya interaction. Instead, the helical order arises from frustrated isotropic short-range superexchange between the 4f moments facilitated by pd-hybridization with the main group elements. Employing a spin Hamiltonian with isotropic exchange and single-ion anisotropy we replicate the experimentally observed helical modulation. Funding: European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant No. 856538, project "3D MAGiC")

MA 15.13 Tue 12:45 H 2013

**Surface magnon spectra of nodal loop semimetals** — ●ASSEM ALASSAF<sup>1</sup>, LÁSZLÓ OROSZLÁNYI<sup>2</sup>, and JÁNOS KOLTAI<sup>3</sup> — <sup>1</sup>Department of Physics of Complex Systems, ELTE Eötvös Loránd University, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary — <sup>2</sup>Department of Physics of Complex Systems, ELTE Eötvös Loránd University, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary; MTA-BME Lendület Topology and Correlation Research Group, Budafoki út 8., H-1111 Budapest, Hungary — <sup>3</sup>Department of Biological Physics, ELTE Eötvös Loránd University, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary

In this paper, we establish a connection between the bulk topological structure and the magnetic properties of drumhead surface states of

nodal loop semimetals. We identify the magnetic characteristics of the surface states and compute the system's magnon spectrum by treating electron-electron interactions on a mean-field level. We draw attention to a subtle connection between a Lifshitz-like transition of the surface

states driven by mechanical distortions and the magnetic characteristics of the system. Our findings may be experimentally verified, e.g. by spin-polarized electron energy loss spectroscopy of nodal semimetal surfaces.