FROM CHEMICAL BONDS TO TOPOLOGY

Leslie Schoop¹

¹Department of Chemistry, Princeton University, Princeton, NJ, USA E-Mail: lschoop@princeton.edu

In the discipline of chemistry, it is common to have guidelines and heuristics that help to predict how chemical reactions will proceed. We are interested to expand these heuristics to understand if we can predict topological materials. In this talk, I will show how delocalized chemical bonds in certain structural networks allow us to define chemical descriptors that predict band inversions. Using these descriptors, we found a layered, antiferromagnetic van der Waals material with very high mobility. These properties have previously not coexisted in a material that can be mechanically exfoliated. We further implemented our heuristics to discover novel complex topological phases, including magnetic ones, and phases that are in competition with complex structural distortions. I will show how structural distortions can have a positive effect on topological band structures.

ELECTRICAL MANIPULATION OF AN ANTIFERROMAGNETIC WEYL SEMIMETAL STATE

Satoru Nakatsuji^{1,2,3}

¹ Department of Physics, School of Science, The University of Tokyo, Tokyo 113-0033, Japan

² Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba 277-8581,

Japan

³Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

E-Mail: satoru@scphys.s.u-tokyo.ac.jp

Electrical manipulation of emergent phenomena due to nontrivial band topology is a key to realize next-generation technology using topological protection. Recent discovery of the magnetic Weyl fermions in the antiferromagnet Mn₃Sn has attracted significant attention [1], as the magnetic Weyl semimetal exhibits various exotic phenomena such as chiral anomaly [1], large anomalous Hall effect (AHE) [2], anomalous Nernst effect [3,4], magneto-optical effects [5], and magnetic spin Hall effect [6], which have robust properties due to the topologically protected Weyl nodes. Given the prospects of antiferromagnetic (AF) spintronics for realizing high-density devices with ultrafast operation, it would be ideal if one could electrically manipulate an AF Weyl semimetal. Here we demonstrate the electrical switching of a topological AF state and its detection by AHE at room temperature [7]. In particular, we employ a polycrystalline thin film of the AF Weyl metal Mn₃Sn, which exhibits zero-field AHE. Using the bilayer device of Mn₃Sn and nonmagnetic metals (NMs), we find that an electrical current density of $\sim 10^{10}$ - 10^{11} A/m² in NMs induces the magnetic switching with a large change in Hall voltage, and besides, the current polarity along a bias field and the sign of the spin Hall angle of NMs determines the sign of the Hall voltage. Notably, the electrical switching in the antiferromagnet is made using the same protocol as the one used for ferromagnetic metals. Our observation may well lead to another leap in science and technology for topological magnetism and AF spintronics.

This is the work in collaboration with Hanshen Tsai, Tomoya Higo, Kouta Kondou, Takuya Nomoto, Akito Sakai, Ayuko Kobayashi, Takafumi Nakano, Kay Yakushiji, T. Koretsune, M. Suzuki, Ryotaro Arita, Shinji Miwa, YoshiChika Otani, Muhammad Ikhlas, Tahahiro Tomita, Hua Chen, and Allan MacDonald.

[1] K. Kuroda, T. Tomita et al., Nature Materials 16, 1090-1095 (2017)

[2] S. Nakatsuji, N. Kiyohara, T. Higo, Nature 527, 212-215 (2015)

[3] M. Ikhlas, T. Tomita, T. Koretsune, M.-T. Suzuki, D. Nishio-Hamane, R. Arita, Y. Otani and S. Nakatsuji, Nature Physics **13**, 1085-1090 (2017)

[4] A. Sakai, Y.P. Mizuta, A.A. Nugroho, R. Sihombing, T. Koretsune, M.-T. Suzuki, N. Takemori, R. Ishii, D.N. Hamane, R. Arita, P. Goswami and S. Nakatsuji, Nature Physics, 14, 1119–1124 (2018)

[5] T. Higo *et al.*, Nature Photonics **12**, 73-78 (2018); T. Matsuda *et al.*, Nature Communications **11**, 2863 (2020)

[6] M. Kimata et al., Nature 565, 627–630 (2019)

[7] H. Tsai, T. Higo, K. Kondou, T. Nomoto, A. Sakai, A. Kobayashi, T. Nakano, K.

Yakushiji, R. Arita, S. Miwa, Y. Otani, and S. Nakatsuji, Nature 580, 608-613 (2020)

TOPOLOGICAL PHYSICS IN THE 2D KAGOME NETWORK

<u>Riccardo Comin¹</u>

¹ Department of Physics, Massachusetts Institute of Technology, Cambridge, 02139, Massachusetts, USA E-Mail: rcomin@mit.edu

The kagome network is one of the possible tilings of two-dimensional space, one with the same point symmetries as the hexagonal lattice of graphene. Recent theoretical developments suggest that the combination of unusual magnetism, spin-orbit coupling, and geometric frustration in kagome metals may lead to a wide range of novel topological physics, such as fractional quantum Hall effect and intrinsic anomalous Hall effect. In these phenomena, a major role is played by the topologically nontrivial flat bands and massive Dirac cones, both of which are predicted to exist from the unique geometrical hopping pathways of kagome lattice. Despite these predictions, the experimental band structure of kagome compounds has long remained unreported.

In this talk, I will report on the experimental band structure of various kagome compounds belonging to the family of transition metal stannides, and in particular Fe₃Sn₂, FeSn, and CoSn. In these systems which intertwine robust magnetism and electronic topology, we observed various manifestations of topological physics. These include the realization of the Kane-Mele model for 2D Dirac fermions with a spin-orbit-induced topological gap, as well as the discovery of the elusive flat bands and its nontrivial topology.

In sum, transition metal-based kagome lattices have emerged a new platform for intriguing phenomena arising from the combination of topology, magnetism, and correlations. I will discuss the prospects and outlook for further exploration of novel topological physics in this materials family.

ORBITAL MAGNETISM AND ISOSPIN POMERANCHUK EFFECT IN MOIRE HETEROSTRUCTURES

Andrea F. Young¹

¹Department of Physics, University of California, Santa Barbara 93106, USA E-Mail: andrea@physics.ucsb.edu

Moire flat bands host a wide range of correlated states at low temperatures. My talk will focus on the role of orbital magnetism in these systems, in which the electron system spontaneously polarizes into one or more spin- and valley-isospin flavors.

In the first part of the talk, I will focus on the observation of quantized anomalous Hall effects in a variety of moire systems. In this spectacular manifestation of orbital magnetism, the ground state at certain integer filling factors is spontaneously polarized into a single valley-projected moire miniband, leading to robust magnetic hysteresis and a quantized Hall effect at zero magnetic field. We observe a variety of novel phenomena in this regime, including ultra-low power current induced switching and gate-tuned reversal of magnetic order that can be tied to the magnetization of the topological edge states.

In the second part of the talk, I will discuss the more general role orbital magnetism plays in the phase diagram of these materials at high temperatures. In particular, we find that even when the ground state is isospin unpolarized, a finite polarization can obtain at high temperatures. We ascribe this effect—observed generically in twisted bilayer graphene—to an isospin analogue of the Pomeranchuk effect long studied in ³He, in which the high entropy associated with isospin excitations of the orbital magnets favors fluctuating magnetic order at high temperatures.

References:

Serlin *et al.*, arXiv:1907.00261 Polshyn *et al.*, arXiv:2004.11353 Tschirhart *et al.*, arXiv:2006.08053 Saito *et al.*, arXiv:2008.10830

QUANTUM TRANSPORT IN THIN FILM HETEROSTRUCTURES OF TOPOLOGICAL INSULATORS

Ryutaro Yoshimi¹

¹RIKEN Center for Emergent Matter Science (CEMS) 2-1 Hirosawa, Wako-shi, Saitama, 351-0198 Japan

E-Mail: ryutaro.yoshimi@riken.jp

Topological insulators are a new class of semiconductors displaying charge-gapped insulating behavior in the bulk but hosting a spin-polarized massless Dirac electron state at the surface. Quantum transport in surface Dirac electron systems has been attracting much attention for the half-integer quantum Hall effect (QHE) and quantum anomalous Hall effect (QAHE) [1]. Fabricating layered structures of thin film is one of the useful techniques to efficiently control the surface states of a topological insulator. We have fabricated topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ (BST) thin films by molecular beam epitaxy (MBE), in which the carrier density can be widely controlled by Bi/Sb ratio. Precise tuning of the Fermi level by field-effect transistor (FET) enables us to observe the QHE [2] and QAHE [3] in BST and Cr-doped compound Cr_x(Bi_{1-y}Sb_y)_{2-x}Te₃ (CBST). designed heterostructures Furthermore, we have sandwich of (Zn,Cr)Te/(Bi,Sb)₂Te₃/(Zn,Cr)Te in which a sizable exchange gap at the TI surface state is induced by the proximity coupling. The proximity coupling realized in the all-telluride based heterostructure will enable a realistic design of versatile tailor-made topological materials coupled with ferromagnetism, ferroelectricity, superconductivity, and so on.

- [1] C.-Z. Chang et al., Science 340, 167 (2013)
- [2] R. Yoshimi et al., Nature Communications 6, 6627 (2015)
- [3] J. G. Checkelsky, R. Yoshimi et al., Nature Physics 10, 731 (2014)
- [4] M. Mogi, R. Yoshimi et al., Appl. Phys. Lett. 107, 182401 (2015)
- [5] R. Watanabe, R. Yoshimi et al., Appl. Phys. Lett. 115, 102403 (2019)

TOPOLOGICAL PROTECTION OF WEYL FERMIONS VISUALIZED ON THE ATOMIC SCALE

Haim Beidenkopf¹, Nurit Avraham¹, Noam Morali¹, Rajib Batabyal¹, Abhay Kumar Nayak¹, Pranab Kumar Nag¹, Binghai Yan¹, Yan Sun², Claudia Felser²

¹Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot

7610001, Israel.

²Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany.

E-Mail: haim.beidenkopf@weizmann.ac.il

Topological electronic materials host exotic boundary modes, that cannot be realized as standalone states, but only at the boundaries of a topologically classified bulk. Topological Weyl semimetals, whose bulk electrons exhibit chiral Weyl-like dispersion, host Fermi-arc states on their surfaces. The Fermi-arc surface bands disperse along open momentum contours terminating at the surface projections of bulk Weyl nodes with opposite chirality. Such reduction of the surface degrees of freedom by their segregation to opposite surfaces of the sample, that reoccurs in all topological states of matter and even exhibited by topological defects [1], provides topological protection from their surface elimination. We have confirmed the Weyl topological classification of both the inversion symmetry broken compound TaAs [2] and the time reversal symmetry broken Co₃Sn₂S₂ [3] by spectroscopic visualization of their Fermi-arc surface states through the interference patterns those electrons embed in the local density of states. This has allowed us to examine their unique nature and level of protection against perturbations. In TaAs the Fermi arc bands are found to be much less affected by the surface potential compared to trivial bands that also exist on its surfaces. In contrast, in Co₃Sn₂S₂ the dispersion of the topological Fermi-arc bands, and even their inter-Weyl node connectivity, are found to vary with the surface termination. A possible resolution of this discrepancy will be discussed.

[1] Abhay Kumar Nayak *et al.*, "Resolving the Topological Classification of Bismuth with Topological Defects" Science Advances **5**, eaax6996 (2019)

[2] Rajib Batabyal *et al.*, "Visualizing weakly bound surface Fermi arcs and their correspondence to bulk Weyl fermions" Science Advances **2**, e1600709 (2016)

[3] Noam Morali *et al.*, "Fermi-arc diversity on surface terminations of the magnetic Weyl semimetal Co₃Sn₂S₂", Science **365**, 1286 (2019)

BEYOND TOPOLOGICAL QUANTUM CHEMISTRY

Maia G. Vergniory¹

¹Donostia International Physics Center, Donostia-San Sebastian, Spain Ikerbasque,

Basque Foundation for Science, Bilbao, Spain

E-Mail: maiagvergniory@dipc.org

Topological quantum chemistry (TQC) framework has provided a complete description of the universal properties of all possible atomic band insulators in all space groups considering the crystalline unitary symmetries. It links the chemical and symmetry structure of a given material with its topological properties. While this formalism filled the gap between the mathematical classification and the practical diagnosis of topological materials, an obvious limitation is that it only applies to weakly interacting systems. It is an open question to which extent this formalism can be generalized to strongly correlated system that can exhibit symmetry protected topological Mott insulators. In this talk I will first introduce TQC and its application and then I will address this question by combining cluster perturbation theory and topological Hamiltonians within TQC. This simple formalism will be applied to calculate to the phase diagram of the Hubbard model for a diamond chain. The results are compared to numerically exact calculations from density matrix renormalization group and variational Monte Carlo simulations together with many-body topological invariants.

M.G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B.A. Bernevig, Z. Wang, "A complete catalogue of High-Quality Topological Materials ", Nature 566, 480-485 (2019)
B. Bradlyn, L. Elcoro, J. Cano, M.G. Vergniory, Z. Wang, C. Felser, M.I. Aroyo, B.A. Bernevig, "Topological quantum chemistry", Nature 547, 298-305 (2017).
M. Iraola *et al.*, in preparation