Topological Quantum Materials:
Designed Chern Insulators, Natural Nodal Loop Semimetals

Warren E. Pickett

University of California Davis

Collaborators on Chern: Hongli Guo, Shruba Gangopadhyay, Okan Köksal, Rossitza Pentcheva
Collaborators on NLS: Yundi Quan, T. Siegrist, A. P. Ramirez, D. S. Dessau, M. Subramanian

Topological quantum materials have provided an extremely active area of research over the past decade. Although topological insulators that may provide useful boundary currents and associated properties are still very few, they are relatively well understood. Two other topological classes provide the strongest current interest, Chern insulators for which proposed materials have had bandgaps of only 1-3 tens of meV, and nodal loop semimetals whose full understanding still requires study.

Chern insulators are exciting both as a novel electronic phase and for their potentially useful boundary transport properties. Honeycomb lattices occupied by heavy transition metal ions have been proposed by Okamoto and coworkers as Chern insulators, but finding a concrete example has been challenging due to an assortment of broken symmetry phases that thwart the topological entanglement. Building on accumulated knowledge of the behavior of the 3d series, we "tune" spin-orbit and interaction strength together with strain to design two Chern insulator systems (one with Ru, one with Os) with bandgaps up to 130 meV and Chern numbers $C = -1$ and $C = 2$ respectively.[1] We find, in this class, that a trade-off between larger spin-orbit coupling and strong interactions leads to a larger gap, whereas the stronger SOC correlates with the larger magnitude of the Hall conductivity. Symmetry lowering in the course of structural relaxation becomes an important feature that will be discussed. This design of Chern insulators follows the Materials Genome Initiative model, but with the emphasis on human-computer synergy rather than high-throughput computation.

The X As_3 class of semimetals, unexplored since their discovery in the 1980s by Bauhofer and von Schnering, have been found [2] to be nodal loop semimetals (NLSs) for X =Ca, Sr, Ba, and Eu. Unlike previously studied NLSs where loops appear in pairs, these display a single loop of accidental degeneracies crossing the Fermi energy with a gap elsewhere in the zone: the nodal loop region dominates the transport. Density functional calculations reveal that monoclinic $CaAs_3$, the sole insulating member of this class, would be a NLS in the absence of spin-orbit coupling (SOC). The position and characters of the nodal Fermi surfaces and associated boundary states will be discussed. The stark low symmetry of monoclinic $CaAs_3$ (with only inversion symmetry) makes it the "hydrogen atom" of NLSs; unlike all other classes, space group symmetry does not provide any "protection" of its loop of accidental degeneracies.

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1. Hongli Guo, Shruba Gangopadhyay, Okan Köksal, Rossitza Pentcheva, and Warren E. Pickett, Wide gap Chern Mott insulating phases achieved by design, npj Quantum Mate- rials (2017, in press).

2. Yundi Quan, Zhiping P. Yin, and Warren E. Pickett, A single nodal loop of accidental degeneracies in minimal symmetry: triclinic $CaAs_3$, (2017, submitted).