MAR14-2013-020432

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Associating Specific Materials with Topological Insulation Behavior[1]

XIUWEN ZHANG, University of Colorado, Boulder, CO 80309 and Colorado School of Mines, Golden, CO 80401

The first-principles (a) total-energy/stability calculations combined with (b) electronic structure calculations of band inversion, spin-polarization and topological invariants (Z2) has led to the design and prediction of specific materials that are topological insulators in this study. We classify bulk materials into four types of band-inversion behaviors (TI-1, TI-2, BI-3, BI-4), based on the number of band inversions and their distributions on various time reversal invariant k points. Depending on the inversion type in bulk, the corresponding surface states have different protections e.g., protected by time reversal symmetry (in TI-1 materials), spatial symmetry (in TI-2), or not protected (in BI-3, BI-4). Subject 1 Discovery of new TI by screening materials for a Z2 metric: Such high-throughput search in the framework of Inverse Design methodology predicts a few previously undocumented materials that are TI-1 in their ground state crystal structure. We also predict dozens of materials that are TI-1 however in structures that are not ground states (e.g. perovskite structure of II-Bi-O3). Subject 2 Design Principle to increase the gap of TI-1 materials: In HgTe-like cubic topological materials, the insulating gap is zero since the spin-orbit splitting is positive and so a 4-fold half-filled p-like band is near the Fermi level. By design of hybridization of d-orbitals into the p-like bands, one can create negative spin-orbit splitting and so a finite insulating gap. Subject 3 Unconventional spin textures of TI surface states: Despite the fact that one of our predicted TI-1 KBaBi has inversion symmetry in the bulk–a fact that that would preclude bulk spin polarization–we find a Dresselhaus-like spin texture with non-helical spin texture. This originates from the local spin polarization, anchored on the atomic sites with inversion asymmetric point groups, that is compensated due to global inversion symmetry in bulk.

[1]In collaboration with: Jun-Wei Luo, Qihang Liu, Julien Vidal, and Alex Zunger, and supported in part by National Science Foundation DMREF. X.Z. acknowledges the administrative support of REMRSEC at Colorado School of Mines, Golden, Colorado.