MAR11-2010-000668

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Tunable multifunctional topological insulators in ternary Heusler and related compounds

CLAUDIA FELSER, University of Mainz

Recently the quantum spin Hall effect was theoretically predicted and experimentally realized in quantum wells based on the binary semiconductor HgTe. The quantum spin Hall state and topological insulators are new states of quantum matter interesting for both fundamental condensed-matter physics and material science. Many Heusler compounds with C1b structure are ternary semiconductors that are structurally and electronically related to the binary semiconductors. The diversity of Heusler materials opens wide possibilities for tuning the bandgap and setting the desired band inversion by choosing compounds with appropriate hybridization strength (by the lattice parameter) and magnitude of spin–orbit coupling (by the atomic charge). Based on first-principle calculations we demonstrate that around 50 Heusler compounds show band inversion similar to that of HgTe. The topological state in these zero-gap semiconductors can be created by applying strain or by designing an appropriate quantumwell structure, similar to the case of HgTe. Many of these ternary zero-gap semiconductors (LnAuPb, LnPdBi, LnPtSb and LnPtBi) contain the rare-earth element Ln, which can realize additional properties ranging from superconductivity (for example LaPtBi) to magnetism (for example GdPtBi) and heavy fermion behaviour (for example YbPtBi). These properties can open new research directions in realizing the quantized anomalous Hall effect and topological superconductors. Heusler compounds are similar to a stuffed diamond, correspondingly, it should be possible to find the "high Z" equivalent of graphene in a graphite-like structure with 18 valence electrons and with inverted bands. Indeed the ternary compounds, such as LiAuSe and KHgSb with a honeycomb structure of their Au-Se and Hg-Sb layers feature band inversion very similar to HgTe which is a strong precondition for existence of the topological surface states. These materials have a gap at the Fermi energy and are therefore candidates for 3D-topological insulators. Additionally they are centro-symmetric, therefore, it is possible to determine the parity of their wave functions, and hence, their topological character. Surprisingly, the compound KHgSb with the strong SOC is topologically trivial, whereas LiAuSe is found to be a topological non-trivial insulator.