First-Principles Design of Low-Dimensional Quantum Materials with Nontrivial Band Topology

Mina Yoon
University of Tennessee, USA

Abstract

We discover new class of electrides [1,2], the first electride with nontrivial band topology, based on 1D building blocks by coupling materials database searches and first-principles-calculations-based analysis. This new class of electrides, composed of 1D nanorod building blocks, has crystal structures that mimic β-TiCl3 with the position of anions and cations exchanged. Unlike the weakly coupled nanorods of β-TiCl3 , Cs3 O and Ba3 N retain 1D anionic electrons along the hollow interrod sites; additionally, strong inter-rod interaction in C3 O and Ba3 N induces band inversion in a 2D superatomic triangular lattice, resulting in nontrivial band topology of Dirac nodal lines [2]. This new material could be served as an ideal template to explore various quantum phases. Using a tight-binding Hamiltonian based on two-dimensional (2D) honeycomb lattices, we construct a phase diagram in terms of exchange coupling and spin-orbit coupling (SOC), which spans four different phases, such as topological insulator, large/small gap quantum anomalous Hall (QAH) insulator, and ferromagnetic semiconductor [3]. We reveal that 2D honeycomb lattices consisting of some post-transition metals, such as Sn, Pb, and Bi, undertake ferromagnetic transition as the lattice constant increases and significant changes in SOC strength, which makes them an ideal material to explore the versatile phases solely by changing lattice constants. First-principles density functional calculations demonstrate that 2D honeycomb SnF can show QAH effect with SOC gap of ~0.25eV and Curie temperature (Tc) of ~780K [3]. Our calculations propose a new avenue to the room-temperature QAH effect in realistic 2D materials systems.

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