Mina Yoon, J Material Sci Eng 2018, Volume 7
DOI: 10.4172/2169-0022-C8-113

First-principles design of low-dimensional quantum materials with nontrivial band topology

Mina Yoon
University of Tennessee, USA

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-$TiCl_3$ with the position of anions and cations exchanged. Unlike the weakly coupled nanorods of β-$TiCl_3$, Cs_3O and Ba_3N retain 1D anionic electrons along the hollow inter-rod sites; additionally, strong inter-rod interaction in C_3O and Ba_3N 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 (T_c) of ~780K [3]. Our calculations propose a new avenue to the room-temperature QAH effect in realistic 2D materials systems.

Recent Publications

1. First-Principles Prediction of Themodynamically Stable Two-Dimensional Electrides, W. Ming, M. Yoon, M.-H. Du, F. Liu, K. Lee, and S. W. Kim, J. Am. Chem. Soc. 138, 15336 (2016).
2. First-Principles Prediction of New Electrides with Nontrivial Band Topology Based on One-Dimensional Building Blocks, Changwon Park, Sung Wng Kim, Mina Yoon, Phys. Rev. Lett. 120, 26401 (2018).
3. Quantum Phase Engineering of Two-Dimensional Post-Transition Metals: Toward a High-Temperature Quantum Anomalous Hall Insulators, L. Zhang, C. Park, and M. Yoon (2018, to be published)

Biography

Mina Yoon received her PhD degree in Theoretical Condensed Matter Physics in 2004, from Michigan State University. She is a Research Scientist at ORNL and a Joint Professor of Physics at University of Tennessee, Knoxville. The primary focus of her research lies in the fundamental understanding of growth mechanisms, novel properties, functionalization, and potential technological applications of surface-based and low-dimensional materials. Especially, her interest is in utilizing these materials as light, environmentally friendly, and efficient energy storage/generation and optoelectronic application by making use of their unique low-dimensional properties. Her theoretical approach ranges from atomistic modeling by first-principles quantum mechanical approaches and many-body potential approaches, to continuum elasticity theory and phenomenological modeling.

myoon@ornl.gov