MAR16-2015-000364

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Designing topological states by pressure, strain, and functionalization

UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Thuwal 23955, Saudi Arabia

Various examples of the design of topological states by means of first-principles calculations are discussed. The presentation focusses on the design parameters (1) pressure, (2) strain, and (3) functionalization. $TiTe_2$ is found to be unusually accessible to strain effects and the first compound that under hydrostatic pressure (up to experimentally reasonable 30 GPa) is subject to a series of four topological phase transitions, which are related to band inversions at different points of the Brillouin zone. Therefore, $TiTe_2$ enables experimental access to all these transitions in a single compound. Phase transitions in $TlBiS_2$ and $TlSbS_2$ are identified by parity analysis and by calculating the surface states. Zero, one, and four Dirac cones are found for the (111) surfaces of both $TlBiS_2$ and $TlSbS_2$ when the pressure grows, which confirms trivial-nontrivial-trivial phase transitions. The Dirac cones at the $\overline{\mathrm{M}}$ points are anisotropic with large out-of-plane component. $TlBiS_2$ shows normal, topological, and topological crystalline insulator phases under hydrostatic pressure, thus being the first compound to exhibit a phase transition from a topological to a topological crystalline insulator. While monolayer arsenic and arsenic antimonide are semiconductors (direct band gap at the Γ point), fluorination results for both compounds in Dirac cones at the K points. Fluorinated monolayer arsenic shows a band gap of 0.16 eV due to spin-orbit coupling and fluorinated arsenic antimonide a larger band gap of 0.37 eV due to inversion symmetry breaking. Spin-orbit coupling induces spin splitting similar to monolayer MoS_2. Phonon calculations confirm that both materials are dynamically stable. Calculations of the edge states of nanoribbons by the tight-binding method demonstrate that fluorinated arsenic is topologically nontrivial in contrast to fluorinated arsenic antimonide.