Search for new topological insulators: ternary Li$_2$AgSb-class semiconductors and related compounds

HSIN LIN, Northeastern U., TANMOY DAS, LANL and Northeastern U., Y.J. WANG, Northeastern U., L.A. WRAY, LBNL and Princeton U., S.-Y. XU, M.Z. HASAN, Princeton U., ARUN BANSIL, Northeastern U. — Topological insulators host a rare quantum phase of electrons which is characterized by a topological invariant number of bulk states of combined spin-orbit and time-reversal symmetry origin. Despite recent progress the available classes of topological insulators are still quite limited for use in device applications and experimental exploration of exotic topological phenomena. For this reason, the search for new materials with greater structural flexibility and tunability in various local order broken symmetry phases is continuing worldwide with great intensity. Here we discuss our effort based on first-principles calculations to show that the adiabatic continuation method can provide a very powerful tool for predicting non-trivial topological phases with the example of ternary intermetallic series, Li$_2$M$'$X ($M'$=Cu, Ag, Au, and Cd, $X$=Sb, Bi, and Sn) as well as other compounds with zinc-blende type sublattice.

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