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Topological insulator and Dirac semimetal in tetragonally strained alkaline earth - pnictide antiperovskites WEN FONG GOH, WARREN PICKETT, University of California, Davis — Compounds with antiperovskite structure have been suggested to be potential topological insulators, due to their small band gap or gapless electronic characteristics. Using first principles calculations, we survey the entire class of $3 \times 5 \times 5$ cubic alkaline earth-pnictide antiperovskites, viz. $\mathrm{Ae_3Pn_APn_B}$, where $\mathrm{Ae = Ca, Sr, Ba}$ and $\mathrm{Pn_A, Pn_B = N, P, As, Sb, Bi}$, and classified these compounds into either trivial insulators or topological semimetals. For the trivial insulators, strain can invert the band ordering to produce topological insulators, while for the topological semimetals, where the band ordering has been inverted by spin-orbit coupling but leaving a gapless bulk state, strain can open up a gap while maintaining the inverted band ordering. Among the antiperovskites that show topological semimetals, $\mathrm{Ca_3BiP}$, a narrow gap semiconductor, is used as an example to illustrate the role played by the spin-orbit coupling and strain in the topological insulator to Dirac semimetal phase transition. Results show that it can be driven into a topological insulating phase under uniaxial compression, or a Dirac semimetallic state under uniaxial expansion. The band inversion diagram, topological surface states and Fermi arc will be presented.

Wen Fong Goh
University of California, Davis

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