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 Z_2 topological insulator in 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 antiperovskite compounds, viz. $Ae_3Pn_APn_B$, where Ae = Ca, Sr, Baand $Pn_A, Pn_B = N, P, As, Sb, Bi$, and have classified these compounds into trivial insulator or topological semimetal. 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 leaves a gapless bulk state, strain can open up a gap while maintaining the inverted band ordering. Among the topological semimetals, the narrow gap semiconductor Ca₃BiP, 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, and a Dirac semimetallic state under uniaxial expansion. The topological surface states and Fermi arc will be presented and discussed.

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