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Design and investigation of potential Sn-Te-P and Zr-Te-P class of Dirac materials PRASHANT SARSWAT, SAYAN SARKAR, MICHAEL FREE, University of Utah — A motivation of new Dirac materials design and synthesis by perturbing the symmetry, was explored by substitution of a Sn vacancy by P that maintains the intrinsic band inversion at the L point but also the direct bandgap shrinkage upon the incorporation of spin-orbit coupling. In a similar line of investigation, Zr-Te-P was also systematically studied. The synthesis of both Sn-Te-P and Zr-Te-P system of compounds resulted in the formation of long needles type crystals and the bulk porous deposits. The exotic morphology of the P-doped SnTe needles possesses the pierced surface throughout its extension. First principle based calculations were also carried out for these sets of compounds using General Gradient Approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional. In order to ensure structural optimization, a limited memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) algorithm was employed and the total energy in PBE exchange-correlation functional was considered for the calculation of the formation energy per atom. The new modifications have a potential to establish the new class of Dirac materials ushering upon new frontiers of interest.

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