Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic structure and electronic properties of two-dimensional InBi WEI LI, Univ of Delaware, ANDERSON JANOTTI COLLABORATION — We use first-principles calculations to investigate the structure and electronic properties of InBi. We find that InBi can be considered as 2D layered material in its ground state, and that van de Waals interaction is essential to correctly describe the separation between layers. Using hybrid functional calculations, including spin-orbit effects, we study the electronic structure of bulk and individual layer of InBi. Although InBi is a semimetal in bulk, we find that one-layer InBi has a small gap of 0.05 eV. The band inversion between the In-s and Bi-p bands indicates that the single-layer InBi is a topological insulator material. We also discuss the effects of biaxial and uniaxial strain on the band gap of single-layer InBi, and investigate the evolution of the electronic band structure of free standing InBi as a function of number of layers.

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Date submitted: 13 Nov 2016 Electronic form version 1.4