Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Topological crystalline insulators from crystal field effect in monolayer IV-VI semiconductors JUNWEI LIU, XIAOFENG QIAN, LIANG FU, MIT — Two-dimensional (2D) topological crystalline insulators (TCIs) were recently predicted in thin films of the SnTe class of IV-VI semiconductors, which can host metallic edge states protected by mirror symmetry. As thickness decreases, quantum confinement effect will increase and surpass the inverted gap at a critical thickness, turning 2D TCIs into normal insulators. Surprisingly, based on first-principles calculations, here we demonstrate that (001) monolayers of rocksalt IV-VI semiconductors XY (X=Ge, Sn, Pb and Y= S, Se, Te) are 2D TCIs with the fundamental band gap as large as 260 meV in monolayer PbTe. This unexpected nontrivial topological phase stems from the strong crystal field effect in the monolayer, which lifts the degeneracy between $p_{x,y}$ and p_z orbitals and leads to band inversion between cation and anion p_z orbitals. Our work offers a new strategy to find atomically thin 2D topological materials.

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Date submitted: 10 Nov 2014 Electronic form version 1.4