

Abstract Submitted
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Three-Dimensional Topological Insulators in I-III-VI₂ and II-IV-V₂ Chalcopyrite Semiconductors¹ DI XIAO, Oak Ridge National Lab, WANXIANG FENG, JUN DING, YUGUI YAO, Institute of Physics, Chinese Academy of Sciences — Using first-principles calculations, we investigate the band topology of the ternary chalcopyrite family. Our method is based on the adiabatic continuity of the Hamiltonian combined with direct calculation of the Z₂ topological invariants in inversion-symmetry breaking systems. We show that a large number of these compounds are candidates for three-dimensional topological insulators. Moreover, The topological order can be tuned and controlled by lattice strain. The excellent physical properties of these compounds make them an appealing platform for novel quantum phenomena.

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