Dirac point and topologically nontrivial phase MINSUNG KIM, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — It has been known that the topological phases of matters can be realized in both insulating and metallic band structures. Topological insulators have nontrivial band inversion between the valence and conduction bands, and topological Dirac semimetals have band crossings along high-symmetry paths in a Brillouin zone. In this work, we investigate a topological band structure where the valence band has nontrivial band topology and accidental band crossings occur giving rise to Dirac points that are protected by relevant point group symmetry. We discuss possible material realization of such topological phase using first-principles calculations based on density functional theory. We also examine the topological phase transitions between the bands constituting the Dirac points.

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