Stacking-Dependent Topological Phase Transitions in Layered Hydrogenated III-V Compounds

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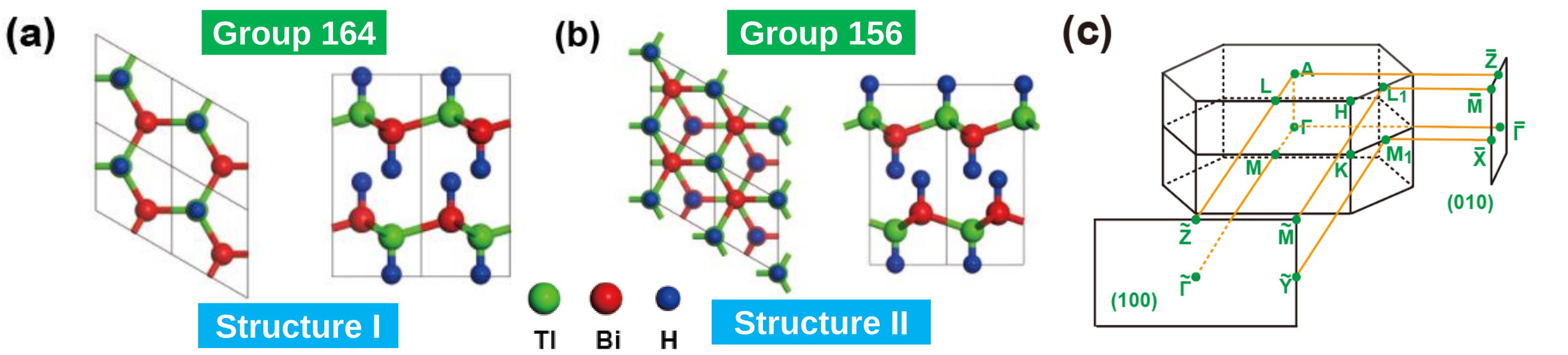
Abstract

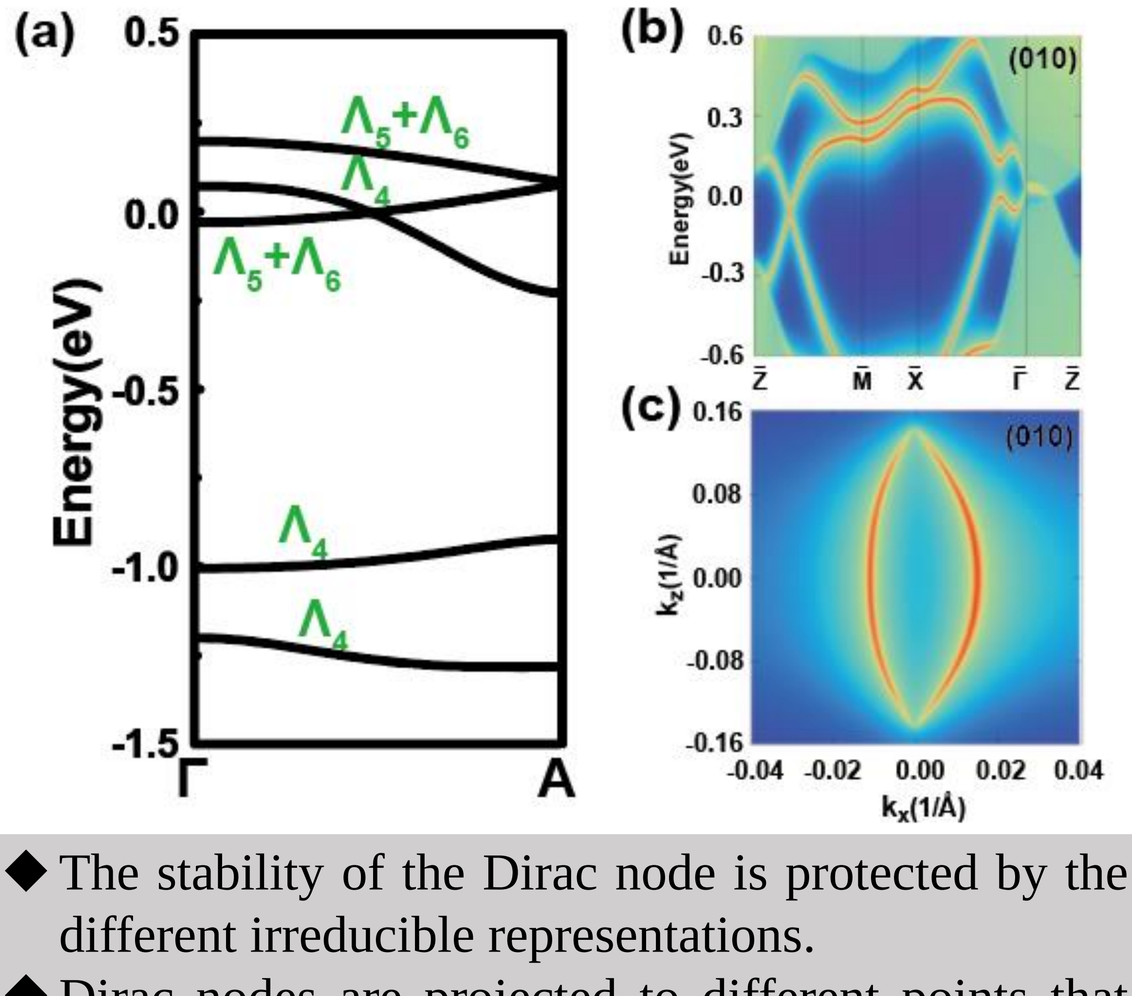
Quantum spin Hall (QSH) insulators and topological semimetals (TSMs) are two classes of topological phases, both having an inverted order in their band structures in the Brillouin zone (BZ). The existence of a given compound as QSH insulator or TSM is a rather consequential distinction because these two topological phases have very different physical properties. Here, we theoretically predict the topological properties of hydrogenated III-V compound, namely $TlBiH_2$, that exhibits dual topological characteristics, QSH insulator in two-dimensional (2D) monolayer and topological Dirac semimetal or topological triply degenerate semimetal in three-dimensional (3D) crystals upon van der Waals (vdW) stacking. The nontrivial surface states with Fermi arcs on the (010) or (100) surfaces are shown to connect the projection of bulk band crossings. Our findings provide an ideal material platform for realizing TSMs and exploring fundamental topological phase transition.

Structures & Models



Results

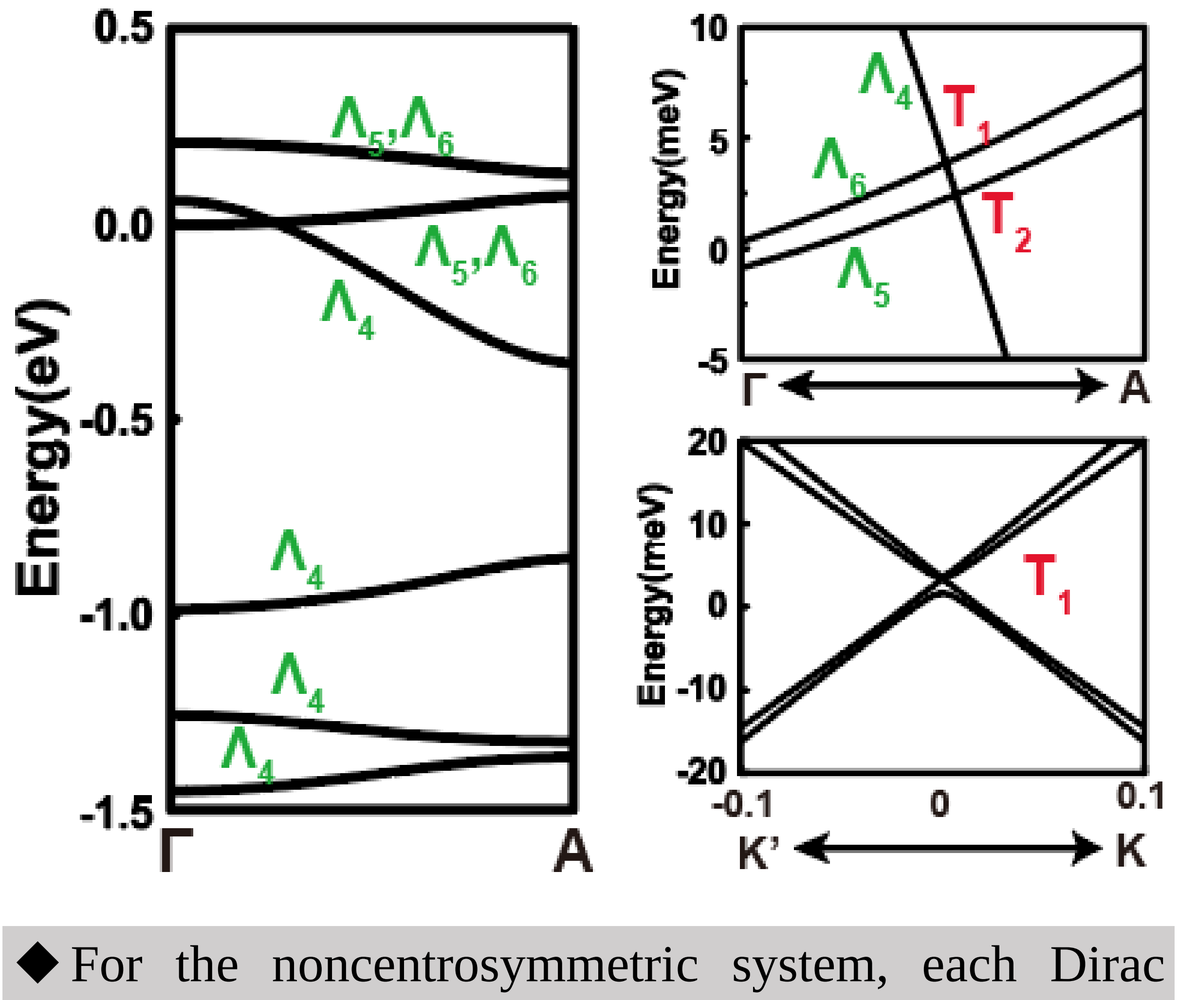
Structure I



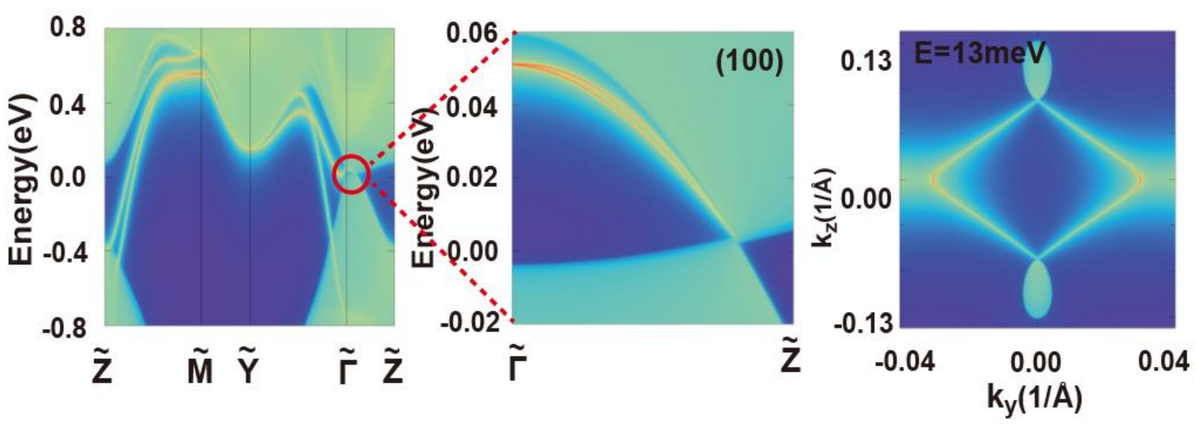
◆ The stability of the Dirac node is protected by the different irreducible representations.

◆ Dirac nodes are projected to different points that are separated from the projected bulk states and connected by Fermi arcs.

Structure II



◆ For the noncentrosymmetric system, each Dirac point can split into two adjacent triply degenerate points along the high-symmetry line ΓA .



◆ Two branches of Fermi arcs coexist at the energy level E = 13 meV.

References

1. Liu J, Wang H, Fang C, et al. Nano Lett. 2016, 17(1): 467-475.
2. Wang J, Sui X, Shi W, et al. Phys. Rev. Lett. 2017, 119(25): 256402.
3. Wang Z, Sun Y, Chen X Q, et al. Phys. Rev. B, 2012, 85(19): 195320.
4. Gibson Q D, Schoop L M, Muechler L, et al. Phys. Rev. B, 2015, 91(20): 205128.