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Weyl semimetal emerging from $LaBiTe_3$-class topological insulators JIANPENG LIU, DAVID VANDERBILT, Rutgers University — We study the topological-to-normal transition in $LaBiTe_3$ and $LuBiTe_3$ by tuning the strength of the spin-orbit coupling (SOC). For centrosymmetric 3D topological insulators (TIs), the strong Z_2 index can be changed only by an accidental band touching at an odd number of time-reversal invariant momenta in the Brillouin zone (BZ), achieved at some critical value of an external parameter λ. These band-touching points (BTPs) are "Dirac-like," carrying zero chiral charge. For general noncentrosymmetric TIs, however, one expects to see a stable Weyl semimetal phase over some finite interval of λ. As λ is varied, one expects first the appearance of $2(2n+1)$ Dirac-like BTPs in the BZ, which then split into pairs of Weyl points carrying opposite chiral charges. These BTPs then migrate in the BZ and finally annihilate after exchanging partners, leaving behind an inverted strong Z_2 index. Based on first-principles calculations, we predict that this phenomenon can be realized as the SOC is tuned in $LaBiTe_3$ and $LuBiTe_3$. We also construct a low-energy effective model to describe the topological phases in these materials. Preliminary results suggest that other interesting phases could be observed when a Zeeman field is applied.

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