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Prediction of weak and strong topological insulators in layered semiconductors.

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We investigate a new class of ternary materials such as LiAuSe and KHgSb with a honeycomb structure in Au-Se and Hg-Sb layers. We demonstrate the band inversion in these materials similar to HgTe, which is a strong precondition for existence of the topological surface states. In contrast with graphene, these materials exhibit strong spin-orbit coupling and a small direct band gap at the point. Since these materials are centrosymmetric, it is straightforward to determine the parity of their wave functions, and hence their topological character. Surprisingly, the compound with strong spin-orbit coupling (KHgSb) is trivial, whereas LiAuSe is found to be a topological insulator. However KHgSb is a weak topological insulators in case of an odd number of layers in the primitive unit cell. Here, the single-layered KHgSb shows a large bulk energy gap of 0.24 eV. Its side surface hosts metallic surface states, forming two anisotropic Dirac cones. Although the stacking of even-layered structures leads to trivial insulators, the structures can host a quantum spin Hall layer with a large bulk gap, if an additional single layer exists as a stacking fault in the crystal. The reported honeycomb compounds can serve as prototypes to aid in the finding of new weak topological insulators in layered small-gap semiconductors.

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