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Tunable topological electronic structures in Sb(111) bilayers: A first-principles study FENG-CHUAN CHUANG, CHIA-HSIU HSU, CHIA-YU CHEN, ZHI-QUAN HUANG, Natl. Sun Yat-sen U., Taiwan, VIDVUDS OZOLINS, UCLA, HSIN LIN, ARUN BANSIL, Northeastern U. — Electronic structure and band topology of a single Sb(111) bilayer in the buckled honeycomb configuration are investigated using first-principles calculations with the inclusion of spin-orbit coupling. While a trivial band insulator is predicted for the free-standing thin film, a band inversion at the Brillouin zone center can be induced by tensile strain, resulting in a topological insulator with a nontrivial topological invariant $Z_2 = 1$. Our study points at the possibility of realizing the quantum spin Hall state for an Sb(111) single bilayer on a suitable substrate. Moreover, the presence of buckling provides an advantage in controlling the band gap through an out-of-plane external electric field, which breaks the inversion symmetry and lifts the spin degeneracy. A topological phase transition driven by gating is demonstrated, and six spin-polarized Dirac cones are found at the critical point. With a tunable gap and reversible spin polarization, Sb thin films are promising candidates for spintronic applications.

Feng-Chuan Chuang
Natl. Sun Yat-sen U., Taiwan

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