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Two-dimensional Topological Crystalline Insulator Phase in Sb/Bi Planar Honeycomb with Tunable Dirac Gap CHIA-HSIU HSU, ZHI-QUAN HUANG, CHRISTIAN CRISOSTOMO, LIANG-ZI YAO, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., YU-TZU LIU, BAOKAI WANG, CHUANG-HAN HSU, CHI-CHENG LEE, HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — We predict planar Sb/Bi honeycomb to harbor a two-dimensional (2D) topological crystalline insulator (TCI) phase based on first-principles computations. Although buckled Sb and Bi honeycombs support 2D topological insulator (TI) phases, their structure becomes planar under tensile strain. The planar Sb/Bi honeycomb structure restores the mirror symmetry, and is shown to exhibit non-zero mirror Chern numbers, indicating that the system can host topologically protected edge states. Our computations show that the electronic spectrum of a planar Sb/Bi nanoribbon with armchair or zigzag edges contains two Dirac cones within the band gap and an even number of edge bands crossing the Fermi level. Lattice constant of the planar Sb honeycomb is found to nearly match that of hexagonal-BN. The Sb nanoribbon on hexagonal-BN exhibits gapped edge states, which we show to be tunable by an out-of-the-plane electric field, providing controllable gating of edge state important for device applications.

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