Prediction of Large-Gap Two-Dimensional Topological Insulators Consisting of Bilayers of Group III Elements with Bi

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We use first-principles electronic structure calculations to predict a new class of two-dimensional (2D) topological insulators (TIs) in binary compositions of group III elements (B, Al, Ga, In, and Tl) and bismuth (Bi) in a buckled honeycomb structure. We identify band inversions in pristine GaBi, InBi, and TlBi bilayers, with gaps as large as 560 meV, making these materials suitable for room-temperature applications. Furthermore, we demonstrate the possibility of strain engineering in that the topological phase transition in BBi and AlBi could be driven at ~6.6% strain. The buckled structure allows the formation of two different topological edge states in the zigzag and armchair edges. More importantly, isolated Dirac-cone edge states are predicted for armchair edges with the Dirac point lying in the middle of the 2D bulk gap. A room-temperature bulk band gap and an isolated Dirac cone allow these states to reach the long-sought topological spin-transport regime. Our findings suggest that the buckled honeycomb structure is a versatile platform for hosting nontrivial topological states and spin-polarized Dirac fermions with the flexibility of chemical and mechanical tunability.

[1] Feng-Chuan Chuang, Liang-Zi Yao, Zhi-Quan Huang, Yu-Tzu Liu, Chia-Hsiu Hsu, Tanmoy Das, Hsin Lin, and Arun Bansil, Nano Lett. 14, 2505 (2014).