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Prediction of Large-Gap Two-Dimensional Topological Insulators Consisting of Hydrogenated Bilayers of Group III Elements with Bi CHRISTIAN P. CRISOSTOMO, LIANG-ZI YAO, ZHI-QUAN HUANG, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, MARVIN A. ALBAO, U. of the Philippines Los Banos, ARUN BANSIL, Northeastern U. — We use first-principles electronic structure calculations to predict a new class of two-dimensional (2D) topological insulators (TIs) in hydrogenated binary compositions of group III elements (B, Al, Ga, In, and Tl) and bismuth (Bi). We identify band inversions in unhydrogenated pristine GaBi, InBi, and TlBi bilayers, with gaps as large as 556 meV for the TlBi case, making these materials suitable for room-temperature applications. Double-sided hydrogenation in which hydrogen was added on opposite sides also exhibited band inversions in the case of GaBi, InBi, and TlBi just as in the unhydrogenated pristine ones. Furthermore, we report the gap to be 885 meV for the hydrogenated TlBi case. Hydrogenation enhace the band gap without changing the band topology. Moreover, our study also aim to demonstrate the possibility of strain engineering in that the topological phase transition in systems whose phase was nontrivial could be driven by suitable strain. Finally, the effect of placing hydrogen to topological edges was also demonstrated. 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. The robustness of III-Bi upon hydrogenation shows that these materials are possible to synthesize by growing on substrates.

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