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Chemically-induced Large-Gap Quantum Anomalous Hall Insulator States in III-Bi Honeycombs CHRISTIAN P. CRISOSTOMO, ZHI-QUAN HUANG, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Dept of Phys, Natl Sun Yat-Sen Univ, HSIN LIN, Graphene Research Ctr and Dept of Phys, Natl Univ of Singapore, ARUN BANSIL, Dept of Phys, Northeastern Univ — The search for new novel materials has increased due to their interesting properties and promising applications. Quantum anomalous Hall (QAH) effect was recently realized in magnetic topological insulators (TIs) but only observable at extremely low temperatures. In this letter, we predict large-gap QAH insulating phases in chemically functionalized III-Bi honeycombs using first-principles electronic structure calculations. QAH insulator phases were found in functionalized AlBi and TlBi, while GaBi and InBi were identified as semimetals with non-zero Chern number. Remarkably, TlBi exhibits robust and large-gap QAH insulator phases with band gap as large as 466 meV for one-sidedly functionalized and buckled honeycomb. Furthermore, the electronic band spectrum of functionalized TlBi nanoribbon with zigzag edge is shown to possess only one chiral edge band crossing the Fermi level within the band gap. With the recent progress of III-V materials, our results suggest that III-Bi honeycomb would provide a new platform for developing novel spintronics devices based on the QAH phase.

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