

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Prediction of Quantum Anomalous Hall Insulator in Functionalized GaBi Honeycomb CHRISTIAN CRISOSTOMO, SUNG-PING CHEN, ZHI-QUAN HUANG, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Using first-principles electronic calculations, we predict functionalized GaBi honeycomb under tensile strain to harbor quantum anomalous hall (QAH) insulating phase. A single band inversion at Γ point was found in spin-polarized band structure of half-fluorinated planar strained GaBi. In order to confirm the topological properties, we evaluated the Chern number (C) and found that $C = 1$, indicating the presence of QAH phase. Additionally, the same value was also obtained by using hydrogen atoms, instead of fluorine atoms, as the adsorbate in both planar and buckled GaBi. Moreover, the electronic spectrum of a half-fluorinated GaBi nanoribbon with arm-chair or zigzag edges possess only one edge band crossing the Fermi level within the band gap. Finally, a suitable substrate which could induce the similar effect of half-hydrogenation or half-fluorination on the GaBi honeycomb could be used for spintronic devices.

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Date submitted: 06 Nov 2015

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