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Nontrivial topological electronic structures in a single Bi(111) bilayer on different substrates FENG-CHUAN CHUANG, ZHI-QUAN HUANG, CHIA-HSIU HSU, YU-TZU LIU, HUA-RONG CHANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Electronic structures, minimum energy configurations, and band topology of strained Bi(111) single bilayers placed on a variety of semiconducting and insulating substrates are investigated using first-principles calculations [1]. A topological phase diagram of a free-standing Bi bilayer is presented to help guide the selection of suitable substrates. Numerous substrates were studied to determine whether they are able to support 2D TIs. The insulating hexagonal-BN is identified as the best candidate substrate material for supporting nontrivial topological insulating phase of Bi bilayer thin films. A planar hexagonal Bi layer is predicted under tensile strain, which we show could be realized on a SiC substrate. The Bi bilayer becomes metallic under the compressive strain induced by Si and Ge substrates. [1] Zhi-Quan Huang, Feng-Chuan Chuang, Chia-Hsiu Hsu, Yu-Tzu Liu, Hua-Rong Chang, Hsin Lin, and Arun Bansil, Phys. Rev. B 88, 165301 (2013).

Feng-Chuan Chuang
Natl. Sun Yat-sen U.

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