Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A comparative study of topological electronic structures of bilayers of group IV and V atoms ZHI-QUAN HUANG, YU-TZU LIU, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, HSIN LIN, Graphene Research Centre and Department of Physics, National University of Singapore, Singapore 117542, CHIA-YU CHEN, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, WAN-SHENG SU, National Center for High-Performance Computing, 28 Nan-Ke 3rd Road, Hsin-Shi, Tainan, ARUN BANSIL, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA — The topological electronic structures of free-standing bilayers of group-IV (C, Si, Ge, Sn, and, Pb) and V (As, Sb, and, Bi) atoms under isotropic strain have been studied using first-principles calculations. For group IV elements, heavier elements with larger spin–orbit coupling possess larger gaps at K, but a lower conduction band at Γ, making the system metallic. Only a few group-IV bilayers remain insulating due to small gaps at Γ. In contrast, for group V elements, spin-orbit coupling changes the ordering of bands at Γ. While As and Sb bilayers are found to be topologically trivial without isotropic strain, strength of spin-orbit coupling in Bi bilayer is large enough to induce band inversions, making the system a topological insulator. Sb bilayer also goes into a topological insulating phase if the spin-orbit coupling is artificially enhanced.

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Date submitted: 15 Nov 2013 Electronic form version 1.4