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**Predicted Growth of Two-Dimensional Topological Insulators Consisting of Hydrogenated III-V Thin films on Si(111) Substrate** FENG-CHUAN CHUANG, CHRISTIAN CRISOSTOMO, LIANG-ZI YAO, CHUN-CHEN YEH, SHU-MING LAI, ZHI-QUAN HUANG, CHIA-HSIU HSU, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, MARVIN ALBAO, U. of the Philippines Los Baos College, ARUN BANSIL, Northeastern U. — We have carried out systematic first-principles electronic structure calculations of growth of ultrathin films of compounds of group III (B, Al, In, Ga and Tl) with group V (N, P, As, Sb and Bi) elements on Si(111) substrate, including effects of hydrogenation. A total of six compounds (GaBi, InBi, TlBi, TlAs, TlSb and TlN) are identified to be nontrivial in unhydrogenated case; whereas for hydrogenated case, only four (GaBi, InBi, TlBi and TlSb) remains nontrivial. The band gap is found to be as large as 855 meV for the hydrogenated TlBi film, making this class of III-V materials suitable for room temperature applications. TlBi remains topologically nontrivial with a large band gap at various hydrogen coverages, indicating the robustness of its band topology against bonding effects of substrates. Two bilayers (BLs) of AlBi, InBi, GaBi, TlAs and TlSb are found to support a topological phase over a wide range of strains, in addition to BBi, TlN and TlBi which can be driven into the nontrivial phase via strain. One and two BL films of GaBi and 2 BL films of InBi and TlAs on Si(111) surface possess nontrivial phases with a band gap as large as 121 meV in the case of 2 BL film of GaBi. Persistence of the nontrivial phase upon hydrogenations in the III-V thin films suggests that these films are suitable for growing on various substrates.

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