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Hydrogenated ultra-thin tin films predicted as two-dimensional topological insulators ZHI-QUAN HUANG, BO-HUNG CHOU, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., YU-TZU LIU, HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Using thickness-dependent first-principles electronic structure calculations, we predict that hydrogenated ultra-thin films of tin harbor a new class of two-dimensional (2D) topological insulators (TIs). A single bilayer (BL) tin film assumes a 2D-TI phase, but it transforms into a trivial insulator after hydrogenation. In contrast, tin films with 2 and 3 BLs are found to be trivial insulators, but hydrogenation of 2 to 4 BL films results in a non-trivial TI phase. For 1 to 3 BLs, H-passivation converts the films from being metallic to insulating. Moreover, we examined iodine-terminated tin films up to 3 BLs, and found these to be non-trivial, with the films becoming semi-metallic beyond 1 BL. In particular, the large band gap of 340 meV in an iodine-terminated tin bilayer is not sustained in the iodine-terminated 2BL and 3BL tin films.

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