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Prediction of two-dimensional topological insulator by forming surface alloy on Au/Si(111) substrate ZHI-QUAN HUANG, FENG-CHUAN CHUANG, CHIA-HSIU HSU, HSIN-LEI CHOU, CHRISTIAN CRISOSTOMO, SHIH-YU WU, CHIEN-CHENG KUO, Natl. Sun Yat-sen U., WANG-CHI YEH, Natl. Dong Hwa U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Two-dimensional (2D) topological insulators (TIs), which can be integrated into the modern silicon industry, are highly desirable for spintronics applications. Here, using first-principles electronic structure calculations, we show that the Au/Si(111)-root3 substrate can provide a new platform for hosting 2D-TIs obtained through the formation of surface alloys with a honeycomb pattern of adsorbed atoms. We systematically examined elements from groups III to VI of the periodic table at 2/3 monolayer coverage on Au/Si(111)-root3, and found that In, Tl, Ge, and Sn adsorbates result in topologically non-trivial phases with band gaps varying from zero to 72 meV. Our scanning tunneling microscopy and low-energy electron diffraction experiments confirm the presence of the honeycomb pattern when Bi atoms are deposited on Au/Si(111)-root3 in accord with our theoretical predictions. Our findings pave the way for using surface alloys as a potential new route for obtaining viable 2D-TI platforms.

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