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Tunable topological electronic structure of silicene on semiconducting Bi/Si(111)-root3xroot3 substrate: a first-principles CHIA-HSIU HSU, ZHI-QUAN HUANG, BO-HUNG CHOU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Using first-principles calculations to obtain the crystal and electronic structures, we show that the 1x1 phase of silicene is energetically more favorable than the root3xroot3 silicene superstructure on a semiconducting Bi/Si(111)- root3xroot3 substrate. The band gap of the system is found to be influenced strongly through the participation of Bi-orbitals, which possess a larger spin-orbit coupling strength compared to Si. In particular, the non-trivial (topological) band gap of a few meV in freestanding 1x1 silicene enlarges to 150 meV and becomes trivial in the presence of the substrate. We further show how an out-of-the-plane external electric field can be used to tune the band gap and restore the non-trivial topological phase.

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