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Quantum spin Hall phases in tin-based films on a SiC substrate: An *ab initio* study.[1] MARCELO MARQUES, FILIPE MATUSALEM, Instituto Technologico de Aeronautica (ITA), Sao Jose dos Campos-SP, Brazil, FRIEDHELM BECHSTEDT, Institut fur Festkorpertheorie und -optik, Friedrich-Schiller-Universitat, Jena, Germany, LARA KUHL TELES, Instituto Technologico de Aeronautica (ITA), Sao Jose dos Campos-SP, Brazil — The deposition of stanene overlayers on 4H-SiC(0001) substrates is studied by means of density functional theory, including van der Waals interaction, and approximate quasiparticle electronic structure calculations. The influence of the Sn overlayer geometry, the surface passivation by H and F as well as the chemical functionalization of the Sn layer by fluorine and hydrogen are investigated in detail. We computed the Z_2 invariant for the systems in which are Dirac cones preserved after deposition on SiC surfaces. The studied systems give rise to local minima on the total energy faces. The reactivity of the clean SiC surfaces widely destroys the band structures of freestanding stanene-like sheets, but Dirac cones and topological character survive for passivated substrate systems. Stanene-derived linear bands survive at the K point (or at the Γ point for fluorostanene) and near the Fermi level for 2×2 stanene and fluorostanene sheets on SiC 3×3(0001) substrates passivated with H or F. The topological character of stanene and fluorostanene, as quantum spin Hall phase, is preserved, when the SiC substrate is passivated, as indicated by $Z_2 = 1$.

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