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Investigating the Electronic and Structural Properties of Stanene

BRENDAN FERRIS, ANTONIO CANCIO, Ball State Univ — We investigate the structural and electronic properties of two-dimensional tin, or stanene, under compressive and tensile biaxial strain using density functional theory (DFT). Stanene possesses a buckled honeycomb-like structure and is a potential candidate for a quantum spin hall (QSH) insulator in which a quantum hall effect is generated in the absence of a magnetic field due to strong spin-orbit coupling (SOC). This effect, in combination with a strain-tunable band gap, makes stanene an interesting material for spintronic applications. Stanene is stable in both a high-buckled configuration which is metallic and a low-buckled configuration which gives rise to a QSH effect, and a transition between the two can be induced through strain. For a monolayer of tin, the high-buckled phase is more stable; we investigate whether multiple layers of tin or a combination of tin and germanium can ensure the low-buckled phase remains the most stable configuration. We use ABINIT, a plane-wave pseudopotential DFT code that accurately reproduces all-electron calculations of ground-state energies and densities, and which is used to determine the ground state atomic structure and electronic band structure.

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