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Investigating the Electronic and Structural Properties of Stanene
BRENDAN FERRIS, ANTONIO CANCIO, Ball State University — We investigate the structural and electronic properties of two-dimensional tin, or stanene, under compressive and tensile strain using density functional theory (DFT). We investigate optimized lattice parameters for several variant structures found in the literature, and the effects of strain on the band structure. Stanene is among a class of atomically thin materials, similar to that of graphene, with a buckled honeycomb-like structure. They are 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). A combination of a QSH effect and strain tuneable band gap make stanene an interesting material for spintronic applications. We use ABINIT, a plane-wave pseudo-potential DFT code that accurately reproduces all-electron calculations of ground-state energies and densities, and which can be used to determine the ground state atomic structure. This then enables simple excited state properties like band structure and band gap estimations to be calculated. Strain is applied by fixing atoms in close-to-equilibrium positions.

Antonio Cancio
Ball State University

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