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Structural and electronic properties of a single layered α-tetragonal B_{50} sheet. CHERNO KAH, MING YU, CHAKRAM S JAYANTHI, SHIYU WU, Univ of Louisville — Ultrathin single-crystalline boron nanosheets with α-tetragonal B_{50} symmetry (α-t-B_{50}) have recently been synthesized [1]. In this presentation, the relaxed structure of this new type of boron sheet is determined using a robust self-consistent and environment-dependent semi-empirical Hamiltonian developed within the LCAO framework that includes MD and power quenching schemes. Upon relaxation, the sheet symmetry is broken and the icosahedral B_{12} units in the sheet are found to be distorted. This stability of the sheet was investigated through a calculation of the vibrational frequencies. The sheet electronic density of states exhibits no energy gap at the Fermi level, suggesting a metallic character similar to that of the bulk α-t-B_{50}. Finally, the cohesive energy of the α-t-B_{50} sheet is found to be higher than that of the recently reported icosahedral B_{12}-δ_6 sheet [2]. [1] Adv. Sci. 2, 1500023 (2015) [2] Nanotechnology 26, 405701 (2015)

Cherno Kah
Univ of Louisville

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