Abstract Submitted
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Electronic Properties of Curved and Defective 2-D BN Nanostructures[1] KORY BEACH, HUMBERTO TERRONES, ALDO RAELIARIJAONA, ROSS SIEGEL, FRED FLORIO, Rensselaer Polytech Inst — Density functional theory (DFT) with local density approximation (LDA) pseudopotentials is used to calculate the band structure and density of states of various novel 2-D BN nanostructures. Three types of systems are studied: Schwarzites, a Haeckelite, and an h-BN monolayer. Schwarzites are negatively curved structures in which the curvature is due to the introduction of octagonal rings of alternating boron and nitrogen atoms. In particular, three families of Schwarzites are analyzed: P, G and IWP. The Haeckelites on the other hand, are flat layers composed of squares and octagons of BN. It is found that all these BN allotropes are metastable in which the band gap is direct and smaller than the most stable system, h-BN.

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