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**Two-dimensional boron based nanomaterials: electronic, vibrational, Raman, and STM signatures** DANIEL V. P. MASSOTE, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, NEERAV KHARCHE, VINCENT MEUNIER, Department of Physics, Rensselaer Polytechnic Institute — Because boron has only three electrons on its outer shell, planar mono-elemental boron nanostructures are expected to be much more challenging to assemble than their carbon counterparts. Several studies proposed schemes in which boron is stabilized to form flat semiconducting sheets consisting of a hexagonal lattice of boron atoms with partial hexagon filling (PRL 99 115501, ACSNano 6 7443-7453) . Other structures were proposed based on results from an evolutionary algorithm (PRL 112 085502). These structures are metallic and one even features a distorted Dirac cone near the Fermi level. Experimental evidence for 2D boron is still lacking but the recently proposed molecular synthesis of a flat all-boron molecule is a promising route to achieve this goal (Nat.Comms. 5 3113). Our research aims at providing a first-principles based description of these materials' properties to help in their identification. DFT is used to calculate phonon dispersion and associated Raman scattering spectra. We report some marked discrepancy between our findings and results from the recent literature and address the deviation using two methods for phonon dispersion. We also simulated STM images at various bias potentials to reveal the electronic symmetry of each material.

Daniel V. P. Masso
Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 121

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