Abstract Submitted
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Electronic Structure Properties of Graphene/Boron Nitride Layered Systems[1] MAX PETULANTE, University of Maryland, NAM LE, LILIA WOODS, University of South Florida — We explore the properties of systems composed of two or three layers of graphene and hexagonal boron nitride (hBN) using the Vienna Ab-Initio Simulation Package (VASP), a software package for performing first principles simulations based on density functional theory (DFT). Particular attention is given to the contribution of inter-layer dispersion interactions, which are modeled within VASP by the "DFT-D2" method of Grimme. We obtain the binding and van der Waals energies, and inter-layer separations for the most stable stacking configurations of each of the following systems: hBN/graphene, graphene/hBN/graphene, hBN/graphene/hBN, hBN/hBN/graphene, and graphene/graphene/hBN. We observe that the addition of hBN layers to graphene structures induces a band gap, ranging from 0.024 eV, for the graphene/hBN/graphene arrangement, to 0.16 eV, for the hBN/graphene/hBN arrangement. These results, specifically band gaps on the same order as those of silicon and germanium, indicate that graphene/hBN layered structures may have applications in electronics.

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