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Electronic structure and lattice matching in graphene/h-BN stacked thin films[1] YUKI SAKAI, Department of Physics, Tokyo Institute of Technology and Department of Physics, University of California, Berkeley, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology, MARVIN COHEN, Department of Physics, University of California, Berkeley and Materials Science Division, Lawrence Berkeley National Laboratory — In this work, we study the electronic structure and possibility of lattice matching of thin films composed of graphene and hexagonal boron nitride (h-BN) within the framework of the density functional theory. Since graphene and h-BN have different in-plane lattice constants intrinsically, we first study relative stabilities of commensurate thin films with lattice matching and incommensurate thin films without lattice matching by comparing total energies in order to clarify the stable geometries of graphene/h-BN thin films. As a result, we find some stacking patterns where commensurate thin films are more stable than incommensurate thin films. We also find that the energy gain due to interlayer interaction depends on the number of layers in thin films. In addition, we report electronic properties of these thin film systems. Some commensurate thin films are found to possess finite band gaps, while induced band gaps should be almost canceled out in incommensurate phases. We also discuss the electric field effect on the electronic properties of graphene/h-BN thin films.

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