Abstract Submitted
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Moire pattern interlayer potentials in van der Waals materials from high level ab initio calculations JEIL JUNG, NICOLAS LECONTE, University of Seoul, Korea, SEBASTIEN LEBEGUE, Universite de Lorraine, France, TIMOTHY GOULD, Griffith University, Australia — Stacking-dependent interlayer interactions are important for understanding the structural and electronic properties in incommensurable two dimensional material assemblies where long-range moiré patterns arise due to small lattice constant mismatch or twist angles. We study the stacking-dependent interlayer coupling energies between graphene (G) and hexagonal boron nitride (BN) single layers for different possible combinations such as G/G, G/BN and BN/BN using high-level EXX+RPA *ab initio* calculations. The total energies differ substantially when compared with conventional LDA, but for stacking-dependent total energy differences we find that the dominance of short-range covalent-type binding over the longer-ranged van der Waals tails near equilibrium geometries renders the LDA as a reasonable starting point for ab initio calculation based analyses for the systems we have studied. Our calculations are useful input for study of strains originated by interlayer interactions in incommensurable 2D van der Waals crystals.

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