Interaction and relative motion of h-BN layers

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The discovery of graphene gave rise to considerable interest to bilayer and few-layer 2D materials. Nevertheless, whereas a wide set of phenomena and applications related to the interaction between the layers have been considered for bilayer and few-layer graphene, the studies of interaction between the layers of hexagonal boron nitride (h-BN) have been mostly restricted to structural and energetic characteristics. In particular, the processes analyzed for graphene include collective atomic-scale slip-stick motion of a graphene flake attached to STM tip on graphene surface [1], formation of dislocations (incommensurability defects) in stacking of the layers [2,3], self-retracting motion of the layers at their telescopic extension [4,5], a new mechanism of fast diffusion and drift of a graphene flake on a graphene surface [6,7], schemes and operational principles of nanosensors based on the displacement of the layers [8]. Similarly interesting phenomena and applications related to relative motion and interaction of the layers can be expected for bilayer and few-layer h-BN and theoretical studies of interaction between h-BN layers are necessary for their prediction and detailed analysis. Though there is a number of publications [9,10] on in-plane motion of h-BN layers, their results are rather contradictory and have been obtained with the aim to study the balance between van der Waals and electrostatic forces without relation to measurable physical quantities.

We have performed density functional theory (DFT) calculations using the vdW-DF2 functional [11] to obtain the potential surface of interlayer interaction of h-BN layers shown in figure 1. The adequacy of our calculations is confirmed by good agreement between calculated interlayer interaction energies for the symmetrical points of the potential surface with the values obtained recently by high-level ab initio local second-order Møller-Plesset perturbation theory [10]. Analogously to the expression suggested previously for fitting the potential surface of interaction energy of graphene layers [12], a simple expression that describes the potential surface of interaction energy of h-BN layers is introduced with the parameters fitted to the results of the DFT calculations. Based on this approximation, a wide set of physical quantities related to interlayer interaction and relative motion of h-BN layers are estimated. This set includes the barriers to relative motion and rotation of layers, shear mode frequencies and shear modulus for bilayer and bulk h-BN, length and formation energy of incommensurability defect (dislocation) in bilayer h-BN. The critical unit elongation of one of the layers of bilayer h-BN at which the transition to the incommensurate phase takes place is also estimated. Possible applications of the suggested approximation for the potential surface of interaction energy h-BN layers for further calculations of mechanical properties and simulations of dynamical phenomena related to motion and oscillation of h-BN layers are discussed. The DFT calculations performed here also represent a necessary intermediate step (as well as similar calculations for bilayer graphene [12]) before theoretical consideration of mechanical properties of graphene-h-BN heterostructures related to interlayer interaction.

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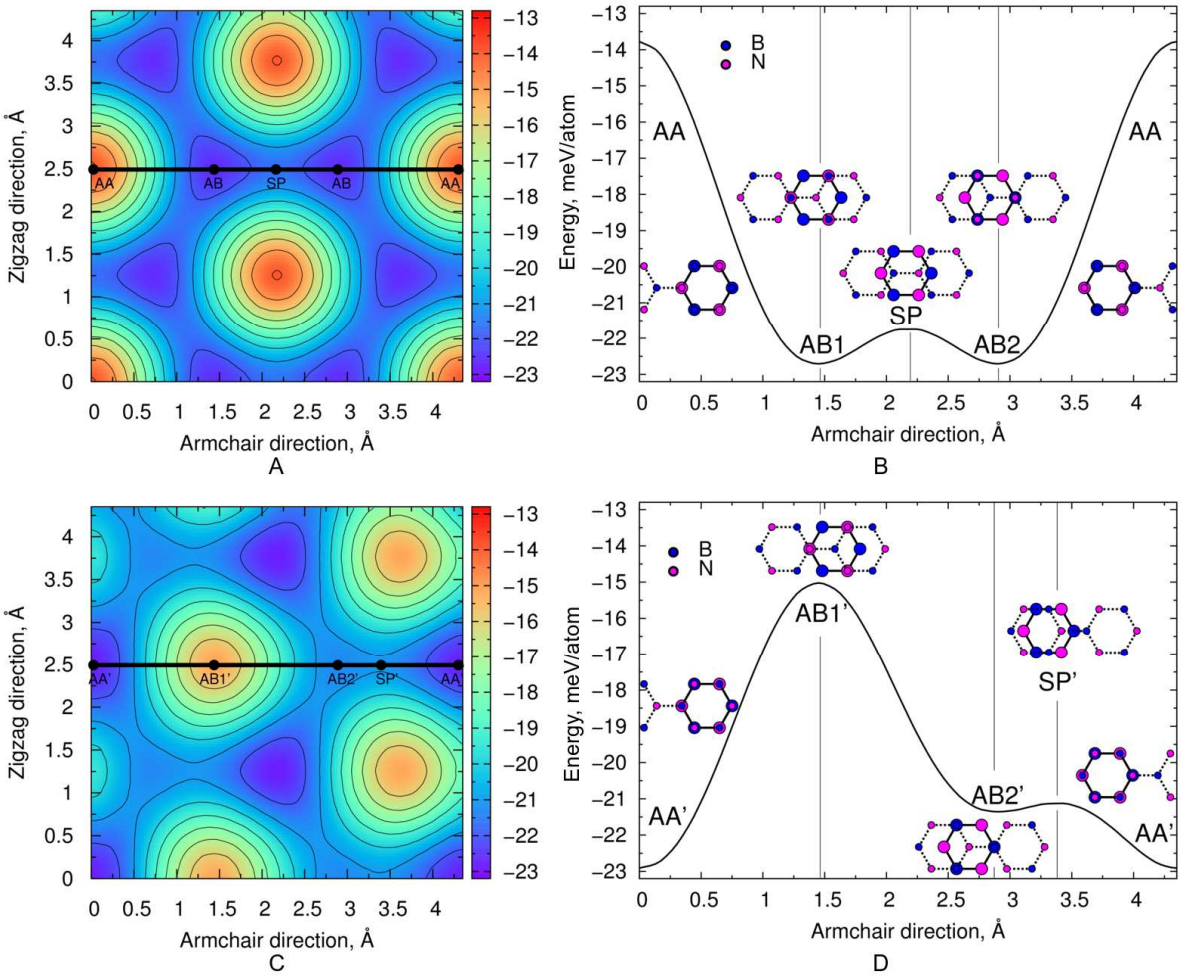

Figure 1: Calculated potential surfaces of interlayer interaction energy (in meV per atom) of h-BN at interlayer spacing equal to 3.33 Å as a function of the relative displacement (in Å) of the layers. Upper (A and B) and lower (C and D) panels correspond to different stacking modes. B and D. Sections of potential surfaces shown on panels A and C, respectively, along thick lines.