Theory of graphene-boron nitride heterostructures

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The efforts for developing graphene-based nanoelectronic devices, e.g., high-speed transistors, require high electron mobilities. At present, an important source of disorder in graphene samples are substrates underlying the graphene layer. Typical disorder effects can be corrugation of the graphene sheet, charge traps, or dangling bonds. A promising candidate to replace silicon dioxide as a standard insulating substrate material is hexagonal boron nitride (h-BN). Since 2010, several experimental groups reported the fabrication of graphene devices on h-BN substrates with highly improved electron mobilities and carrier inhomogeneities, reaching a quality comparable to suspended graphene [1,2,3].

Recently, Ponomarenko et al., [4] showed that h-BN is not only suited for the reduction of graphene-substrate interaction, but also opens new paths towards the functionalization of graphene. By embedding several layers of h-BN between two graphene layers Ponomarenko et al. induced a tunable metal-insulator transition in one graphene layer while changing the carrier density in the other graphene layer. Hence, understanding the physics of h-BN/graphene systems is also crucial in the context of graphene-heterostructures, a field of rising interest.

h-BN is a BN polymorph with remarkable similarity to graphite: It consists of alternating B and N atoms forming two-dimensional layers of strong sp^2 bonds arranged in a honeycomb lattice with a lattice constant very close to that of graphene. The h-BN sheets are weakly bound by long-range adhesive forces at an equilibrium distance of 3.3 Å. The electronic structure, however, exhibits clear differences: the chemically inequivalent sublattices make h-BN an insulator with a band gap of 6.0 eV. Experiments show that graphene stacks quasi-randomly orientated on a h-BN substrate and keeps its zero band gap [1,2].

In this work, we investigate the adhesion behavior and the electronic structure of graphene on h-BN from first-principles (results can be found in [5]). We show that a weak nonlocal attraction between the h-BN and the graphene layers requires methods beyond standard density-functional theory (DFT) to simulate the adhesion correctly. We calculate adhesion energies (Fig. 1c) using the random-phase approximation (RPA) within the framework of the adiabatic connection fluctuation-dissipation theorem (ACFDT) and compare the results to standard DFT methods. We also discuss mechanisms to release the stress resulting from the lattice mismatch and leading to the formation of moiré superstructures (Fig. 1b). Another part of our work is devoted to the band structure and energy gaps of graphene on h-BN. We derive a low-energy tight-binding description of graphene on h-BN from first-principles calculations and find mass terms that change their sign with the stacking configuration (Fig. 1d). This leads to an absolute gap in the moiré structure that is at least an order of magnitude smaller than the maximum local values of the mass term. Finally, we discuss the real space shape of the low-energy states and how they manifest in, for instance, local probe experiments. Particularly, the issue of sublattice

polarization and the occurrence of so-called snake states in regions where the mass term changes its sign, is presented.

References

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Figures
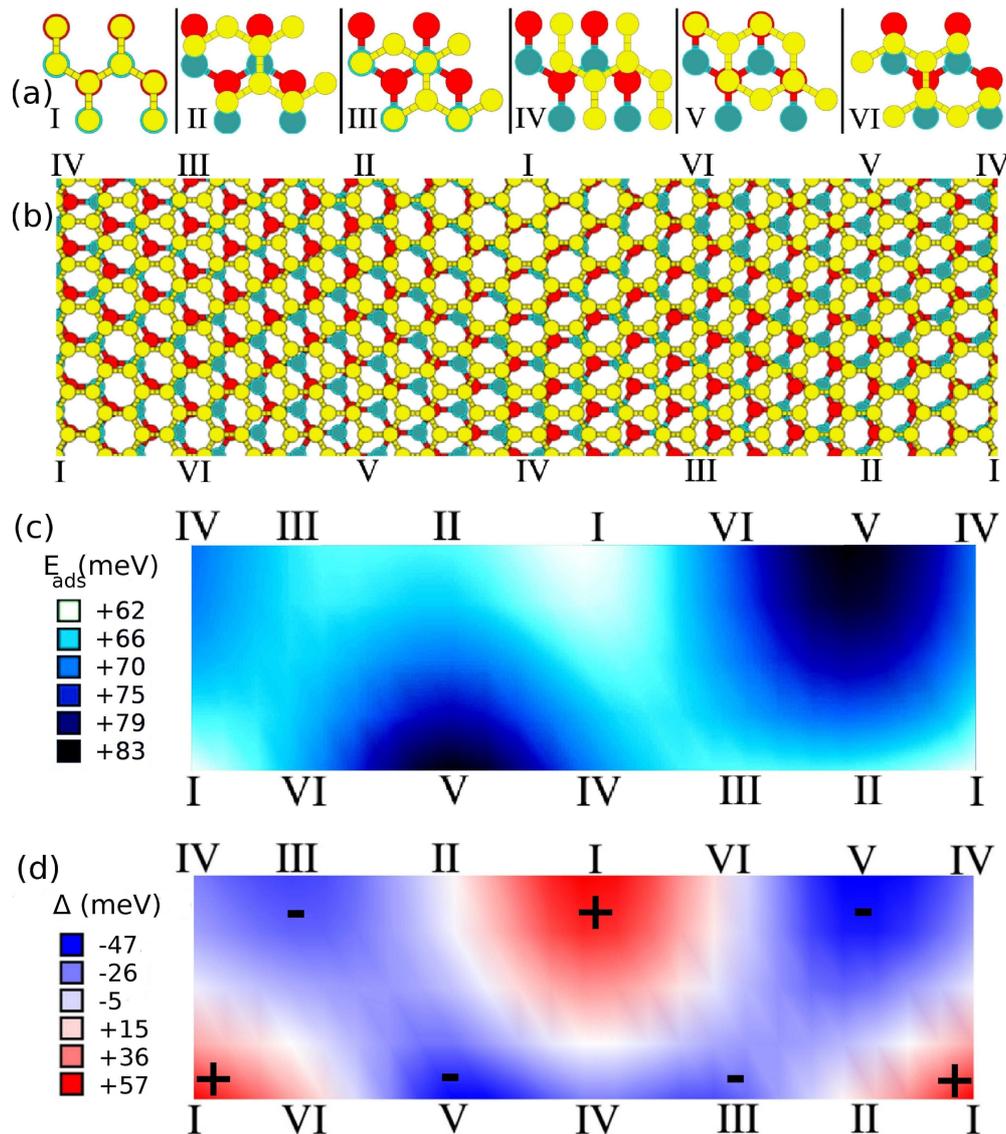
Figure 1: (a) Top view of different stacking configurations for graphene on h-BN with the carbon atoms (yellow), boron (red) and nitrogen (green). (b) Moiré structure with persisting lattice mismatch. A lattice mismatch of 1.8% corresponds to a 55x55 moiré unit cell. For clarity, a smaller moiré unit cell (13x13) is shown. (c) Adhesion energy (E_{ads}) landscape in the moiré pattern. (d) The same for the local mass terms.