Investigation of graphene interactions with hexagonal boron nitride layers - the density functional studies

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Boron nitride (BN) is a material that has attracted a lot of interest of scientists as a counterpart of graphene. Many similarities of those materials, along some very significant differences drifted physicists' attention not only to monolayers of hexagonal BN, but to structures combining both those materials as well. Moreover, hexagonal BN has been proven a very good substrate for graphene layers, due to very similar morphology and insulating properties.

First, we present a theoretical study of structural and electronic properties of graphene and boron nitride vertical heterostructures. The study is based on the ab initio calculations in the framework of the density functional theory. We determine the existance and magnitude of the energy gap in such structures under different conditions. Further, we investigate effects of van der Waals interactions in given systems using DFT-D2 scheme of Grimme [1] employing *SIESTA* numerical package with norm-conserving pseudopotentials.

Another part of our study deals with the properties of graphene on bulk h-BN substrate. We attempt to determine the possible morphology of these interfaces and the stability of the resulting structures. It is also interesting question to which extent the substrate influences the electronic properties of graphene. Our studies are based on the ab initio calculations in the framework of the density functional theory (DFT) with different energy functionals containing van der Waals correction using *VASP* software with PAW pseudopotentials.

Our research fits into very popular trend of investigating heterostructures based on graphene and BN and sheds light on basic physics of those materials.

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[1] S. Grimme, *J. Comp. Chem*. **27**, 1787 (2006).

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