# Similarities in the physico-chemistry of the C/BN and SiC/AlN(GaN) interfaces: *ab initio studies*

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The increased interest in certain III-V nitride compounds, in particular zinc-blende (c-BN) and hexagonal (h-BN) boron nitride is due to the fact that this material has many properties similar to that of diamond, such as wide band gap, extreme hardness, high thermal conductivity, and good transmittance over a large spectral range [1]. These unique physical properties make it be an appropriate material for technological development micro-, and/or nanoelectronic devices and also of optoelectronic ones operating in the visible/ultra-violet regions of electromagnetic spectrum. Physical and chemical properties of BN have been studied in great detail, both theoretically and experimentally [2]. Less attention has been paid to C/BN heterostructures, although h-BN is the best substrate for graphene-based 2D electronics. It has been demonstrated experimentally [3] that not only vertically stacked graphene/h-BN hybrid structures can be grown [4,5] but also in-plane graphene/h-bN atomic layer can be integrated into a lateral heterostructure with randomly distributed domains by CVD method. Creation of such heterostructures requires a physical insight into microscopic details of interfaces' morphology.

In this work, we present *ab-initio* DFT based studies on diamond/BN heterostructure interfaces. We employ a slab approach by creating the supercells with 208 atoms, representing, in particular, the c-BN stacked on the [001] diamond surface and h-BN on the [111] one. Such abrupt interfaces contain 'oversaturated' or 'undersaturated' tetrahedral bonds with more than ¼ or less than ¼ electron per bond, respectively. This bond heteropolarity leads to macroscopically charged interfaces that are energetically unstable and undergo various reconstructions. We propose some reconstruction patterns, which involve one mixed atomic layer (e.g. N/C or B/C) in the case of C/c-BN interfaces, or some number of substituted atoms in the case of C/h-BN ones. We compare the total energies of the abrupt and reconstructed interfaces to find the preferred bonding configurations, as well as, the resulting valence electron charge densities. Additionally, we compare the obtained results for C/c-BN, C/h-BN interfaces with the respective ones for 3C-SiC/GaN(AlN) and 4H-SiC/wz-GaN(AlN) interfaces. The analysis shows that the charge density distribution is more pronounced in the case of SiC/nitride heterostructures [6] than C/nitirdes ones. Finally, we compute the formation enthalpies, valence band offsets (VBO's), induced interface charges, and electric fields. The present studies shed light on the physics of C/nitride and SiC/nitride interfaces and provide microscopic knowledge on interface morphology.

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