



First principle study of the attachment of graphene onto non-doped and doped diamond (111)

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ABSTRACT

Density function theory (DFT) calculations have in the present study been used to study the adhesion of a graphene monolayer onto a non-, B-, or N-doped diamond (111) surface. Semiempirical dispersion corrections were used to take the Van-der-Waals corrections into consideration. In case of non-doped diamond as a substrate, DFT calculations (based on the local density approximation (LDA)) have shown a strong binding between graphene and the diamond (111) surface at a shorter distance (2.47 Å). The binding energy was -14.5 kJ/mol per C_{graphene} atom. In comparison, the generalized gradient spin density approximation (GG(S)A) was found to predict a weaker (-9.6 kJ/mol) interfacial bond at a distance of 3.10 Å. For the situation with B-, or N-, doped diamond, the optimized shorter diamond-graphene distance was found to be 3.01 and 3.24 Å, respectively. The corresponding adhesion energies per C_{graphene} atom was -9.9 kJ/mol (B-doping) and -9.6 kJ/mol (N-doping), which are quite similar to the non-doped situation (-9.6 kJ/mol). For all situations in the present study, the graphene layer was found to remain its aromatic character. However, a minor charge transfer was observed to take place from the graphene adlayer towards the non-doped and doped diamond (111) substrates.

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1. Introduction

Graphene is an aromatic structured monolayer carbon packing to a two-dimensional honeycomb crystal, with a high stability of a perfect six-carbon ring structure. Graphene is also known to be a semi-metal with zero band gap. Hence, there is no overlap between the conduction band and valence band, but only one single point will converge at the Fermi level (called the Dirac point). The electron transport in graphene is highly mobile (with about $200,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) [1], and temperature-independent within the range of 10 to 100 K [1–3]. The resistivity of graphene is even lower than that of silver (which is $10^{-6} \Omega \text{ cm}$). [4] These unusual transport properties of graphene are quite attractive for various applications within the area of electronics. [5–8] Due to its unique structural geometry, graphene also shows a variety of structural-related properties. Examples of properties are high opacity, [9] various chemical modifications, [10–12] high thermal conductivity at room temperature, [13] and spin transport. [14] Thus, graphene shows promising potential applications in fields such as optics, [15] electrochemistry, [7] and for electrochromical devices [16].

Thus, it is common to construct a transistor based on graphene positioned on top of metals, such as Cu [17], or positioned on top of Si-based hybrid substrates, such as SiC [18] and SiO_2 . [19] However, the transistor constructed from graphene on top of the metal surfaces most often shows undesired properties. The structural mismatch between graphene and the metal substrates would then cause folding, or defects,

within the graphene layer [20]. Moreover, graphene that is deposited on a conventional SiO_2/Si substrate, in the form of a field-effect transistor, shows a smaller breakdown current density than the maximum achieved one for a carbon nanotube [21]. When substituting SiO_2 with hexagonal boron nitride, the carrier mobilities of graphene can be increased [22]. Hexagonal boron nitride (hBN) is also an alternative for epitaxial graphene. However, it is not possible to avoid doping of graphene by either B or N atoms. Moreover, the effectiveness of hBN as a substrate depends strongly on the stacking order between BN and graphene [23,24], and hBN as a substrate can also influence the properties of graphene [25–28]. Thus, diamond has recently been suggested to be used as a substrate for the deposition of an epitaxial monolayer of graphene [21,29,30]. Diamond is a material that consists of only sp^3 -hybridized carbon bonds. It would avoid inducing any impurity into graphene. Diamond shows very attractive properties, such as large electrochemical potential window, high thermal conductivity at room temperature, hardness, and chemical inertness [31]. Thus, synthetic diamond, which can function as a heater spreader, is a natural candidate as a bottom dielectric substrate in graphene-based devices.

For a non-terminated diamond (111) surface, the projection of the first carbon layer onto the xy-plane will result in a carbon–carbon distance of 1.45 Å. This C–C distance is very similar to the C–C bond length in graphene (1.42 Å). Graphene on top of a diamond-like carbon substrate, has been used as a high frequency transistor by Wu et al. [32] Moreover, Okada et al. have studied the formation of graphene onto diamond nanowire surfaces [33], and Yu has studied some graphene-on-diamond devices with increased current-carrying capacity [21]. Some

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theoretical work, considering graphene attached to a diamond substrate, has also been performed [34–36]. Ma et al. have revealed that diamond substrate will induce one gap opening and spin injection in the supported graphene [34]. Hu et al. have found that the main effect of a diamond surface as an inert substrate is the formation of charge transfer complexes between graphene and a diamond (111) surface, and tiny gaps opening in graphene adhered onto a diamond (100) substrate [35]. Selli et al. have studied the electronic structure quantum transport properties of the buckling of a graphene layer that is covalent binding to the diamond substrate [36]. However, there is still a lack of detailed knowledge considering, e.g., the effect of dopants (e.g., B and N) in the diamond substrate when interacting with graphene.

Due to the promising structural similarity between graphene and the diamond (111) surface, the focus in the present investigation has been on the possibility to form graphene on top of non-doped, and on B- and N-doped, diamond (111) substrates. The B and N dopants within the diamond lattice are expected to cause an extent of defects in the diamond electronic structure. It is therefore quite interesting to investigate if these defects can improve the interaction between the graphene monolayer and the diamond substrate. More specifically, the purpose with the present work has been to study the stability and electronic structure of the graphene/diamond (GD) interface systems, using various DFT techniques under periodic boundary conditions. The adhesion energy of graphene, and its electronic properties when adhered to diamond (111), have thereby been calculated and compared for non-, B- and N-doped diamond (111) surfaces.

2. Computational details

The geometrical structures, total energies and electronic properties of the various diamond (111)/graphene interlayers, have been investigated using Density Functional Theory (DFT), as implemented in the CASTEP software (Materials Studio 5.5) from Biovia, Inc [37–39]. The CASTEP program uses an ultrasoft pseudopotential plane-wave approach under periodic boundary conditions [40]. The electronic and

structural properties of the interlayer systems were calculated and analyzed using both the Perdew Burke Ernzerhof (PBE) [augmented with the Tkatchenko–Scheffler Van-Der-Waals (TS–vdW) correction] generalized gradient (spin density) approximation (GG(S)A) [41], and the Local Density Approximation (LDA) with semi-empirical dispersion corrections [39,42]. The PBE functional is a common exchange-correlation functional that accurately describes the chemical interactions on surfaces. [41] In the present study, interfacial diamond//graphene distances larger than 2.5 Å (i.e., non-covalent bonds like Van der Waals (vdW) interactions) has been found to be crucial for the formation and stability of the diamond//graphene system. However, the vdW interactions are not properly described in the standard DFT methods. Thus, semiempirical dispersion-corrections were introduced to improve the non-bonding interactions in the standard DFT description. [43–45] For this purpose, the Tkatchenko–Scheffler van der Waals (TS–vdW) [46] scheme, and the OBS (Ortmann, Bechstedt, and Schmidt) [44] scheme, were implemented in semi-empirical dispersion correction methods. These semi-empirical dispersion corrections have been shown to improve non-covalently bonding interactions, and thereby to account for the relative variation in dispersion coefficients of differently bonded atoms. [44,46] The dispersion-corrected total energy E_{total} is described as:

$$E_{total} = E_{DFT} + s_i \sum_{i=1}^N \sum_{j>i}^N f(S_R R_{ij}^0, R_{ij}) C_{6,ij} R_{ij}^{-6} \quad (1)$$

where E_{DFT} is the standard DFT total energy. The other terms describe the semiempirical dispersion-correction energy. The E_{total} sum covers all N atoms in the system. For a long range order, the potential for the dispersion of interatomic interaction is given by the $C_{6,ij} R_{ij}^{-6}$ term. The parameter $C_{6,ij}$, which is a material-depending factor, is the dispersion coefficient for an atom pair i and j , at the distance R_{ij} . Moreover, the damping function $f(R_{ij}^0, R_{ij})$ is used with the purpose to match the long-range expression to the short-range. For the short to medium range, the function of dispersion interaction is modified by the parameters s_i and S_R . In the existing schemes, heteronuclear R_{ij}^0 and $C_{6,ij}$ are coefficients approximated from semiempirically determined homonuclear parameters.

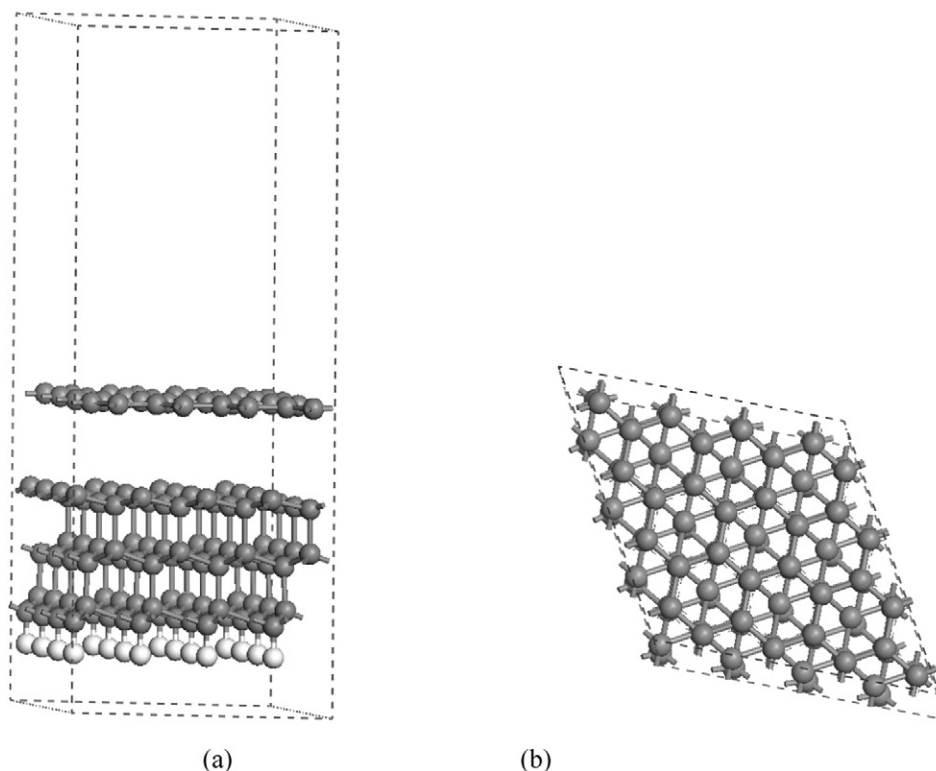


Fig. 1. Side view (a) and top view (b) of the graphene//diamond (111) interface system.

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