Ab initio studies of graphene layers on insulating substrates

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Graphene is one of the most promising materials for applications in the future nanoelectronics and the large-area graphene has been synthetized on metal surfaces by chemical vapor deposition. However, to utilize graphene's unique features in electronic devices, one needs to place it onto an insulating substrate. This procedure requires a multiple step transfer process and, therefore, several attempts have been undertaken to achieve the transfer-free synthesis of graphene. So far, the metal-catalyst-free synthesis of graphene has been tried on the whole plethora of substrates such as MgO, GaN, h-BN, Si_3N_4, Al_2O_3, ZrO_2, HfO_2, and also directly on SiO_2 [1, 2].

However, the deeper understanding of the physicochemistry of graphene/substrate interfaces would facilitate the development of the better growth techniques. Therefore, we have undertaken the *ab initio* studies of the graphene layers of the substrates MgO, GaN, h-BN, Si_3N_4, and SiO_2 substrates. We attempt to find out 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 the energy functionals containing van der Waals (vdW) correction that turned out to be important in our studies of the graphene and h-BN vertical heterostructures [3]. To perform the computations, we have employed the *SIESTA* and *VASP* numerical packages with norm-conserving and PAW pseudopotentials, respectively. For systems containing more than 500 atoms, we have used also Density Functional based Tight Binding (DFTB) method [4]. However, the studies are far from being complete yet, we can conclude that they provide hints how the graphene layers can form on the variety of substrates studied.

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