Structural and energetic properties of hydrogenated graphene on Ni(111) surface.

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Graphene, precursor of 2D materials has been the subject of recent intensive research due to the novelty of its various properties [1]. However, it is zero band gap material which limits its potential electronic applications. One way of opening the gap is the incorporation of heteroatoms (e.g., hydrogen, nitrogen, halogens) and molecular groups [2] into graphene sheet. Recently graphane (fully hydrogenated graphene) with a band gap around 4.5 eV has been reported [3]. Moreover, graphone (only one side of graphene is hydrogenated), leads to the indirect band gap semiconductor exhibiting magnetic behavior [4]. In addition, it has been demonstrated that graphone can be successfully synthesized on Ni(111) surface in reversible manner, which is crucial for hydrogen storage [5]. Thus, the influence of the substrate on graphone formation is worth a theoretical considerations.

Therefore, in present study, we demonstrate results of extensive first principles calculations of the freestanding graphone, and graphone formed on the Ni(111) supported surface, in the framework of density functional theory with van der Waals approach included. Our studies reveal formation of graphone on the ferromagnetic Ni(111) surface rather than formation in the vacuum condition [6]. Generally, our results for freestanding partially hydrogenated graphene shows two minima, which stands for the chemical and physical adsorptions, whereas for the graphone on a Ni(111) surface only one deep potential occurs, with no energy barrier for this chemical adsorption.

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