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First-Principles Calculations of Hydrogen Adsorbed in Multi-Layer Graphene

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Abstract : Graphene-based materials have attracted much attention because they are candidates for post silicon materials. Since controlling of impurities is necessary to achieve nano device, we study hydrogen impurity in multi-layer graphene. We perform local spin Density approximation (LSDA) in which the plane wave basis set and pseudopotential are used. Previously hydrogen monomer and dimer in graphene is well theoretically studied. However, hydrogen on multilayer graphene is still not clear. By using first-principles electronic structure calculations based on the LSDA within the density functional theory method, we studied hydrogen monomers and dimers in two-layer graphene. We found that the monomers are spin-polarized and have magnetic moment 1 μB. We also found that most stable dimer is much more stable than monomer. In the most stable structures of the dimers in two-layer graphene, the two hydrogen atoms are bonded to the host carbon atoms which are nearest-neighbors. In this case two hydrogen atoms are located on the opposite sides. Whereas, when the two hydrogen atoms are bonded to the same sublattice of the host materials, magnetic moments of 2 μB appear in two-layer graphene. We found that when the two hydrogen atoms are bonded to third-nearest-neighbor carbon atoms, the electronic structure is nonmagnetic. We also studied hydrogen monomers and dimers in three-layer graphene. The result is same as that of two-layer graphene. These results are very important in the field of carbon nanomaterials as it is experimentally difficult to show the magnetic state of those materials.

Keywords : first-principles calculations, LSDA, multi-layer gra-phene, nanomaterials
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