Theoretical study of the effect of nickel and gold impurities on electronic properties of graphene using density functional theory

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Abstract

In this paper, the electronic properties of graphene in the presence and absence of the gold and nickel atoms are calculated using the density functional theory. The electronic structure, density of states, stability, band gap, and spin polarization are studied. The calculations are performed with SIESTA software. For this reason, the local density approximation (LDA) and generalized gradient approximation (GGA) are used to calculate the exchange-correlation potential. Pure graphene layers do not show any spin polarization, but in the presence of impurity, they show the spin polarization depending on the gold and nickel impurities location. Furthermore, gold and nickel impurities affect the flatness of the surface. There is a hybridization between H*s* and C*p* orbitals in graphene with impurities of gold and nickel. Moreover, *d* orbitals of gold and nickel have hybridization with *p* orbitals of carbon.

Keywords: Graphene, Density functional theory, generalized gradient approximation

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