Magnetic properties of interstitial Fe in graphene nanosheet

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Abstract

In this paper electrical and magnetic properties of interstitial Fe in graphene nanosheet have been investigated. The calculations have been performed in the framework of density functional theory and the GGA approximations within Quantum Espresso package. The band structure calculation show that direct band gap of graphene nanosheet along M direction. According to this calculation, the electronic and magnetic properties of this structure depend to the Fe atom, which will be attained the magnetic metal or magnetic semiconductors.