Electronic and Optical properties of interstitial Fe in graphene nanosheet

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Abstract

In this paper electronic and optical properties of interstitial Fe in graphene nanosheet have been studied. The calculations have been performed using pseudo-potential method in the framework of perturbation density functional theory and the LDA approximations within Quantum Espresso package. Our results show the gap energy become zero and the graphene nanosheet display metallic properties. Furthermore, the optical properties have been presented in terms of the real and imaginary parts of dielectric function.