ELECTRON STRUCTURE AND ELECTRIC CONDUCTIVITY OF GRAPHENE WITH A NITROGEN IMPURITY

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S u m m a r y

On the basis of the tight-binding model with the use of exchange-correlation potentials, the electron structure and the electric conductivity of graphene with a nitrogen impurity have been studied in the framework of density functional theory. The wave functions of $2s$ and $2p$ states of neutral noninteracting carbon atoms are selected as the basis ones. Band hybridization was found to result in the splitting of the electron energy spectrum near the Fermi level. In the nitrogen-doped graphene, owing to the overlapping of $2p$ energy bands, the mentioned gap is realized as a quasi-gap, in which the electron density of states has a much lower value in comparison with the other spectral region. It is found that an increase in the nitrogen concentration reduces the electric conductivity of graphene, although the density of states at the Fermi level grows at that. Hence, the reduction of the electric conductivity is associated with a sharper decrease in the relaxation time for electron states.