# On the calculation of the charge transfer due to atom adsorption on graphene

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In the recent years, increasing attention has been focused on the adsorptive properties of the carbon nanostructures. As to graphene, any atom interacting with monolayer carbon sheet is in fact adsorbed on it. Moreover, under some conditions adsorption leads not only to the doping of graphene but can manifests itself as the energy gap opening. The most part of the theoretical studies in the field are based on the density-functional formalism. Here we present the model approach to the problem.

Recently we have proposed simple model for the graphene density of states (DOS) [1], which permits us to obtain an analytical expression for the adatom's local DOS. With this in hand we have calculated the corresponding occupation numbers for the adatom's states taking part in the charge-transfer processes. This scenario has been applied to the alkali metals [1], atomic hydrogen [2], and the halogens. It was found that hydrogen and alkali metals act as donors, while halogens appear themselves as acceptors. Furthermore, their charges are: 1) 0.2 – 0.4 for hydrogen, 2) increase from 0.8 to about of 1 in the row of Li → Cs, 3) change around − 0.5 for the halogens.

Furthermore, we have studied the effect of the carbon orbitals hybridization type on the adatom's occupation number and demonstrated that this effect is not crucial for the charge transfer value. The role of the adsorption bond length and graphene work function has been also analyzed.

[1] S.Yu. Davydov, G.I. Sabirova. *Phys. Solid State* **53**, (2011).
[2] S.Yu. Davydov, G.I. Sabirova. *Tech. Phys. Lett*. **36**, 1154 (2010).