Computational study of functional groups (-F and -Cl) on graphene

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The graphene is an aromatic system, and can be thought of as being composed of benzene rings with the hydrogen atoms substituted by carbon atoms from adjacent rings. Any changes in the edge geometry such as termination, reconstruction, distortion would modify the electronic properties of grapheme. [1]. The considered models of this study are the representative models of graphene that the ends of graphene are saturated by hydrogen atoms (Fig.1). Three models are considered: pristine model(C28H14),with -F functional group (C28F8H13) and with -Cl functional group (C28ClH13) .In the first step, the structures are allowed to relax by all atomic geometrical optimization at the DFT level of BLYP exchange-functional and 6-31G* standard basis set .Subsequently, the CS tensors are calculated in the optimized structures using the same level of the theory. All DFT calculations are performed by the Gaussian 98 package [2]. The three structures had the same number of atoms, the functional groups were members at the top of the graphene instead of H atom (Fig.1a, 1b). Values of band gap detect significant changes in which the values of band gaps for the pristine model, with -F functional group and with -Cl functional group are 0.94, 0.92 and 0.91 ev respectively. This trend means that Cl functional group has more influence on the band gap of pristine model. The calculated dipole moment indicated that the polarizibility of graphene with the Cl functional group was more than F functional groups.

Geometry optimization has showed that edge functionalization did not significantly alter the graphene structure. The calculated energies indicated that when the edge of graphene dangling bond is bonded by F atom the structure become more stable than is bonded by Cl atom. The calculated total energies indicated graphene functionalized with F is the most stable model. The changes of the calculated CS tensors in two different functional group regarding to the pristine models are also shown by changes of the structural properties.

Fig:1a

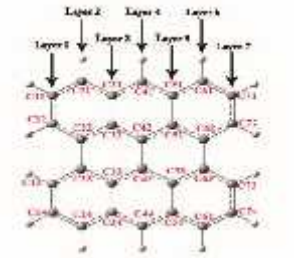

Fig 1: The pristine model of graphene

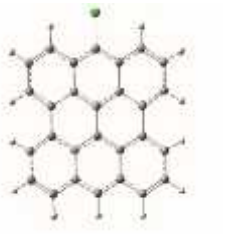

Fig:1b

Refrence:

[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V.Grigorieva, A.A. Firsov, Science 306 (2004) 666.

[2] Frisch, M.J. et al., GAUSSIAN 98, Gaussian, Inc., Pittsburgh, PA, 1998.