Improved the conductivity of the carbon nanotubes by iodine doping: a DFT study

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Abstract

Since its discovery, significant researches have tried to understand and use the electronic transport properties of carbon nanotubes (CNTs) to create more efficient new components. One way to improve significantly the conductivity of CNT bundles is to put them in interaction with iodine vapor. [1,2] However little is known about the origin of such an improvement at the atomic scale. The major target of this theoretical/experimental study is to analyze the interaction between iodine complexes and carbon based nanostructures and to rationalize it to predict induced changes in the electronic structures by chemical doping by halogens species. The final goal will be to compare electronic transmission of two crossed carbon nanotubes by junction molecules both theoretically and experimentally.

At the very beginning of this work, we have focused our computational effort on the comparison of the adsorption modes and the induced modifications of the electronic structures (Fermi level shifts and hybridization of bands) by atoms and molecules belonging to the family of halogens, I and I_2 on a graphene layer, which can be considered as a reasonable model of large CNT (Fig. 1). Our first results are in good agreement with previous studies [3-4]. They confirm that the molecule prefers to adsorb on a specific site, as soon as the concentration remains low, < 2%, with an adsorption energy of around -0.4 eV, when van der Waals forces are included. More interestingly the molecular state is more stable than the dissociated one. However experimentally charged complexes like I_3^- or I_5^- are detected [2]. By looking at the interaction of stable molecule with highly reactive sites like monovacancy, we propose a mechanism of formation of these ions compatible with the hole-doping observation of the carbon nanostructures. Finally by varying the concentration of I_2 absorbates one should be able to tune the density of states and doing so the conductivity of CNTs.

References

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Figures

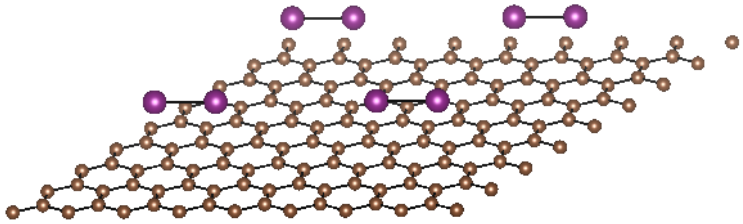

Figure 1: The coverage of admolecules. The sketch diagram shows four admolecules on CNTs with a large radius curvature, with 4x4 primitive cells.