Investigation of chemical effects of c-hexane absorbed on pristine and defected graphene

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Abstract- In the present paper, adsorption of c-hexane on pristine and defective graphene sheet and the changes of chemical properties of graphene due to its adsorption is studied in the framework of van der Waals density functional theory.

Graphene is a carbon-based material formed in the hexagonal honey-comb geometry. The reason for the tremendous increase of interest in graphene is its novel electronic, structural and chemical properties [1]. In this work, we aim to investigate the chemical effects of organic molecules adsorbed on pristine and defected graphene. The theoretical method of choice is density functional theory in the LDA and GGA exchange-correlation approximations[2].

In the initial stage of the work, we calculate the formation energy of defects as a function of defect density by defining different supercells of sizes 3x3, 4x4 and 5x5. As seen in literature, two kinds of defects important : vacancy and adatom [3]. Vacancy formation can be obtained only in one type of geometry, while there are many geometries to obtain adatom formations. The most valuable type of adatom formation is bridge, where the adatom is placed top on the bond of any two carbon atoms.

Up to now, formation energies of single vacancy and adatom are obtained in both 3x3 and 4x4 supercells for LDA and GGA pseudopotentials, and the calculations for 5x5 sized supercell is going on. As I expected, there is a slight difference between the formation energies for different pseudopotentials.

Up to now, several investigations of adsarption of graphene are done with various types of molecules[4]. Especially, some organic molecules are worth to study, such as c-hexane and tolune. Toluene is mainly used as paint thinner, spray paint , dyes, etc., while C-hexane is mostly used in nylon molding resin and production of nylon fibre. This project is limited to c-hexane adsorption, adsorption of toluene on graphene is going to be studied in my future works.

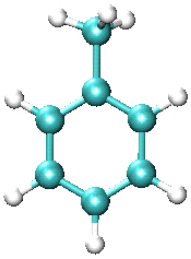

Figure 5: Toluene [5]

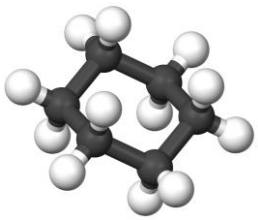

Figure 6: C-hexane [6]

Investigation of c-hexane adsorption on graphene will be studied in three binding geometries. First, flat type geometry will be considered. In this type of adsorption van der Waals interactions will be required. In the other two geometries, c-hexane will be bounded to the adatom, and to the unsaturated atom of vacancy. In this manner, DOS and band structures will be compared**.** Lastly, coverage effects will be studied.

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[6] http://commons.wikimedia.org/wiki/File:Cyclohexane-chair-3D-balls.png