Study of Interaction between Carbon Nanosheets and water Pollutants by Density Functional Theory (DFT)

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The unique electronic and mechanical properties of graphene has attracted a lot of attention to this matter. Single layer graphene is the two dimensional matter wich made of hexagonal carbon network with diameter of single atom and non localized π electrons and it is used in production of electrical capacitors and so in adsorption of organic pollutants molecules dilute aqueous solutions and it is by creating a complex with interaction of non electrostatical and electrostatical attraction. Both kinds of intractions depend on the surface features of adsorbent, adsorbate and the chemistry of the solution. In this project the interactions between organic molecule 2,4- di chloro phenoxyacetic acid with carbon nanosheet has been investigated. All the calculations are done by using density functional theory, B3LYP hybrid function and the basic set 6-31G(d) for optimization of the complexes. The analysis of natural bond orbitals (NBO) and the frequency calculations of all structures which are studied are done by B3LYP (Beck, 3parameters, Li yang- Parr) method and basic set 6-31G(d) in the 298 K. Based on the results obtained, complexes produced by the chemical adsorption between 2,4- di chloro phenoxyacetic acid molecule and carbon nanosheet is spontaneously but the constitution of the complexes produced by physical adsorption thermodynamically is not possible. By using the results of NBO studies, energy valuses of HOMO and LUMO and so the related functions has been calculated.

Keywords : 2,4- di chloro phenoxyacetic acid, carbon nanosheet, density functional theory, complex.