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Investigation of adsorption of aromatic dyes by carbon nanotubes: A DFT study of NMR parameters

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ABSTRACT

In this study, the adsorption of aromatic dyes on the surface of carbon nanotubes was investigated by quantum mechanical calculations. Exploring a novel sensor for detection of toxic aromatic compounds, interaction of pristine single-walled carbon nanotubes (5, 0) zigzag CNT (SWCNT) was investigated using the density functional theory (DFT) within the local density approximation. It was found that the pristine CNT can effectively interact with aromatic dyes. So that their electronic and structural properties are changed upon exposure to aromatic compounds. In the most stable configuration, the binding energy is negative (E_{ad}= -3.922 kcal/mol) and suggesting that the absorption reaction is possible. The impacts of the estereoelectronic effect associated with donor-acceptor electron delocalizations on the structural and electronic properties and reactivity of zigzag open-end single wall carbon nanotubes (SWCNTs) as nano adsorbents in interaction with aromatic dyes was studied based on the DFT calculations. The total electronic energy, orbital energies, density of state (DOS), LUMO-HOMO energy bond gaps, Adsorption energies (E_{Ad}) were calculated. Moreover, Nuclear Magnetic Resonance (NMR) shielding tensors were calculated by using the Gauge Independent Atomic Orbital (GIAO) method in order to determination of intramolecular interactions and chemical properties of molecules.

Keywords: Arimatic Dye, Adsorption, CNTs, Density functional theory (DFT), Energy gap, NMR

1. INTRODUCTION

The prediction of the carbon nanotubes (CNTs) by Iijima [1], which can be metallic or semiconductor in character, depending on their chirality and their diameter; their properties have suggested a variety of applications in the nanoelectronics. CNTs have recently revealed as materials of different properties and various applications in gas storage, sensors and in environment applications. In 1994 Rubio et al. [2] theoretically suggested the existence of the boron nitride nanotubes (CNTs), which were synthesized, by Chopra et al. [3]. CNTs possess excellent mechanical properties, high thermal conductivity, chemical stability; unique properties including tensile strength, stiffness and deformation are the features of CNTs, and resistance to the oxidation, among other properties. CNT has a smaller band gap of a material that is interesting for applications in nanoscale devices. Previously adsorption of different molecules toward nanostructures has been studied [4, 5]. Aromatic Dyes are hazardous substances and are considered as one of the environmental pollutants. Moreover, photocatalytic decomposition of toxic chemicals that have caused severe environmental pollution has been widely studied. Carbon nanotubes are new adsorbents with