4TH National Conference of Iran Chmistry, Chemical Enginereeng And Nano

THEORETICAL STUDY OF INTREACTION OF 4-AMINO PHENYL AZOBENZENE WITH (SWCNTs), A DFT METHOD

Masoud Arabsalmani, Fatemeh Azarakhshi*, Nilofar Tajdini

Department of Chemistry, Varamin-Pishva Branch, Islamic Azad University, Varamin, Iran
masoudarab6969@gmail.com
***Corresponding author- E-mail: fa_azarakhshi@yahoo.com**
nilofar_tajdini@yahoo.com

Abstract: The electronic and structural properties of single wall carbon nanotubes (SWCNTs) interacted with 4-amino phenyl-azobenzene were theoretically investigated by using the B3LYP density functional theory (DFT) calculations. The amount of thermodynamic parameters of this reaction in the gas and aqueous phase suggesting thermodynamic favourability for adsorption of 4-amino phenyl-azobenzene on (5, 0) zigzag CNT in both phases. The binding energy (BE) for the optimized structure of azo dye-CNT was calculated -3.92 (kcal/mol) and results showed that the physical adsorption reaction was occurred. The bonding-antibonding orbital interactions on the structural properties and reactivity of azo dye and CNNT, HOMO-LUMO bond gap and the total density of states (DOS) were quantitatively investigated by the NBO approach based on B3LYP/6-311+G** level of theory.

Keywords: Carbon nanotubes, DFT, Azo dye, Adsorption, NBO, Electronic effect.

1. INTRODUCTION

In the last decades, carbon-based materials have been widely studied. The discovery of carbon forms such as fullerenes, carbon nanotubes and graphene have brought a big interest because these materials exhibit remarkable properties to be applied in several technological areas [1]. In particular, carbon nanotubes are promising materials for several applications such as components in water filters [2,3], environmental sensors [4], electronic nanodevices [5], efficient gas storage elements and sensors in medicine [6]. Colours make many problems and these are major sources of environmental pollution and should be treated before discharge to environment. Nanotubes are new adsorbents with extend application for adsorption of different compounds. In this study the single-walled carbon nanotubes as adsorbent to reactive 4-amino phenyl-azobenzene was theoretically investigated.

2. COMPUTATIONAL DETAILS

First principle calculations of all the geometry optimizations, thermodynamic functions, natural bond orbital (NBO) for (5, 0) zigzag CNT interacted with 4-amino phenyl-azobenzene molecule are performed using Gaussian quantum package [7] at the level of density functional theory (DFT) with B3LYP/6–31G* basis set [8]. The 4-amino phenyl-azobenzene molecule was made in the different positions of the site to be close to the C30H10 nanotube and its adsorption has been calculated by using the Eqn (1). In addition, δBSSE is representing the basis set super position error.

$$E_{adsorption} = E_{(Chrysene\text{-}B12N12\ nanoring)} - (E_{Chrysene} + E_{B12N12\ nanoring}) + \delta BSSE \qquad (1)$$

In order to investigation of electronic and structural properties of (SWCNTs) interacted with 4-amino phenyl-azobenzene the stabilization energies associated with electronic delocalization, HOMO/ LUMO energy gap (Eg), frontier molecular orbitals (FMO) analyses were quantitatively investigated by the NBO (Natural Bond Orbital) analysis [9].

3. RESULTS AND DISCUSSION

Thermodynamic parameters [ΔH, ΔG (in kcal/mol) and ΔS (in cal $mol^{-1}K^{-1}$)] and relative energies $\Delta E0$ ($E0= ZPE + Eel$ (in kcal/mol), for the energy minimum azo dye–CNT at 25 ºC and 1 atm pressure was calculated at the level B3lyp/6-31g*, all parameters are negative in gas and aqueous phase and the adsorption reaction is exothermic (Tables 1, 2). In order to obtain