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

Comparing the adsorption HCN gas on the surface of (8, 0) zigzag models of boron nitride nanotube and boron phosphide nanotube: A computational study

M. Rezaei-Sameti*, E. Mehrabi
Department of Physical Chemistry, Faculty of Science, Malayer University, Malayer, 65174, Iran
mrsameti@malayeru.ac.ir

Abstract: In this research, we study the adsorption of HCN gas on the outer and inner surface of boron nitride nanotube and boron phosphide nanotube and comparing the adsorption parameters. The optimized parameters, adsorption energy, HOMO-LUMO orbital and other quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), and electronegativity (χ) of the nanotubes were calculated. The computational results reveal that the adsorption of HCN gas on the outer surface of two nanotubes is exothermic. The adsorption energy results showed that doping Ge impurity in BNNTs and BPNNTs increase the sensivity of nanotube for adsorption of HCN molecule. The adsorption of HCN molecule on the surface of Ge doped of BNNTs was more stable and favourable than other models. The energy gap between LUMO and HOMO orbital changed slightly from 2.83 to 3.09 eV, with adsorbing HCN gas on the surface of BPNTs. The comparison results show that gap energy of BNNTs is in range 6.30 to 4.05 eV.

Keywords : BNNTs, BPNTs, HCN adsorption, Ge-doped

Introduction

Hydrogen cyanide (HCN) is a toxic liquid or colourless gas which boils at 26°C. It is produced from the smoke of various tobacco and nitrogen containing organic materials [1]. Hydrogen cyanide is a poison compound and it can also be taken up through the skin [2]. It is highly lethal to man and animals, since it inhibits the consumption of oxygen by the bodily tissue. Therefore, it is important to develop sensitive sensors to detect the presence of toxic HCN [3–5]. In the current work, DFT calculations are performed to study the adsorption of HCN gas on the surface of BNNTs and BPNTs. For this aim, at first step all structures of nanotube/HCN complex at different configurations have been optimized, and then, the electronic structure properties, quantum parameters, adsorption energies, energy gap, net charge transfers, electronic densities of states (DOS spectrum), HOMO and LUMO orbitals of all representative models of BPNTs and BNNTs are investigated.

Materials and method

The quantum molecular descriptors electronic, chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), and electronegativity (χ) of the nanotubes are calculated as follows:

$$\mu = -(I + A)/2$$
$$\eta = (I - A)/2$$
$$\chi = -\mu$$
$$\omega = \mu^2/2\eta$$
$$S = 1/2\eta$$
$$E\ gap = E_{LUMO} - E_{HOMO}$$

Where I ($-E_{HOMO}$) is the ionization potential and A ($-E_{LUMO}$) the electron affinity of the molecule. chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), the maximum amount of electronic charge, ΔN, and electrongativity (χ) of the nanotubes [5] are calculated.