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Carbon monoxide interaction with the pristine and Ge-doped (8, 0) zigzag models of boron nitride nanotube: A DFT study

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Abstract: The aims of this project, to investigate the interaction of the carbon monoxide molecule with the pristine and Ge-doped BNNTs at various configurations. 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 are calculated. The results indicate that the adsorption of carbon monoxide from O and C head in the vertical direction of inner surface of pristine BNNTs is favourable than other those models in thermodynamically approach. The Fermi level energy of whole models is close to HOMO energy and is in range −2.41 to –3.86 eV; it is probably the most important factor in determining the current and the direction of natural flow of electrons.

Keywords: BNNTs, DFT, CO interaction, Ge- doped

Introduction

Boron nitride nanotubes shortly after the prediction in theory, are successfully synthesized by experimental methods [1-2]. BNNTs have attracted large amounts of attention due to potentially unique and significant properties, morphology and other excellent properties, *e.g.*, high elastic modulus, superb structural stability, anti-oxidation ability, chemical inertness and surface polarization [3-4]. The carbon monoxide molecule is highly toxic to human beings and animals as they inhibit the consumption of oxygen by body tissues. CO gas is colourless, odourless, and tasteless, and thus, human beings do not have timely alertness to their presence. Therefore, gas sensors with high sensitivity to this gas are highly desired. Many efforts have been made to reduce and monitoring the amount of carbon monoxide [5-6].
Following our previous research [7-8], in this work, we investigate the interaction of CO gas with the pristine and Ge-doped (8,0) zigzag BNNTs at the various possible adsorption geometries including the C and O atoms of CO close to the Ge atom of the with CO molecular axis being vertical and parallel to the surface of the tube.

Materials and method

In this work, at the first time all representative models of CO adsorption on surface (4, 4) armchair BNNTs ((*a*-*h*)models, Figs.1-2) are individually optimized by using density function theory at the B3LYP level of theory using the Gaussian 03 set of programs . The adsorption energy (E_{ads}) of CO on the surface of undoped and Ge-doped BNNTs calculated by Eq.(1)

$$E_{ads} = E_{BNNTs-CO} - (E_{BNNTs} + E_{CO}) \quad (1)$$

Where $E_{BNNTs-CO}$ obtained from the scan of the potential energy of the BNNTs–CO, E_{BNNTs} is the energy of the optimized BNNTs structure, and E_{CO} is the energy of an optimized CO. The quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), the maximum amount of electronic charge, ΔN, and electronegativity (χ) of the nanotubes [5] are calculated.

Results and Discussion

Quantum molecular descriptors and adsorption energy for CO adsorption on surface of undoped and Ge-doped BNNTs at representative (*a*-*h*) models (see Figs. 1).