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Interaction carbon monoxide on the surface of pristine and As-doped (٨, ٠) zigzag models of Aluminium nitride nanotube: A quantum and NQR approach

S. Azadi Doureh[١], M. Rezaei-Sameti[٢], E. Samadi Jamil[٣]

[١]Department of Physical Chemistry, Faculty of Science, Malayer University, Malayer, ٦٥١٧٤, Iran, sedigheh.azadi@yahoo.com

[٢٣]Department of Physical Chemistry, Faculty of Science, Malayer University, Malayer, ٦٥١٧٤, Iran, mrsameti@malayeru.ac.ir

Abstract: In the present project we study the effects of adsorption CO molecule and As-doped on the electrical and optical properties of AlNNTs at various configurations. From optimized structures, the 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 by using DFT theory. The results indicate that the adsorption energy of all models is negative and is favourable in view of thermodynamic approach. The result show that the Fermi level energy of whole models is close to HOMO energy, it is probably the most important factor in determining the current and the direction of natural flow of electrons. The results demonstrate that As doping decrease the sensivity of AlNNTs to adsorb of CO gas.

Keywords: AlNNTs, DFT, CO adsorption, As- doped, NQR

Introduction

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 [١-٢]. Since after discovery and synthesize BNNTs, many researches have done to investigate the properties and application of BNNTs. 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 [٣-٥]. In this project, we study the adsorption of CO gas with pristine and As-doped (٨٠٠) zigzag AlNNTs at the various possible adsorption geometries including the C and O atoms of CO close to the As atom of the with CO molecular axis being vertical and parallel to the surface of the nanotube.

Computational method

For study the adsorption of CO molecule on the surface of pristine and As-doped AlNNTs, The surface

and E_{CO} is the energy of an optimized CO. The quantum molecular descriptors: electronic chemical

of undoped and As-doped AlNNTs calculated by Eq.(١)

$$E_{ads} = E_{AlNNTs-CO} - (E_{AlNNTs} + E_{CO})$$

potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), the maximum amount of electronic charge, ΔN, and