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Original Research Article

The AIM, NBO thermodynamic, and quantum study of the interaction nitramide molecule with pristine, B, As and B&As doped of AlNNTs

Sedigheh Azadi doureh and Mahdi Rezaei–Sameti*

Department of Applied Chemistry, Faculty of Science, Malayer University, Malayer, 65174, Iran

*Corresponding author Fax number: mrsameti@gmail.com , mrsameti@malayeru.ac.ir

ABSTRACT

In this work, by using density functional theory, the adsorption of Nitramide (NH_2NO_2) molecule on the surface of pristine, B, As and B&As doped (4,4) armchair aluminum nitride nanotube (AlNNTs) is investigated. From optimized structures the adsorption energy, deformation energy, natural bond orbital (NBO), atom in molecule (AIM), quantum parameters, reduced density gradient (RDG) and molecular electrostatic potential (MEP) are calculated. The calculated results indicate that the adsorption energy values of NH_2NO_2 on the surface of pristine, As, B and B&As doped AlNNTs complex are negative and favorable in viewpoint of thermodynamic. Moreover the adsorption of NH_2NO_2 molecule on the surface of B&As doped AlNNTs is more stable and favorable than other models. It is notable that with doping B&As atoms in AlNNTs the deformation energy of NH_2NO_2 and nanotube are less than other models. The results of AIM and RDG outcomes demonstrate that nature of binding NH_2NO_2…AlNNTs is covalent bond type, indicates strong interactions. The results of NBO & Mullikan partial charge transfer, HOMO-LUMO, total charge transfer parameters (ΔN) and molecular

electrostatic potential (MEP) display that the charge transfer occurred from NH_2NO_2 molecule toward nanotube surface and electrical properties of system change significantly from original state. The results of this study reveal that the B&As doped AlNNTs is a good adsorbent for NH_2NO_2 molecule.

Keywords: Nitramine, B, AS, B&As doped, AlNNTs, DFT, AIM, NBO

Introduction

Shortly after successful discovery and synthesis of carbon nanotubes [1–3], intensive attentions have been dedicated to discovery and synthesis non-carbon nanotubes from the third and fifth group elements, which are neighbors of carbon in the periodic table, are an interesting subject of many researches [4–8]. One of them is Aluminum nitride nanotube (AlNNTs). The results of Zhang et al. indicated that AlNNTs in a hexagonal network is energetically favorable with sp^2 hybridization for both N and Al atoms [9]. Tondare et al., and Wu et al., [10–11] synthesized successfully the AlNNTs through different methods, the results of these study demonstrate that the electronic properties and semiconductor behavior of AlNNTs is independent of length, tubular diameter and chirality. The results of other studies reveal that the one-dimensional nanostructures of AlN have several unique properties such as high thermal conductivity at low temperature, high electrical resistivity, a moderately low dielectric constant, high dielectric breakdown strength, low thermal expansion coefficient close to the one of silicon, good mechanical strength, excellent chemical stability, and nontoxicity [12–13]. Aluminum nitride (AlN) nano materials are widely used in technological applications, mainly in micro and optoelectronics, such as laser diodes and solar-blind ultraviolet photodetectors and semiconductors [14–15]. Tuning the electronic structures of the semiconducting AlNNTs for specific application is evidently important in building specific electronic and mechanical devices