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Investigation of Adsorption of the Nitrosamine Molecule as a Carcinogen Agent on the AlN Nanotubes: A DFT Study

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ABSTRACT

In this study, chemical reactivity of (4,0) and (5,0) AlN nanotubes by interaction with nitrosamine molecule as a carcinogen agent was investigated using the B3LYP/6-311++G (d) level of theory. The HOMO-LUMO gap, electronic chemical potential (μ), hardness (η), softness (S), the maximum amount of electronic charge ($\Delta N_{\max}$), and electrophilicity index (ω) for the monomers and complexes were calculated. The results show that the interaction of NA with nanotubes can change electronic properties of nanotubes. To investigate the interactions between the NA molecule and nanotubes, analysis of atoms in molecules was performed at B3LYP/6-311++G (d) level of theory. The Multiwfn program was used to calculate the electron density of states (DOS). The charge transfer in complexes was calculated using the NBO analysis. The results of this work were compared with the results of adsorption of NA molecule on BN nanotubes. It is expected that the AlN nanotubes can be used as a sensor for detection of NA molecules.

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Graphical Abstract

Introduction

Nanocarbons, such as graphenes, graphynes, carbon nanotubes, and fullerene, have been widely studied [1, 2]. Carbon nanotubes due to their unique physical, chemical, electronic, thermal, optical and mechanical properties, have many applications in nanotechnology and other fields of materials science [3-8]. The metallic and semiconducting behavior of CNTs depends on the diameter and chirality of the nanotubes, which makes their synthesis difficult for specific purposes [9]. Numerous studies have been performed to find the stable structures of the noncarbon nanotubes [10, 11]. Among the various systems, boron-nitride nanotubes (BNNTs) and aluminum-nitride nanotubes (AlNNTs) are of great importance [12-14]. AlN nanotubes have been successfully synthesized with a diameter ranging from 30 nm to 80 nm [15]. These nanotubes have a band gap of 6.2 eV and their gaps are slightly dependent on their correlates. The zigzag AlNNT is seen to be energetically more eligible than the armchair one [16-18]. Due to their great polarity, AlNNTs have noticeably higher reactivity compared with carbon and boron nitride nanotubes. These nanotubes can be potentially used as sensor for detection of various molecules [19-21]. Studies have shown that AlN nanotubes are good candidate for trapping the gaseous molecules [22-24]. It was reported that, nitrosamines are carcinogenic compounds characterized by functional group of $-N-N=O$. Nitrosamines are

mutagen compounds and carcinogens that can damage DNA and induce tumors in humans and animals [25, 26]. Due to the abundance of nitrosamines in different food categories, beverages, drinking water, and cigarette smoke, it is necessary to find out the methods for removing these hazardous materials from the environment. In recent years, the experimental and theoretical studies have been performed on evaluating the adsorption of nitrosamines with zeolites and carbon nanotubes [27, 28]. In our previous work, we investigated the interaction of nitrousamin with BN and $B_{3Al}N$ nanotubes [29], and the results suggested that, the BN and $B_{3Al}N$ nanotubes can be the potential candidates for the nitrosamin molecule detection. In this work, the effect of adsorption of nitrosamin by AlN nanotubes was investigated and the results were compared with the results of the previous work. Also, the effect of increasing the diameter of the tube on the electronic and structural properties of the complexes was studied.

Experimental

Computational methods

Many of the properties of the materials and structures could be examined using theoretical methods [30, 31]. In this study, the zigzag models of (4,0) and (5,0) AlN nanotubes were chosen. All the complexes were optimized at B3LYP/6-311++G (d) level of theory using the Gaussian 09 software package [32]. The basis set superposition error (BSSE) was used to correct the calculation of the interaction energies [33]. The HOMO–LUMO gap, electronic chemical potential, hardness, softness, electrophilicity index, the maximum amount of electronic charge (ΔN_{max}), and dipole moment were calculated for different complexes. The Multiwfn program was utilized to calculate the electron density of the states (DOS) [34]. The NBO and AIM analysis were carried out at the B3LYP/6-311++G (d) level of theory [35, 36].

Results and discussion

All the possible sites for adsorption of the NA molecule by (4,0) and (5,0) AlN nanotubes were examined (Figure 1).

Figure 1. The optimized structures for (4,0) and (5,0) AlN nanotubes

The NA molecule can be placed on the wall of the nanotube with two different molecular orientations, which forms two types of A and B complexes. In A complexes, the hydrogen and oxygen atoms of NA interact with the nanotube, while, in B complexes, N atom of NA interact with the nanotube. Totally, eight stable structures on the potential energy surface were found which are presented in Figure 2.

Figure 2. The optimized structures for NA/(4,0) AlNNT and NA/(5,0) AlNNT complexes

In each structure, the new $H_{\text{molecule}}-N_{\text{nano}}$ and $N(O)_{\text{molecule}}-Al_{\text{nano}}$ bonds were formed between NA and nanotube. The $H_{\text{molecule}}-N_{\text{nano}}$ and $N(O)_{\text{molecule}}-Al_{\text{nano}}$ equilibrium distances between NA nanotubes are given in Table 1. Comparing the length of $H_{\text{molecule}}-N_{\text{nano}}$ and $N(O)_{\text{molecule}}-B_{\text{nano}}$ bonds indicated that the length of $H_{\text{molecule}}-N_{\text{nano}}$ bond is smaller than $N(O)_{\text{molecule}}-Al_{\text{nano}}$ bond. It is expected that in all complexes, $H_{\text{molecule}}-N_{\text{nano}}$ bond to be stronger than $N(O)_{\text{molecule}}-Al_{\text{nano}}$ bond. The results show that the length of $H_{\text{molecule}}-N_{\text{nano}}$ and $N(O)_{\text{molecule}}-B_{\text{nano}}$ bonds in A complexes are smaller than B complexes.

Table 1. Interaction energy (kJ/mol⁻¹), equilibrium distances (D) and dipole moment (μ) for NA/AlNNT complexes

Structure	$\Delta E_{\text{ele}}^{\text{bsse}}$	O(N)...Al(D)	N...H(D)	μ (D)
NA/(4,0) AlNNT				9.02
Aa	-103.74	1.96	1.68	10.22
Ba	-87.34	2.15	1.95	10.01
Ab	-101.52	1.96	1.71	13.98
Bb	-93.93	2.14	1.82	13.06
Ac	-105.51	1.95	1.71	10.77
Bc	-81.71	2.12	2.07	10.59
Ad	-110.74	1.95	1.73	10.41
Bd	-80.60	2.12	2.08	10.40
NA/(5,0) AlNNT				9.00
Aa	-99.30	1.98	1.72	13.93
Ba	-80.13	2.16	2.16	13.78
Ab	-91.89	1.98	1.79	13.93
Bb	-84.54	2.16	1.89	13.13
Ac	-102.55	1.97	1.74	10.93
Bc	-82.87	2.15	2.08	10.92
Ad	-102.79	1.98	1.75	10.58
Bd	-79.10	2.14	2.11	10.57

Our calculations confirmed that the length of $H_{\text{molecule}} \cdots N_{\text{nano}}$ and $N(O)_{\text{molecule}} \cdots B_{\text{nano}}$ bonds increased by enhancing the tube diameter. The interaction energies (ΔE) as a difference between the energy of the complex and the sum of the energies of monomers were summarized in Table 1. These energies were corrected by applying the counterpoise procedure. The results revealed that, the structure A is more stable than the structure B. Due to more electronegativity of atom O compared with N, it is expected that the structure with O...Al interaction to be more stable. Also, in complexes A, the relative stability of complexes is in the order of $d > c > a > b$. Based on Table 1, the interaction energies raised with increasing the tube diameter. Therefore, the stability of the complexes reduced by increasing the tube diameter. Compared to the previous study, our results showed that, the interaction energy of NA/AlNNT complexes is greater than that of the NA/BNNT [29]. Therefore, in comparison to the BNNTs, it is predicted that AlNNTs could be a better candidate for adsorption of NA molecules. The values of dipole moments are presented in Table 1. As can be seen, the dipole moment of the nanotubes increased upon complexation. The dipole moment in complexes A is higher than that of the complexes B. It is expected that, in polar solvents, the solubility of complexes A would be greater than complexes B. To explore the effect of the complexation on the electronic properties of AlN and $B_{3\text{Al}}\text{N}$ nanotubes, the HOMO–LUMO gap, electronic chemical potential (μ), hardness (η), softness (S), electrophilicity index (ω) and ΔN_{max} for NA, nanotubes and complexes were investigated (Table 2).

Table 2. The frontier molecular orbital levels, the energy gap (E_g), hardness (η), softness (S), chemical potential (μ), the maximum amount of electronic charge ($\Delta N_{\max}$) and electrophilicity index (ω) for NA/AlNNT complexes in the gas phase

Complex	HOMO (eV)	LUMO (eV)	E_g (eV)	η (eV)	S (eV)	μ	ω (eV)	$\Delta N_{\max}$
NA/(4,0) AlNNT	-6.20	-2.40	3.81	1.90	0.26	-4.30	4.86	2.26
Aa	-6.15	-2.79	3.35	1.68	0.30	-4.47	5.96	2.67
Ba	-6.20	-2.88	3.31	1.66	0.30	-4.54	6.22	2.74
Ab	-5.77	-2.76	3.01	1.51	0.33	-4.26	6.03	2.83
Bb	-5.88	-2.76	3.12	1.56	0.32	-4.32	5.98	2.77
Ac	-6.08	-2.86	3.23	1.61	0.31	-4.47	6.19	2.77
Bc	-6.08	-2.97	3.10	1.55	0.32	-4.53	6.60	2.92
Ad	-5.97	-2.84	3.13	1.57	0.32	-4.40	6.19	2.81
Bd	-5.99	-2.96	3.03	1.52	0.33	-4.48	6.61	2.95
NA/(5,0) AlNNT	-6.45	-2.29	4.16	2.08	0.24	-4.37	4.59	2.10
Aa	-6.16	-2.78	3.38	1.69	0.30	-4.47	5.92	2.65
Ba	-6.24	-2.84	3.40	1.70	0.29	-4.54	6.07	2.67
Ab	-6.05	-2.78	3.28	1.64	0.30	-4.41	5.94	2.69
Bb	-6.16	-2.76	3.40	1.70	0.29	-4.46	5.86	2.63
Ac	-6.26	-2.82	3.43	1.72	0.29	-4.54	6.01	2.65
Bc	-6.28	-2.88	3.40	1.70	0.29	-4.58	6.17	2.70
Ad	-6.23	-2.83	3.40	1.70	0.29	-4.53	6.03	2.66
Bd	-6.25	-2.89	3.36	1.68	0.30	-4.57	6.22	2.72

The results showed that, the energy gap of all complexes decreased upon complexation. Therefore, conductivity of the nanotubes increased. Also, the chemical softness, chemical potential, electrophilicity index and $\Delta N_{\max}$ of complexes increased and the chemical hardness decreased upon the complexation. Based on Table 2, conductivity of the nanotubes decreased by enhancing the diameter of the tube. In comparison with the previous work, the conductivity of (4,0) AlNNT is greater than (4,0) BNNT. In addition, the energy gap and chemical hardness for NA/AlNNTs complexes are smaller than those reported for NA/BNNT complexes (with the exception of Aa and Ba complexes). On the other hand, chemical softness, chemical potential, electrophilicity index and $\Delta N_{\max}$ for NA/AlNNTs complexes are greater than the corresponding NA/BNNT complexes (with the exception of Aa and Ba complexes). So, it is concluded that the stability and conductivity of NA/AlNNTs complexes are greater than NA/BNNT complexes. The calculated electron density of states (DOS) for the stable complexes is shown in Figures 3 and 4.

Figure 3. The density of states (DOS) for (4,0) AlNNT and NA/(4,0) AlNNT complexes

Figure 4. The density of states (DOS) for (5,0) AlNNT and NA/(5,0) AlNNT complexes

As seen in Figures 3 and 4, in NA/(4,0) AlNNT and NA/(5,0) AlNNT complexes, HOMO states move to less negative energy and LUMO states move to more negative energy. Therefore, it is predicted that the interaction of the NA molecule with nanotubes leads to a change in the conductivity of the nanotubes. The NBO analysis showed some interesting details on the electron density transfer in donor $\rightarrow$ acceptor interactions. The results of the NBO analysis are summarized in Table 3. Upon complex formation,

charge transfer occurs between nanotube and NA molecule. Therefore, the charge transfer can be defined as the sum of the electronic charge of atoms in the NA molecule. Inspection of the results revealed that in the all complexes, the charge transfer is taking place from NA molecule to nanotube. At each site, the amount of charge transfer in B complex is more than A. On the other hand, the amount of charge transfer for complexes NA/(4,0) AlNNT is more than NA/(5,0) AlNNT. In comparison to the previous study, the amount of charge transfer in AlNNT complexes is smaller than that of the BNNT complexes.

The quantum theory of atoms in molecules (QTAIM) is a useful tool to characterize the chemical bonds. To investigate the nature of the interactions between the NA molecule and nanotubes, analysis of atoms in molecules was performed at B3LYP/6-311++G (d) level of theory. The molecular graphs including the critical points and bond paths for NA/AlNNT complexes are shown in Figure 5. The molecular graphs represent two additional critical points in intermolecular region in each complex. The values of electron density ($\rho(r)$), Laplacian of the electron density ($\nabla^2\rho(r)$) and total energy density ($H(r)$) at the bond critical points (BCPs) are given in Table 3. There is a relation between the value of $\rho(r)$ at the $O(N)_{\text{molecule}} \dots AlN_{\text{Nanotube}}$ and $H_{\text{molecule}} \dots N_{\text{Nanotube}}$ BCPs with bonding distances. The results depicted that, at each position, the structure with the shorter bonding distances has greater $\rho(r)$ at bond critical points. With comparing the valves of $\rho(r)$ at the $O(N)_{\text{molecule}} \dots AlN_{\text{Nanotube}}$ and $H_{\text{molecule}} \dots N_{\text{Nanotube}}$ bond critical points, we can observe that, these interactions in the NA/(4,0) AlNNT complexes are stronger and shorter than those in the NA/(5,0) AlNNT complexes.

Figure 5. Molecular graphs indicating the critical points and bond paths for NA/(4,0) AlNNT and NA/(5,0) AlNNT complexes

The values of $\nabla^2\rho(r)$ and $H(r)$ at BCPs of all complexes were found to be positive and negative, respectively, with a partially covalent chemical bond. The covalent nature of these interactions reduced by increasing the tube diameter that is in agreement with the increase in the corresponding bond distances.

Table 3. Calculated BCP data (au) and the charge transfer for NA/AlNNT complexes

Complex	Bond	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	CT	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	CT
		(4,0) AlNNT complexes				(5,0) AlNNT complexes			
Aa	O...Al	0.0512	0.3166	-0.0030	0.095	0.0486	0.2950	-0.0028	0.094
	H...N	0.0591	0.1086	-0.0138		0.0537	0.1091	-0.0107	
Ba	N...Al	0.0417	0.1887	-0.0019	0.147	0.0403	0.1819	-0.0016	0.140
	H...N	0.0426	0.0968	-0.0006		0.0415	0.0925	-0.0001	
Ab	O...Al	0.0476	0.3099	-0.0047	0.107	0.0453	0.2857	-0.0041	0.103
	H...N	0.0548	0.1051	-0.0116		0.0459	0.1020	-0.0069	
Bb	N...Al	0.0418	0.1914	-0.0016	0.131	0.0396	0.1789	-0.0014	0.128
	H...N	0.0427	0.1034	-0.0052		0.0401	0.0952	-0.0026	
Ac	O...Al	0.0526	0.3262	-0.0028	0.100	0.0498	0.3029	-0.0027	0.098
	H...N	0.0558	0.1081	-0.0117		0.0513	0.1076	-0.0093	
Bc	N...Al	0.0437	0.2067	-0.0016	0.153	0.0412	0.1901	-0.0015	0.144
	H...N	0.0443	0.0757	-0.0013		0.0425	0.0807	-0.0009	
Ad	O...Al	0.0526	0.3262	-0.0815	0.106	0.0497	0.3014	-0.0026	0.104
	H...N	0.0558	0.1081	-0.0117		0.0506	0.1081	-0.0089	
Bd	N...Al	0.0437	0.2067	-0.0016	0.160	0.0414	0.1912	-0.0016	0.148
	H...N	0.0442	0.0757	-0.0013		0.0414	0.1912	-0.0016	

Conclusion

In this work, the DFT method was employed to assess the effect of the adsorption of nitrosamine (NA) on the electrical properties of AlN nanotubes. It was found that the NA molecule can be chemically adsorbed by the AlN nanotubes. As the type and the diameter of the tube play an important role in determining the interaction energy of the NA molecule, the NA/(4,0) AlNNT complexes found to be more stable than the NA/(4,0) BNNT complexes. Also, the interaction energy of NA with AlNNTs decreased with increasing the tube diameter. It is energetically favorable for the NA molecule to interact with d position of nanotubes. The energy gap and chemical hardness of nanotube decreased, whereas, the chemical softness, $\Delta N_{\max}$ and electrophilicity index of the nanotube increased upon complexation. Also, the conductivity and reactivity of the nanotube reduced as the tube diameter increased. Based on the NBO results, in all complexes, charge transfer occurred from the NA to the nanotube. The AIM results revealed

that, the O(N)...Al and H...N interactions are partially covalent in nature. It is predicted that, AlN nanotubes can be used as adsorption of NA molecules. In comparison to the BNNTs, it seems that the AlNNTs could be a better candidate for adsorption of NA molecules.

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Conflict of Interest

We have no conflicts of interest to disclose.

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