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ORIGINAL ARTICLE

Theoretical comparison of thermodynamic parameters, NMR analysis, electronic properties of Boron Nitride and Aluminum Nitride nanotubes

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Abstract

In this research, geometrical structures of armchair single walled boron nitride nanotube (SWBNNT) and armchair single walled aluminum nitride nanotube (SWAlNNT) were optimized by Density Functional Theory (DFT) in the gas phase, both having the same length of 5 angstrom and n=9, m=9. B3LYP/6-31G* level of theory have been used to determine and compare electronic properties, natural charge and chemical shielding tensors of nanotubes. The chemical shielding tensors were calculated using GIAO method to obtain structural information and dynamic behavior for optimal boron nitride and aluminum nitride nanotube structures. Also, thermodynamic functions for the boron nitride nanotube (9, 9-5) and the aluminum nitride nanotube (9, 9-5) in the gas phase were carried out with using the B3LYP method and 6-31g* basis set. It is significant that all of NMR parameters and geometrical properties of both nanotubes were determined in 5 layers.

Keywords: *AlNNT; BNNT; Chemical shielding; DFT; Isotropic; Nanotube; NMR.*

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INTRODUCTION

After discovering of carbon nanotubes (CNT) by Iijima [1], Nanotubes were considered because of their structural properties, and unique electric, physical and chemical characteristics. After that, a variety of other non-carbon nanostructures, such as boron nitride (BN), and aluminum nitride (AlN) nanotubes, silicon carbide (SiC), zinc oxide (ZnO) have been synthesized experimentally [2-5]. Boron nitride nanotubes (BNNT) and Aluminum nitride nanotubes (AlNNT) have unique properties and chemical stabilities at high temperatures. BNNTs are excellent candidates for biological and medical application [6]. Boron nitride (BN) nanostructures such as nanotubes [7], Nano capsules [8], and fullerenes have received much attention as promising materials for the electronic industry because of their unique structures and properties. For the first time, BNNTs were predicted theoretically by Rubio and colleagues in 1994 [9] and were synthesized in 1995 by Chopra *et al.,* [10] in the form of pure boron nitride nanotubes. Due to its chemical, optical, electrical, mechanical properties and higher thermal conductivity, it is considered as a known substance in the polymer industry, medicine, electronics and electricity [10-11]. This Nano structure is structurally similar to a pure carbon system. BNNTs and carbon nanotubes (CNTs) are isoelectronic. The sum of atomic numbers of boron and nitrogen is equivalent to the atomic number in the two carbon atoms. Therefore, due to the number of electrons, there is great similarity between carbon nanotubes and boron nitride nanotubes. Since CNTs exhibit different properties due to changes in chirality, controlling the synthesis of these nanotubes is very difficult. Therefore, BNNTs that their properties are independent of

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chirality changes can be suitable alternative to CNTs [12-13]. The properties of BNNTs do not show much dependence on chirality changes. Therefore, structural study and identification of its properties are of great importance. Unlike carbon nanotubes (CNTs), which are metallic or narrow band-gap semiconductors, BNNTs are wide-gap semiconductors with a value of ~5.5 eV [14]. AlN nanotubes are usable for ultraviolet LEDs. Inefficient emission at 210 nm was achieved on AlN nanotubes. AlNNTs have also been discovered to be semiconductors with a wide band gap (ranging from 2.84 to 3.95 eV) [15]. Unlike BNNTs, AlNNTs increases the band gap with its diameter, but depends only slightly on the chirality [16-19]. Furthermore, interactions between AlNNT/BNNT and gas molecules such as H_2, O_2, CO_2, etc., have already been reported [20-21]. Recently, many cases of AlNNTs and BNNTs reactions with other materials have been reported [22-23]. Nature of Interaction between Semiconducting Nanostructures and Biomolecules such as DNA Molecules has been studied [24].

AlNNT/BNNTs have many similar physical properties and structural characteristics [25]. The results on the synthesis of LD boron nitride materials have been reported but most attention on special CVD technique which requires high temperatures (>1000 °C) and ultrahigh vacuum (UHV) for the production of BNNs [26-27]. Synthesis of BNNs under such conditions may cause serious stresses between the substrate and the BNNs as well as significantly increasing the cost of production [28-29]. The application of pulsed laser plasma deposition (PLPD) technique for the synthesis of BNNs [30] and their use as UV detectors [31-32] and gas sensors [33] was reported. In recent decades, III-V semiconductors have gained extensive attention due to their various potential applications. It is noteworthy that semiconductor materials with a wide band gap can be doped with impurities that change its electronic properties in a controllable way. These materials are classified according to the periodic table groups of their constituent atoms [34-36].

In this study, we focused on the structural and dynamic properties of two nanotubes. So that geometrical structure, thermodynamic functional and NMR analysis by using Density Functional Theory (DFT) calculations at B3LYP/6-31G* level of theory in gas phase for BNNT and AlNNT (9,9-5) nanotubes into 5 layers have been investigated and compared.

COMPUTATIONAL DETAILS

In this research, the initial design of the boron nitride nanotube (9, 9) with length of 5 angstrom was performed using the nanotube modeler software (A program for generating xyz-coordinates for Nanotubes and Nanocones, and can also be used to generate some INTs: B-N, Ga-N, Al-N, Al-P and Ga-P) [37]. The quantum chemical calculations were carried out using the Gaussian 09W program package [38]. All of structures were optimized using the Density Functional Theory (DFT) method. DFT calculation accounts for the correlation energy in computationally efficient manner and offers a substantially improved accuracy over conventional approaches and it has become popular for molecular applications [39-40]. At the first step each of the considered pure models of BNNT & AlNNT was allowed to fully relax during the geometrical optimization. The geometries were optimized at the B3LYP/6-31G* level of theory. Then the values of thermodynamic functions [41] of BNNT and AlNNT nanotubes (9, 9) with a length of 5 angstrom in the gas phase and the related frequency calculations and NMR parameters are calculated at the B3LYP/6-31G* level of theory [42-44]. By comparing the values of the calculated parameters, the properties of these compounds have been studied. Finally nuclear magnetic resonance (NMR) parameters at the 11-B, 27-Al and 15-N nuclei of the optimized structures have been calculated. Nuclear Magnetic Resonance (NMR) properties including isotropic and anisotropic chemical shielding tensors (CSI and CSA) are among the important elements in the study of the reactivity and structural properties of chemical compounds by quantum mechanical calculations [45]. Subsequently, chemical shielding tensors (CSI and CSA) have been calculated for the optimized structures at the same level of the theory based on the gauge included atomic orbital (GIAO) approach [46]. These calculations have carried out at the GIAO/B3LYP/6-31G* level of theory, one of the best compromises between accuracy and computer time [44]. Since quantum chemical calculations yield the chemical shielding tensors in the principal axes system (PAS) ($\sigma 33 > \sigma 22 > \sigma 11$) they have been converted to CSI, CSA uses (Eqs. 1 and 2) respectively.

RESULTS AND DISCUSSION

The main reason for choosing boron nitride and aluminum nitride nanotubes is their interesting properties compared to carbon nanotubes. For

example, conductivity in these nanotubes, unlike carbon nanotubes, does not depend on the type of nanotube. The optimal geometrical structure of boron nitride (Fig. 1a) and aluminum nitride (Fig. 1b) nanotubes in the form of 5 layers at B3LYP/6-31G* level are shown in Fig. 1. The values of the electronic energy for BNNT (9,9-5) and AlNNT (9,9-5) are -3608.697 and -13399.574 hartree, respectively.

The values of the bond length of both nanotubes are shown in Table 1. As the table data specifies, the bond length of the outer layers such as 1 and 5 or 2 and 4 are similar. Also, the bond lengths of connector bonds between two layers that have the same position are the same values.

Thermodynamic Functions in Gas Phase

Thermodynamic parameters [41] for the BNNT (9,9-5) and also the AlNNT (9,9-5) in the gas phase were carried out using the B3LYP method and

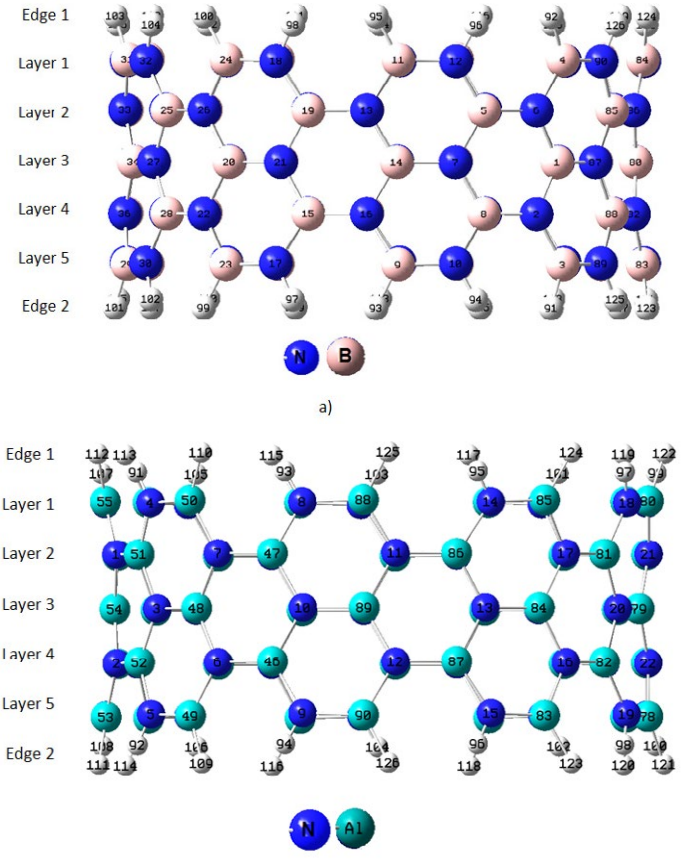


Fig. 1. Geometrical structure of a) BNNT (9,9) b) AlNNT (9,9) with the same length of 5 angstrom.

Table 1. bond length values of the boron nitride and aluminum nitride nanotubes.

Optimized parameters of BNNT (9,9-5) and AlNNT (9,9-5)		
Bonding nuclei	Bond lengths (Å) of B-N	Bond lengths (Å) of Al-N
Layer 1	1.418	1.797
Layer 2	1.453	1.806
Layer 3	1.450	1.805
Layer 4	1.453	1.806
Layer 5	1.418	1.797
Connector bond of Layer 1 and 2	1.445	1.804
Connector bond of Layer 2 and 3	1.456	1.807
Connector bond of Layer 3 and 4	1.456	1.807
Connector bond of Layer 4 and 5	1.445	1.804

6-31g* basis set. Sum of electronic and zero-point Energies (Eel+ZPE), Sum of electronic and thermal Energies (Eel+T), Sum of electronic and thermal Enthalpies (Eel+H), Sum of electronic and thermal Free Energies (Eel+G), and entropy (S) are shown in Table 2. Given the values of the thermodynamic parameters, it can be seen that the AlNNT (9,9) is more stable than BNNT.

Atomic charges of the boron, aluminum and nitrogen atoms in AlNNT and BNNT are shown in Fig. 2. Clearly, the contribution of the negative charge of nitrogen atoms in the aluminum nitride nanotube is higher than the negative charge of nitrogen atoms in the boron nitride nanotubes, since electronegativity of the boron atom is greater than that of the aluminum atom.

NMR Parameters

NMR spectroscopy is a powerful technique for studying the structural and dynamic behavior of molecules in different physical states. Theoretical study of nuclear magnetic resonance properties can be accomplished using advanced methods of quantum mechanics. The NMR parameters calculated by the quantum mechanics method [42-44] have an effective role in investigating the molecular structure of the compounds used. There are several ways to determine the NMR parameters such as Gauge-Including atomic orbitals (GIAO), Individual gauge for localized orbitals (IGLO), Localized orbitals local origin (LORG), Continuous set of gauge transformations (CSGT). In this research, the chemical shielding (CS) tensors were calculated using GIAO method to obtain structural information, dynamic behavior, and intermolecular interactions for optimal boron nitride nanotube and aluminum nitride nanotube. Chemical shielding (CS) tensors includes chemical shielding isotropic (CSI) tensor and chemical shielding anisotropic (CSA) tensor are calculated according to equations (1-9) [42-44]:

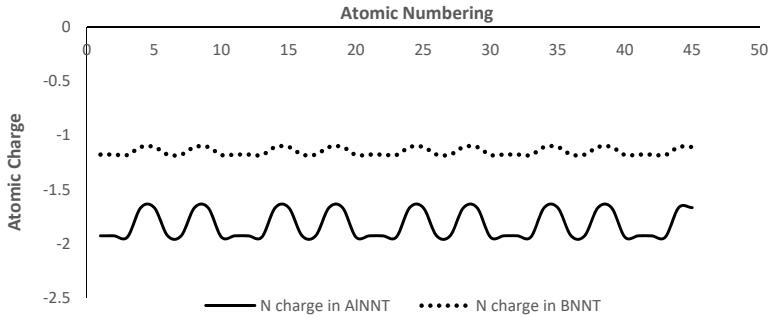
$$\mathrm{CSI(ppm)} = \sigma_{\mathrm{iso}} = \frac{(\sigma_{11} + \sigma_{22} + \sigma_{33})}{3} \quad (1)$$

If $|\sigma_{zz} - \sigma_{iso}| \geq |\sigma_{xx} - \sigma_{iso}|$:

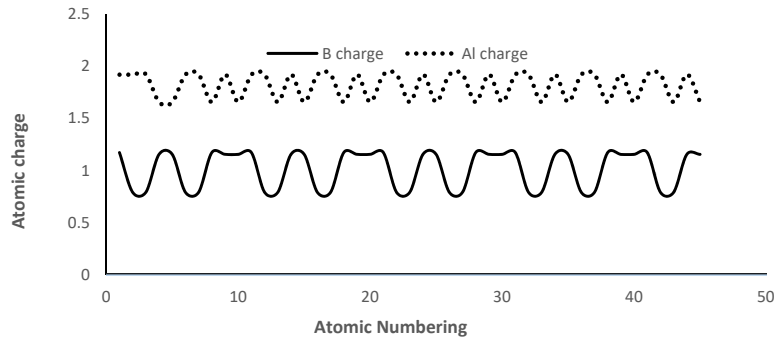
$$\mathrm{CSA(ppm)} = \sigma_{\mathrm{aniso}} = (\Delta\sigma) = \sigma_{33} - \frac{(\sigma_{11} + \sigma_{22})}{2} \quad (2)$$

$$\delta(\mathrm{ppm}) = \sigma_{33} - \sigma_{\mathrm{iso}} \quad (3)$$

$$\eta = \frac{(\sigma_{22} - \sigma_{11})}{\delta} \quad (4)$$



a)



b)

Fig. 2. Atomic charges of a) nitrogen atoms in AlNNT and BNNT b) boron and aluminum atoms in AlNNT and BNNT.

Chemical shielding tensors (CS) are described using parameters (Ω) and (k) and (Δσ) and (η) [42-44].

$$\Omega = \sigma_{33} - \sigma_{11} \quad (5)$$

$$\kappa = \frac{-3(\sigma_{iso} - \sigma_{22})}{\Omega} \quad (6)$$

Where (η) is asymmetry parameter, (σiso) chemical shielding isotropy, (Δσ = σaniso) chemical shielding anisotropy, (Ω) span that describes the peak width and (k), skew that describes the peak shape and (δ) is chemical shift anisotropy. The range of asymmetry parameter changes is 0 ≤ η ≤ + 1, for skew is -1 ≤ k ≤ +1 and for span is Ω ≥ 0 [42-44].

and if $|\sigma_{zz} - \sigma_{iso}| \leq |\sigma_{xx} - \sigma_{iso}|$:

$$\mathrm{CSA(ppm)} = \sigma_{aniso} = (\Delta\sigma) = \sigma_{11} - \frac{(\sigma_{22} + \sigma_{33})}{2} \quad (7)$$

$$\delta(\mathrm{ppm}) = \sigma_{11} - \sigma_{iso} \quad (8)$$

$$\eta = \frac{(\sigma_{22} - \sigma_{33})}{\delta} \quad (9)$$

Nuclear magnetic resonance (NMR) parameters of 45 nucleus boron and 45 nucleus nitrogen in armchair BNNT (9, 9) and 45 nucleus Aluminum and 45 nucleus nitrogen in armchair AlNNT (9, 9), both having length of 5 angstrom, were investigated at GIAO method and B3LYP/6-31G* level of theory and the results are shown in Tables 3 and 7.

The calculated chemical shielding isotropic (CSI) parameters in the BNNT and AlNNT nanotubes divide the nucleus into 5 layers in terms of the electrostatic medium. So that in each layer, the CSI values for its nuclei is approximately the same. CSI parameters of all of boron and nitrogen atoms in BNNT into 5 layers are shown in Tables 4 and 5 respectively and CSI parameters of hydrogen atoms of two edge of BNNT are shown in Tables 6. It is significant that the atomic labels of each layer and also two edges are also indicated in three Tables.

Generally, in symmetric locations of the BNNT and AlNNT (Fig. 1), such as (1, 5) or (2, 4) layers, in each pair of layers the atoms nuclei have the same CSI values. For example, in layers 1 and 5, which are exactly at the end of the BN nanotube, boron nuclei have the same electrostatic medium and σiso equal to 81 ppm. Also, in layers 2 and 4 the boron nuclei have σiso equal to 84 ppm. This means that the shielding of boron nuclei in (2, 4) layers are the highest while this is the minimum at the end of the nanotube.

The calculated chemical shielding isotropic (σiso) parameters in the AlNNT nanotube divide the nucleus into 5 layers in terms of the electrostatic medium. Chemical shielding isotropic of aluminum nuclei Checked out and aluminum nuclei are examined in the same way as boron nuclei in the 5 layers form. So that (1, 5) or (2, 4)

Table 2. The values of thermodynamic functions of BNNT and AlNNT in the gas phase.

Thermodynamic functions/ B3LYP/6-31G*		Compounds	
		BNNT (9,9-5)	AlNNT (9,9-5)
kcal/mol	$G+E_{el}$	-2263995.9	-8408078.9
	$H+E_{el}$	-2263899.3	-8407908.8
	$E_{thermal}+E_{el}$	-2263899.9	-8407909.4
	E_0= ZPE+Eel	-2263941.3	-8407980.3
	E_{el}	-2264491.7	-8408360.0
Cal/molK	S	325	570.866

Table 3. NMR parameters of boron and nitrogen nuclei in different layers of BNNT.

NMR parameters of boron nitride nanotube (9,9-5) / ppm							
Layers	nuclei	CSI	CSA= Δσ	δ	η	Ω	κ
Layer 1	^{11}B	81	51	34	0.50	59.46	-0.43
	^{15}N	151	132	-101	0.75	189.51	0.20
Layer 2	^{11}B	84	32	21	0.10	33.81	-0.87
	^{15}N	141	196	131	0.21	210.31	-0.74
Layer 3	^{11}B	83	34	23	0.16	36.50	-0.79
	^{15}N	142	184	123	0.03	186.85	-0.96
Layer 4	^{11}B	84	32	21	0.10	33.80	-0.87
	^{15}N	141	196	131	0.21	210.69	-0.74
Layer 5	^{11}B	81	51	34	0.50	59.46	-0.43
	^{15}N	151	132	-101	0.75	189.46	0.20

pair of layers, the aluminum nuclei have the same CSI values. According Table 7, chemical shielding isotropic of aluminum nuclei in the layer 3 is the highest and equal to (σiso) = 458 ppm.

Chemical shielding isotropic parameters of all of Al and N atoms in AlNNT into 5 layers are shown in Tables 8 and 9 respectively and CSI parameters of hydrogen atoms of two edge of BNNT are shown in Tables 10. It is noteworthy that the atomic labels of each layer and also two edges are also indicated on three Tables.

As we know, the reason for the replacement of the boron nitride nanotubes instead of the carbon nanotubes is that the sum of atomic numbers of boron and nitrogen is equal to the sum of the atomic numbers of the two carbon atoms. But the main difference between boron and nitrogen atoms is the presence of a non-bonded electron pair in the nitrogen valence layer while there is a shortage of electrons in the boron valence layer. And this is the reason why two nuclei behave differently in the boron nitride nanotubes.

Table 4. Chemical shielding isotropic values of boron nucleus in different layers of BNNT.

Chemical shielding isotropic of boron atoms in boron nitride nanotube (9,9-5)									
Layer 1									
Atomic Number	31-B	24-B	11-B	4-B	84-B	71-B	64-B	51-B	44-B
CSI (ppm)	81.824	81.747	81.825	81.709	81.798	81.753	81.786	81.818	81.837
Layer 2									
Atomic Number	25-B	19-B	5-B	39-B	45-B	59-B	65-B	79-B	85-B
CSI (ppm)	84.373	84.409	84.427	84.364	84.397	84.470	84.445	84.486	84.512
Layer 3									
Atomic Number	1-B	80-B	74-B	60-B	54-B	40-B	34-B	20-B	14-B
CSI (ppm)	83.536	83.464	83.473	83.433	83.464	83.574	83.575	83.563	83.598
Layer 4									
Atomic Number	88-B	75-B	68-B	55-B	48-B	35-B	28-B	15-B	8-B
CSI (ppm)	84.527	84.485	84.451	84.464	84.389	84.369	84.375	84.404	84.430
Layer 5									
Atomic Number	9-B	3-B	83-B	69-B	63-B	49-B	43-B	29-B	23-B
CSI (ppm)	81.808	81.701	81.782	81.765	81.789	81.812	81.835	81.823	81.735

Table 5. Chemical shielding isotropic values of nitrogen nucleus in different layers of BNNT

Chemical shielding isotropic of nitrogen atoms in boron nitride nanotube (9,9-5)									
Layer 1									
Atomic Number	32-N	18-N	12-N	90-N	78-N	72-N	58-N	52-N	38-N
CSI (ppm)	151.318	151.302	151.420	151.641	151.504	151.516	151.352	151.329	151.230
Layer 2									
Atomic Number	26-N	13-N	6-N	33-N	46-N	53-N	66-N	73-N	86-N
CSI (ppm)	141.385	141.313	141.266	141.469	141.383	141.435	141.201	141.381	141.208
Layer 3									
Atomic Number	87-N	81-N	67-N	61-N	47-N	41-N	27-N	21-N	7-N
CSI (ppm)	143.122	143.232	143.129	143.041	142.951	142.911	142.977	143.030	143.029
Layer 4									
Atomic Number	2-N	82-N	76-N	62-N	56-N	42-N	36-N	22-N	16-N
CSI (ppm)	141.281	141.252	141.380	141.198	141.411	141.368	141.472	141.377	141.309
Layer 5									
Atomic Number	10-N	89-N	77-N	70-N	57-N	50-N	37-N	30-N	17-N
CSI (ppm)	151.421	151.643	151.471	151.518	151.353	151.331	151.238	151.326	151.307

Table 6. Chemical shielding isotropic values of hydrogen nucleus in two edges of BNNT.

Chemical shielding isotropic of hydrogen atoms in boron nitride nanotube (9,9-5)									
Edge 1									
Atomic Number	92-H	96-H	95-H	98-H	100-H	104-H	103-H	106-H	108-H
CSI (ppm)	26.947	26.905	26.947	26.915	26.938	26.856	26.948	26.894	26.951
Atomic Number	112-H	111-H	114-H	116-H	120-H	119-H	122-H	124-H	126-H
CSI (ppm)	26.883	26.951	26.899	26.95	26.926	26.949	26.916	26.955	26.925
Edge 2									
Atomic Number	91-H	94-H	93-H	97-H	99-H	102-H	101-H	105-H	107-H
CSI (ppm)	26.947	26.906	26.947	26.917	26.937	26.858	26.947	26.896	26.952
Atomic Number	110-H	109-H	113-H	115-H	118-H	117-H	121-H	123-H	125-H
CSI (ppm)	26.884	26.950	26.901	26.957	26.925	26.950	26.912	26.954	26.925

According to the above, the nitrogen nuclei in the (1,5) edge layers have the highest (σiso), while the value of (σiso) is the lowest for boron atoms in the edge layers. And nitrogen nuclei in the (2, 4) layers have the lowest (σiso). This is in contrast to boron nucleus. This refers to the acidic properties of boron atoms and the alkaline properties of nitrogen atoms. In the comparison mode, the layer that chemical shielding of boron nucleus is higher than previous layer, chemical shielding of nitrogen nucleus is lower than previous layer.

CONCLUSIONS

In this research, h-BNNT and h-AlNNT armchair nanotubes with n= 9, m= 9 and length of 5 angstrom and consisting of 27 hexagonal loops were

Table 7. NMR parameters of aluminum and nitrogen nuclei in different layers of AlNNT.

NMR parameters of aluminum nitride nanotube (9,9-5) / ppm							
Layers	nuclei	CSI	CSA= Δσ	δ	η	Ω	κ
Layer 1	^{27}Al	437	51	34	0.31	56	-0.62
	^{15}N	205	54	-45	0.64	81	0.28
Layer 2	^{27}Al	456	37	-39	0.22	64	0.71
	^{15}N	186	31	-28	0.72	47	0.26
Layer 3	^{27}Al	458	46	-46	0.37	75	0.55
	^{15}N	197	40	-25	0.65	53	0.29
Layer 4	^{27}Al	456	37	-39	0.22	64	0.71
	^{15}N	186	31	-28	0.72	47	0.26
Layer 5	^{27}Al	437	51	34	0.31	56	-0.62
	^{15}N	205	54	-45	0.64	81	0.28

Table 8. Chemical shielding isotropic values of aluminum nucleus in different layers of AlNNT.

Chemical shielding isotropic of aluminum atoms in aluminum nitride nanotube (9,9-5)									
Layer 1									
Atomic Number	50-Al	88-Al	85-Al	80-Al	73-Al	68-Al	63-Al	58-Al	55-Al
CSI (ppm)	437.212	437.514	437.012	437.106	436.823	435.798	436.173	436.301	436.507
Layer 2									
Atomic Number	51-Al	47-Al	86-Al	81-Al	76-Al	71-Al	66-Al	62-Al	56-Al
CSI (ppm)	456.312	456.831	457.944	456.356	459.022	457.630	457.087	456.363	456.699
Layer 3									
Atomic Number	48-Al	89-Al	84-Al	79-Al	74-Al	69-Al	64-Al	59-Al	54-Al
CSI (ppm)	458.566	457.343	457.526	458.201	457.548	459.381	460.191	456.923	461.476
Layer 4									
Atomic Number	52-Al	46-Al	87-Al	82-Al	77-Al	72-Al	67-Al	61-Al	57-Al
CSI (ppm)	456.269	456.785	457.915	456.426	459.032	457.603	457.161	456.407	456.715
Layer 5									
Atomic Number	49-Al	90-Al	83-Al	78-Al	75-Al	70-Al	65-Al	60-Al	53-Al
CSI (ppm)	437.191	437.499	437.038	437.107	436.776	435.828	436.155	436.301	436.501

Table 9. Chemical shielding isotropic values of nitrogen nucleus in different layers of AlNNT.

Chemical shielding isotropic of nitrogen atoms in aluminum nitride nanotube (9,9-5)									
Layer 1									
Atomic Number	4-N	8-N	14-N	18-N	24-N	28-N	34-N	38-N	44-N
CSI (ppm)	205.659	206.029	204.995	206.317	204.807	204.814	205.067	205.454	204.876
Layer 2									
Atomic Number	1-N	7-N	11-N	17-N	21-N	27-N	31-N	37-N	41-N
CSI (ppm)	186.597	186.459	187.271	187.623	186.063	187.536	186.724	186.001	187.724
Layer 3									
Atomic Number	3-N	10-N	13-N	20-N	23-N	30-N	33-N	40-N	43-N
CSI (ppm)	197.099	196.479	196.352	196.853	196.792	195.234	196.091	196.759	195.121
Layer 4									
Atomic Number	2-N	6-N	12-N	16-N	22-N	26-N	32-N	36-N	42-N
CSI (ppm)	186.614	186.424	187.248	187.591	186.008	187.428	186.742	185.995	187.738
Layer 5									
Atomic Number	5-N	9-N	15-N	19-N	25-N	29-N	35-N	39-N	45-N
CSI (ppm)	205.619	206.011	204.977	206.371	204.878	204.743	205.033	205.456	204.842

Table 10. Chemical shielding isotropic values of hydrogen nucleus in two edges of AlNNT.

Chemical shielding isotropic of hydrogen atoms in aluminum nitride nanotube (9,9-5)									
Edge 1									
Atomic Number	91-H	112-H	107-H	113-H	105-H	115-H	103-H	117-H	101-H
CSI (ppm)	31.179	26.944	31.115	26.931	31.129	26.939	31.139	26.940	31.078
Atomic Number	119-H	99-H	122-H	97-H	124-H	95-H	125-H	93-H	110-H
CSI (ppm)	26.948	31.112	26.945	31.185	26.943	31.122	26.946	31.181	26.933
Edge 2									
Atomic Number	92-H	109-H	94-H	126-H	96-H	123-H	98-H	121-H	100-H
CSI (ppm)	31.176	26.934	31.177	26.946	31.122	26.943	31.191	26.94	31.114
Atomic Number	120-H	102-H	118-H	104-H	116-H	106-H	114-H	108-H	111-H
CSI (ppm)	26.948	31.072	26.939	31.141	26.940	31.130	26.931	31.112	26.944

selected. Because the presence of B-N and Al-N polar bonds compared to non-polar C-C bonds, these compounds are more suitable for studying the absorption of other compounds. The results of quantum mechanical calculations at B3LYP/6-31G* level show the structural properties and reactivity of boron nitride B45H36N45 and aluminum nitride Al45H36N45 single-wall armchair nanotube. NMR results also confirm the activation and reactivity of the nanotube edges in comparison with the intermediate layers for reaction with electrophilic and nucleophilic molecules. In general, the examination of NMR parameters in different layers shows the non-homogeneous of the electrostatic medium throughout the nanotube, especially on the two edges.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this review article.

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