Journal of Physical and Theoretical Chemistry
of Islamic Azad University of Iran, 13 (2) 185-200: Summer 2016
(J. Phys. Theor. Chem. IAU Iran)
ISSN 1735-2126

The Effect of Aluminum, Gallium, Indium- Doping on the Zigzag (5, 0) Boron-Nitride Nanotubes: DFT, NMR, Vibrational, Thermodynamic Parameters and Electrostatic Potential Map with Electrophilicity Studies

Reza Soleymani*

Young Researchers and Elite Club, Shahre-Rey Branch, Islamic Azad University, Tehran, Iran.

Received June 2016; Accepted September 2016

ABSTRACT

Influence of Aluminum, Gallium, Indium- Doping on the Boron-Nitride Nanotubes (BNNTs) investigated with density functional theory (DFT) and Hartreefock (HF) methods. For this purpose, the chemical shift of difference atomic nucleus was studied using the gauge included atomic orbital (GIAO) approch. In the following, structural parameter values, electrostatic potential, thermodynamic parameters, chemical hardness, chemical potentials, the Maximum amount of electronic charge transfer, electrophilicity and electronegativity for the tittle structure was studied in different states. Our results show that doping of Aluminum, Gallium, Indium atoms to the nanotube surface leading to changesin theIsotropic Chmical Shift, Anisotropic Chemical Shift, also chemical and the rmodynamic parameters will follow the regular process changes.

Keywords: BNNTs; ACS; ICS; Electrostatic potential; NMR

INTRODUCTION

In recent years, there has been an increasing interest in BN, DFT studies. Very soon after explore of CNT structure, semiconducting behaviors were observed for zigzag & armchair BN nanotubes. In 1995, Chopra succeeded to produce single-walled and multi-walled BNNTs by utilizing the process of arc-discharge techniques [1]. However another synthesis method by laser –technique assisted for BNNT is reported by the other researchers [2-4]. More ever, Lourie et al has introduced a method based on pyrolytically grown CNTs as templates to prepare BNNTs, using chemical vapor deposition CVD. Afterward other different processes methods such as arc-melting high temperature chemical reaction, carbon nanotube templates, and laser ablating have been reported for producing boron nitride nanotubes (BNNTs) [5-10]. Addition empirical and experimental studies, researchers were done theoretical studies on the Boron-Nitride Nanotubes (BNNTs) [11]. In 2010, doping influence of siliconand germanium on the Boron-Nitride Nanotubes were studied by Temer S. Ahmadi et al [12] and other researches. However, most studiesby Ehsan Zahedi et al[13] have been shown the effect of NH_3-doping on BN (10, 0)nanotubestructure. The effect of O_2 doping on BNNTs

*Corresponding author: reza.soleymani@hotmail.com

structure have been studied by M. T. Baei et al [14] over thepast two decades othertheoretical and experimentalstudies has been doneonthe BN semiconducting behavior and structure [10]. Boron nitride (BN) is a compound with hexagonal and cubic structures. Hexagonal boron nitride has a layer structure similar to graphite, and also the most stable and softest multi-network boron nitride types, as lubricating oilsoradditives to cosmetics is used. Cube-shaped structure of boron nitride (C-BN) has diamond structure. BNs hardness is less than diamond & thermal stability is more. BN nano network has two-dimensional structure which have composed of BN layers. The structure of hexagonalboron nitrideisharder thancubic structure. Boron nitridenanotube can bethought of wrapping the graphene sheet such as boron nitride network around itself, where the nitrogen and boronatomsre place carbon atoms. These compounds can befor med by single- layer and multi- layer wallsand their structure can be network state. Nano structured ofboron nitride is resistant not only against degradation in a vacuum, air and some fluids but also don't decompose at temperatures above 900 °C. The particular properties of nanotubes consist mechanical properties(Young's modulus) 1.18 TPa, high heat resistance and also theirs emiconductor properties. The boron nitridenanotubes have been utilized for a wide variety of applications ranging from fiber production to manufactures olar cells [15-20]. More ever,these compounds have high resistance too xidation compared with carbon nanotubes. Boron nitridenanotubes structure are similar tocarbon nanotubes (CNT) and it has better field emitter to compare carbon nanotube structures. Theboron-nitride nanotubes have used for Spintronics [21]. Boron nitride is chemically more ineffective than carbon nanotubes, but its electronic properties is lower than adjustable carbon nanotube (CNT) [22-26].

In this paper, density functional theory (DFT) and hartree fock (HF) and two Basis set including 6-31G (d), 6-31G were used to predict several parameters such asstructural, thermodynamic parameters, the values of electrophilicity, electrostatic potential, zigzag BNNT (5, 0) nanotube structure in pure state and when atomsof aluminum, galliumandindium doping to BN structure that were studied with same diameter and length. These calculations can be helped to study this structure and improving their application in various industries.

COMPUTATIONAL DETAILS

The zigzag BNNT (5, 0) Structure preliminary design by Nanotube Modeler software, and theoretical calculations were done in the gas phase, 1 atmospheric pressure and temperature of 298 ° K on the structure by DFT and HF methods. Density functional theory calculation was used by the hybrid exchange-functional B3LYP method and 6-31G (d) standard basis set and also HF calculation was used by 6-31G basis set. All of calculations are carried out by Gaussian 98w package of program [27]. In order that the computer Pentium 4, 1.7 GHz processor with 4 GB of RAM and Windows 7 operating system has been used. More ever, the gauge included atomic orbital (GIAO) method was used to calculate the value of NMR parameters [28 and 29] and calculation of these parameters is performed using this method. Therefore, Eqs. (1) And (2) are used to evaluate the isotropic chemical-shielding (CSI) [30-33] and anisotropic chemical-shielding parameters (CSA) CS tensors in the principal axes system(PAS) ($\sigma_{33}>\sigma_{22}>\sigma_{11}$)

$$CS^{I}(ppm) = (\sigma_{11}+ \sigma_{22}+ \sigma_{33})/3 \quad (1)$$

$$CS^{A}(ppm) = \sigma_{33}- (\sigma_{11}+ \sigma_{22})/2 \quad (2)$$

Electronegativity can be calculated using the HOMO and LUMO results by the following equation:

$$\chi = =-(E_{HOMO}+E_{LUMO})/2 \quad (3)$$

Electrophilicit are calculated by the related values of HOMO and LUMO [34-40].

$$\omega=\mu^2/2\eta=\chi^2/2\eta \quad (4)$$

$$\chi=-\mu=-(\sigma_E/\sigma_N)_{V(r)} \approx(I+A)/2\approx-1/2(\varepsilon_{HOMO}+\varepsilon_{LUMO}) \quad (5)$$

$$\eta=(\sigma_{2E}/\sigma_{N2})_{V(r)} =(I-A)\approx(\varepsilon_{LUMO}-\varepsilon_{HOMO}) \quad (6)$$

$$\Delta N_{max}=-\mu/\eta \quad (7)$$

However, Molekel package of program was used to calculate the electrostatic potential values and GaussSum software was applied to calculate HOMO and LUMO gap and DOS Spectrum [41]. To see related spectrum to vibration parameter have used by Chemcraft package of program.

RESULT AND DISCUSSION

The influence of Aluminum, Gallium, Indium- Doping on the Zigzag BNNT (5, 0) was investigated by DFT method, the hybrid exchange-functional B3LYP level of theory and 6-31G standard basis set that results showed that atoms were effective completely on the structure properties. Using the compounds in various fields such as telecommunications and electrical industries will be much better and more functional if these be done experimentally. The optimization structure with the number of atoms is shown in fig. 1.

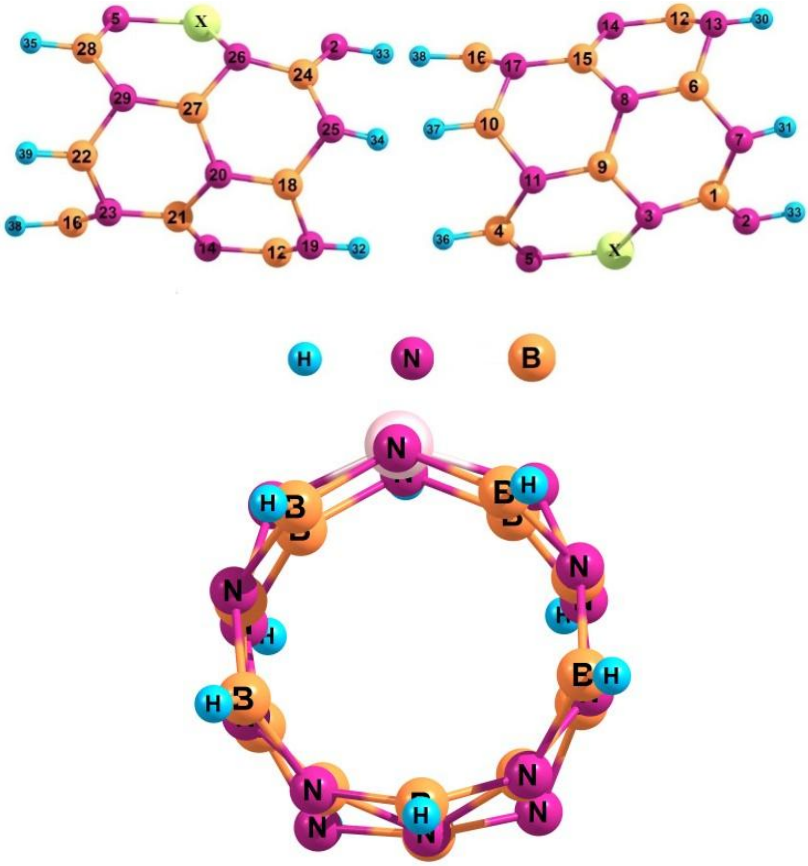


Fig. 1. The different 2D view of the pristine and doped BNNTs in zigzag model of BNNT.

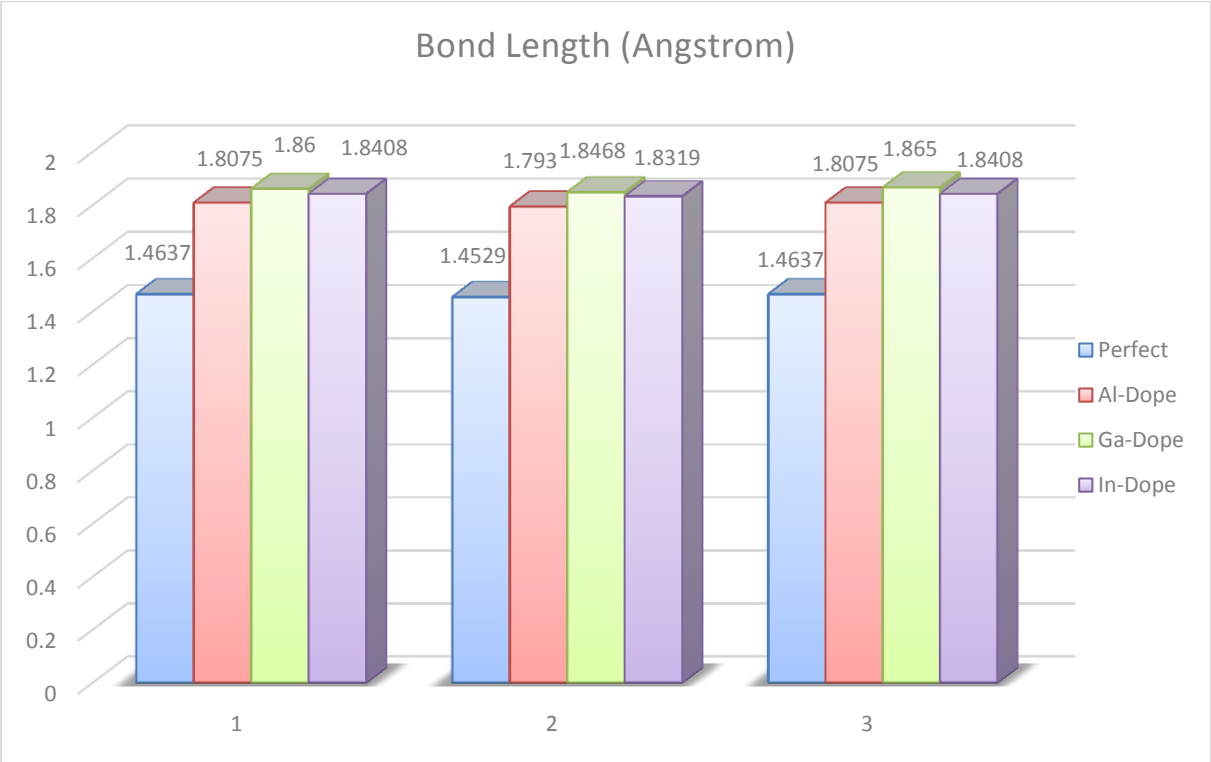
Geometrical parameter

In this section, bond lengths and bond angle were discussed; the unit of them respectively has been reported according to angstrom unit (Å) and base on degree table1. In this table only bond length and bond angles has been studied thataremost affected bydoped atoms. BNNT sstructure in perfect model, Al- Dope, Ga- Dope and In- Dopewere compared with each other. The Numbering of atoms process for studying the length andbondanglesare show ninfigure 1. In fact, inthis study, B30 atoms have replaced with atoms of aluminum, galliumandindium.

3.1.1. Bond length in Zigzag BNNTs

After dopingof aluminum atom instead of boron atom, the most change of bonds will happen when more influence were done by doped atoms that contain X30-N3, X30-N5 and X30-N26 bonds. How the comparing of bonds is shown in figure 2.

The results show that three atoms are affected by doped atoms have significant changes. Process of change can be arranged byelongation Ga- dope> In-dope> Al- dope> Perfect considered (table 1).



1: X30-N3
2: X30-N5
3: X30-N26

Fig. 2. The relationship between X30-N3, X30-N5 and X30-N26 bond lengths in zigzag BNNTs perfect, Al, Ga and In doped.

Table 1. Bond length (angstrom) and bond angle (degree) of perfect and Al, Ga, In- dopingin (5, 0) zigzag model of BNNTs

Method	B3LYP/6-31G (d) for (N, O, B, Al, Ga and H) and LANL2DZ for In			
Bond Length	**Perfect**	**Al Dope**	**Ga Dope**	**In Dope**
X30-N3	1.4637	1.8075	1.8600	1.8408
X30-N5	1.4529	1.7930	1.8468	1.8319
X30-N26	1.4637	1.8075	1.8650	1.8408
N5-B28	1.4616	1.4627	1.4605	1.4295
N5-B4	1.4616	1.4627	1.4605	1.4295
N3-B9	1.4638	1.4571	1.4558	1.4229
N3-B1	1.4524	1.4453	1.4447	1.4270
N26-B24	1.4524	1.4453	1.4447	1.4270
N26-B27	1.4638	1.4571	1.4559	1.4329
Bond Angle				
N26-X30-N5	119.84	114.97	115.35	116.88
N3-X30-N5	119.84	114.97	115.35	116.88
N3-X30-N26	117.60	112.19	110.14	111.74
B9-N3-X30	106.36	105.20	104.06	102.98
B1-N3-X30	116.79	108.46	108.82	109.89
B27-N26-X30	106.36	105.20	104.06	102.98
B24-N26-X30	116.79	108.46	108.82	109.89
B28-N5-X30	116.99	112.53	110.91	110.11
B4-N5-X30	116.99	112.53	110.91	110.11

Studying of other bonds lengthshow B-N bond length will be significant compare the perfect model. The bond of B-N is more changeable than perfect model. In perfect model, Al- doped, Ga- dope, In- dope the B-N is 1.4524 to 1.4638 Angstrom, 1.4453 to 1.4627 Angstrom, 1.4447 to1.4650 Angstrom, 1.4270 to 1.4329 Angstrom respectively. Ahmad Saif et al and Temer S. Ahmadi et al have reportedB-N bond length for zigzag BNNT (10, 0)nanotubes structure 1.45to 1.48 and 1.47 Angstromrespectively [42, 12]. Last work studies indicates any change in the structure ofNanotube that alters structural parameterssuch as length bond [43-45].

Bond Angle in Zigzag BNNTs

The bond angles are the function of doped atoms typeon the surface of boron nitridenanotubes. So that before doping atoms on the surface ofthe nanotube structure in termbond length and bond angle has symmetry and many parts of the structure has asame bond lengthandthe same structure angle. However, E. Zahedi et al [13] has reportedN-B-N angle is variable between 112 to 122 degree and B-N-B angle between 103 to 120 degree. More ever, Temer S. Ahmadi et al has reported N-B-N bond angle is between 116to 120degree and B-N-B bond angle between 118to 120degree for (10, 0) BNNTs structure in perfect model [12]. Addition Ahmad Seif et al, has reported the bond angles of the zigzag BNNT (10, 0) structureare in the range of123degree for B-N-Bangleand N-B-Nangle in the range of 117 degree [42]. All bond angle will undergone many changes bytheeffect of doping different atoms. The range of

variation for the B-N-B angle is between 106.36to116.99degree and for N-B-N angle is in the range of 117.6 to 119. 84 degree that is variable in perfect model. But these angle will be change by Aluminum, Gallium, Indium- doping on the Zigzag (5, 0) Boron-Nitride Nanotubes.

NMR properties

NMR properties were studied by Gauge Independent Atomic Orbital (GIAO) method. Dependent parameter values Nuclear Magnetic Resonance (NMR) includes Chemical Shift Isotropic (CSI) and Chemical Shift Anisotropic (CSA) were investigated and analyzed. First, objective structure is optimized by density functional theory (DFT)method thenthese two parameters were discussed with different atoms doping on the Zigzag (5, 0) Boron-Nitride Nanotubes. The properties and applicationsof these structurescan be studied and compared by studding these characteristics.

ICS parameter

The process of numbering with atoms position are shown in figure 1. BNNTs in perfect model has high symmetry andthis factorcausedthe value of chemical shift of some atoms is equivalent and appears in similar areas. The investigation of E. Zahedi et al [13] shows that therange of CSI for the ^{11}B nuclearin BNNT (10, 0) structure in perfect model appears in 75, 82and85 ppmand whenNH_3- attached, ICS value increase to106 ppm. In some reports the ICS values appearsin the region of 73 and 83 and 84 ppm that these values will change with other doped-atoms.ButE. Zahedi et alhas reported the range of ICS changes for the ^{15}Nnuclear in Perfect model to appear in the area of 112, 144, 147 and 174 ppm and when NH_3 – attach the range will be109 to174 ppm. However, the range of changes for ^{15}N atom is between 104 to 169ppm and for ^{11}B nuclear is between 74to 84ppm that results has reported by Ahmad Seif et al [42]. The position of atoms in the different layer is effective in the value of parameters.This parameter in the zigzag BNNT (5, 0) structure represent the same result. The chemical shift is obtained for ^{15}N nuclear in the range of 90 to 150 ppm in perfect model and for ^{11}B nuclear isin the range of 74 to 78 ppm. When Aluminum, Gallium, Indium- doping on the zigzag (5, 0) Boron-Nitride Nanotubes significant change is observed in layer 2, 3 and 4. Table 2 shows N3, N5, N26 atoms and also B9, B27 atoms are more affected in different chemical environments induced Aluminum, Gallium, Indium- doping on the Boron-Nitride Nanotubes and thus the value of ICS is different from perfect model.

ACS in zigzag (5, 0) BNNTs

Tables 2. And 3 in dicated the values of the ACS for the BNNTs structure same as the ICS value. Because by comparing BNNTs structure and when Aluminum, Gallium, Indium- doping on the Zigzag (5, 0) Boron-Nitride Nanotubes shows that value of chemical shift is changed by doping different atoms on the nanotube structure that more changeable are for atoms in the vicinity of doping atoms. Ehsan Zahedi et al [13] has reported the value of ACS in the range of 32 to 47 ppm for ^{11} B and ^{15}N nuclear between 74 to 232 ppm for the zigzag BNNT (10, 0) structurein perfect model. More ever,Temer S. Ahmadi et alhave reported the value of ACS forsiliconand germanium- doping on the zigzag Boron-Nitride Nanotubes [12]. The N and B atoms are doped by the C and Si and Ge atoms, respectively and the ACS value is variable, for ^{15}N nuclear when carbon atom doped on the nanotube structure the value of ACS is in the range

Table 2. Isotropic Chemical Shift (ppm) values for perfect and Al, Ga, In- doping in (5, 0) zigzag modelof BNNTs

Method		B3LYP/6-31G (d) for (N, O, B, Al, Ga and H) and LANL2DZ for In			
Layer	Labels and Symbol	Isotropic Chemical Shift			
		Perfect	Al Dope	Ga Dope	In Dope
1	B4	74	74	74	73
1	B10	74	74	73	70
1	B16	74	74	74	73
1	B22	74	74	73	70
1	B28	74	74	74	73
		Continued Table 2			
2	N5	90	119	112	125
2	N11	90	80	80	68
2	N17	90	92	92	80
2	N23	90	92	92	80
2	N29	90	80	80	68
3	B9	77	80	81	81
3	B15	77	77	77	76
3	B21	77	77	77	76
3	B27	77	80	81	81
3	X30	77	427	1681	4438
4	N3	126	133	117	139
4	N8	126	125	125	118
4	N14	126	130	131	122
4	N20	126	125	125	118
4	N26	126	133	117	139
5	B24	78	77	76	74
5	B1	78	77	76	74
5	B18	78	79	78	76
5	B6	78	79	78	76
5	B12	78	77	77	76
6	N13	154	156	156	151
6	N2	154	168	164	157
6	N7	154	146	148	140
6	N19	154	156	156	151
6	N25	154	146	148	140

of 74 to 230 ppm and when Si and Ge atoms replaced, the ACS values were between 74 to231 ppmand 74 to 232 ppm respectively. For ^{11}B nuclear, when carbon atom doped on the nanotubestructure the value of ACS was in the range 73 to 84 ppmand when Si and Ge replaced on the structure the values of ACS were between 72 to 85 ppm and 71 to 85 ppm respectively. The value of ACS for ^{15}N and ^{11}B nuclear in the zigzag BNNT (5, 0) structure in perfect model in the range 106 to 222 ppm and 42 to 57 ppm respectively. But Ahmad Seif et al have reported the ACS values for the zigzag BNNT (10, 0) is similar the values of zigzag BNNT (5, 0) structure [42]. Atoms that are closer than doping atoms will have changed by

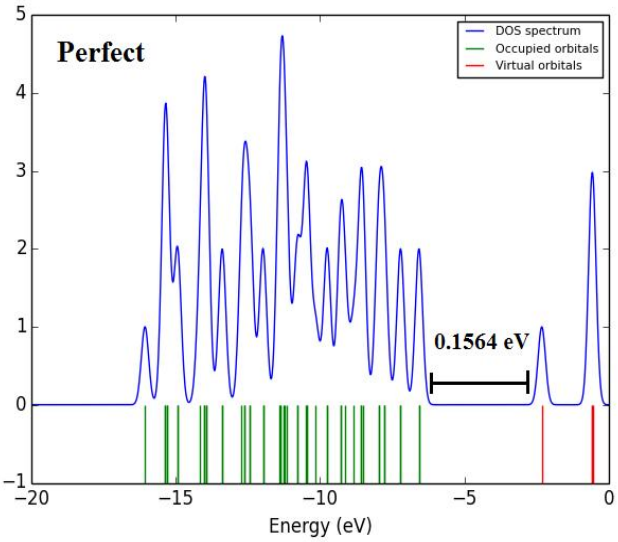
Aluminum, Gallium, Indium- doping on the Boron-Nitride Nanotubes. Table 3 shows N3, N5, N26 atoms and also B9, B27 atoms are more affected in different chemical environments induced Aluminum, Gallium, Indium- doping on the Boron-Nitride Nanotubes thus the value of ACS is different from Perfect model.

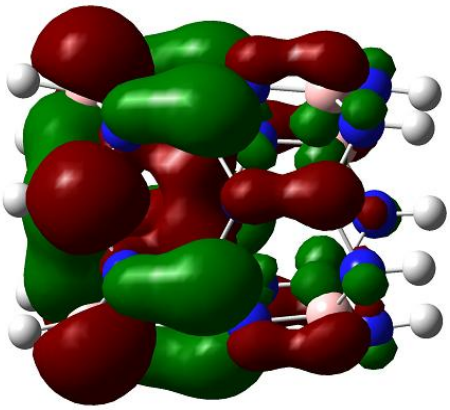
Table 3. Anisotropic Chemical Shift (ppm) values for perfect and Al, Ga, In- doping in (5, 0) zigzag modelof BNNTs

Layer	Method Labels and Symbol	B3LYP/6-31G (d) for (N, O, B, Al, Ga and H) and LANL2DZ for In Anisotropic Chemical Shift			
		Perfect	Al Dope	Ga Dope	In Dope
1	B4	57	56	51	48
1	B10	57	57	37	60
1	B16	57	58	58	59
1	B22	57	57	57	60
1	B28	57	56	51	48
2	N5	222	195	218	281
2	N11	222	222	222	209
2	N17	222	220	220	226
2	N23	222	220	220	226
2	N29	222	222	222	209
3	B9	42	36	35	36
3	B15	42	42	43	43
3	B21	42	42	43	43
3	B27	42	35	35	36
3	X30	42	25	182	355
4	N3	181	142	150	184
4	N8	181	181	179	184
4	N14	181	174	174	181
4	N20	181	181	179	184
4	N26	181	142	150	184
5	B24	44	42	40	38
5	B1	44	42	40	38
5	B18	44	41	41	43
5	B6	44	42	41	43
5	B12	44	43	43	44
6	N13	106	102	102	104
6	N2	106	74	70	70
6	N7	106	112	110	114
6	N19	106	102	102	104
6	N25	106	112	110	114

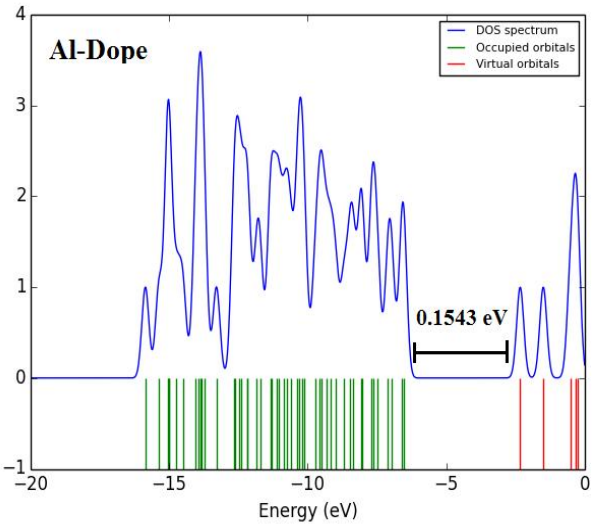
HOMO and LUMO Parameters

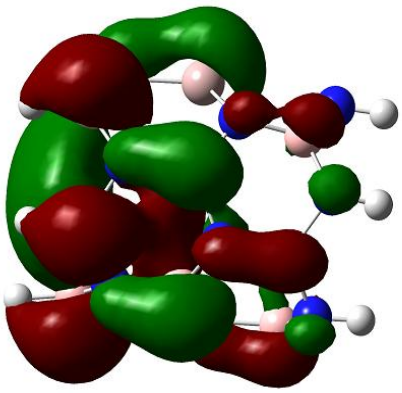
Afteroptimizing the structure by density functional theory at hybrid exchange-functional B3LYP level of theory with 6-31G (d) basis set the value of HOMO and LUMO have been reported for different states to investigate theproperties of the structure and effects onthe chemical properties by doping atoms.Comparing the value of HOMO and LUMO show ninfigure 3.





(a)





(b)

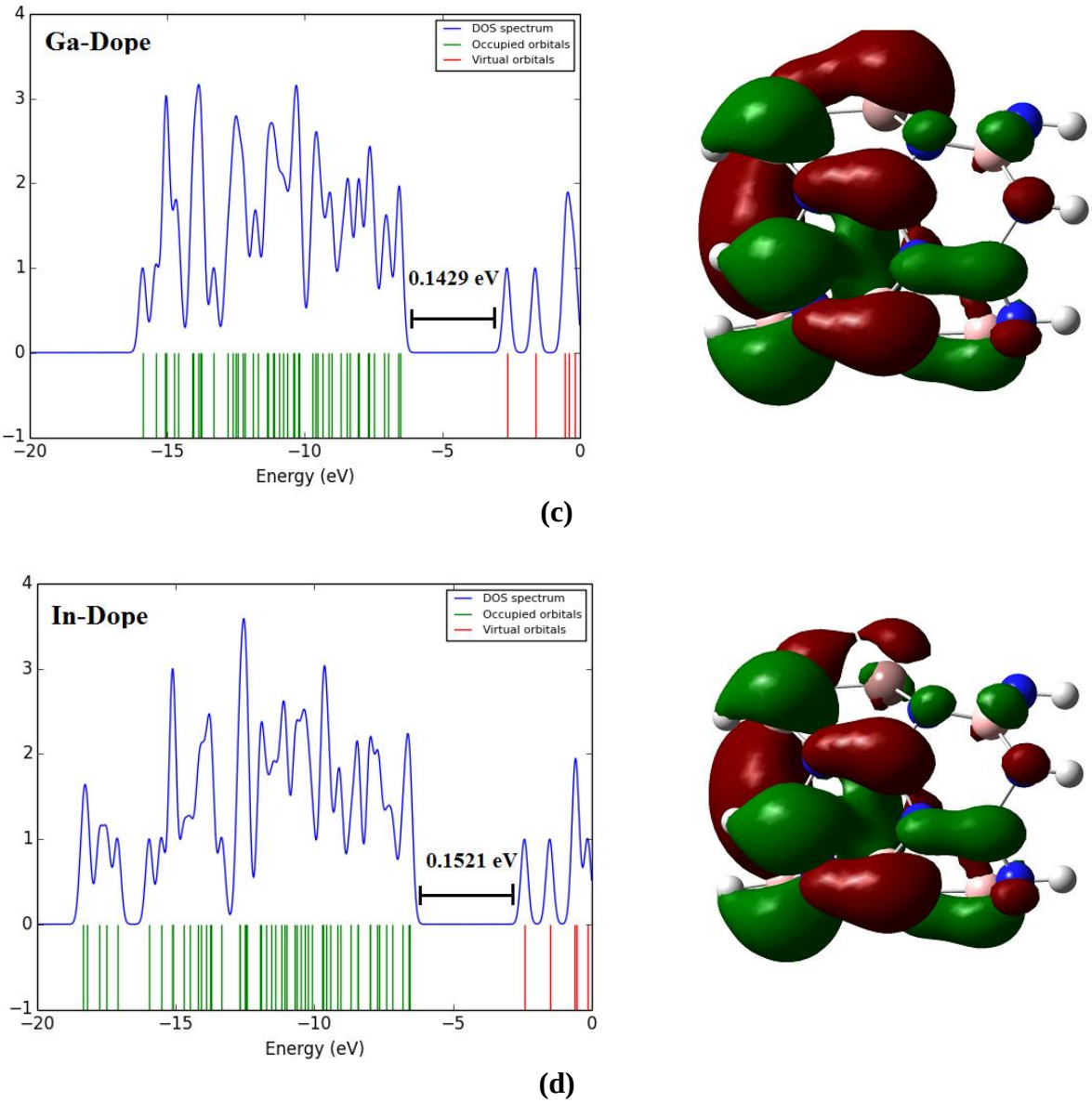


Fig. 3. The view of the DOS spectrum and highlighted HOMO and LUMO orbitals for different zigzag BNNTs perfect (a), Al (b), Ga (c) and In (d) doped.

After computing by density functional theory the results shown in table 4. The trend ofincrease in electrophilicity infour different models areGa- dope> In- dope> Al- dope> Perfectthat results showdoping atoms on the nanotubes surface areassociatedwith an increasing inthe amount electrophilicity. Thistrendisexactly the opposite for chemical hardness values and will followthe reverse process. But the increase inchemical potential will beforAl-dope> Perfect>In- dope> Ga- dope. Different results for this structure in Perfect model and when thedifferent atoms dopedon thezigzag BNNT (5, 0)structure can bestudied by usingHOMO and LUMOGAP. Density-Of-States (DOS) spectra calculated fordifferent modesand shown in figure3. The increasing of HOMO and LUMO GAP is obtained for

four structure for Perfect model> Al-dope> In- dope> Ga- dope. In addition, highlighted HOMO and LUMO orbitals is shown that these results indicatethat Aluminum, Gallium, Indium- doping on the Zigzag BNNTs the forms of HOMO and LUMO orbitals and independent parameters orbitalparametersaredependent on thehybridchange.

Thermodynamic Parameters

Hartree – Fuck method and 6-31 Gbasis set was used for studying thermodynamic parameters. The resultsarereportedinTable 5. The resultsindicatethattheAluminum, Gallium, Indium- doping on the Zigzag BNNT schange all the thermodynamic parameters of structure. But perhaps the significant parameters is the total energylevels in thistable that themore negative will bethe stable structure. This compares with electrone nergy by density functional theory isgiven in table 5, that shows the doping atoms in the nanotube structure havemore stable (-4299794.515 Kcal/ mol) tocompared theother states.

Table 4. Electronic energy (Kcal/mol), dipole moment (Debye), molecular orbitals energies (εHOMO and εLUMO, eV), electronic chemical potential, μ (eV), chemical hardness, η (eV), electrophilicity, ω (eV) and maximum amount of electronic charge transfer for perfect and Al, Ga, In- doping in (5, 0) zigzag model of BNNTs

Method	**B3LYP/6-31G (d) for (N, O, B, Al, Ga and H) and LANL2DZ for In**			
Structure	**Perfect**	**Al Dope**	**Ga Dope**	**In Dope**
E_{ele}	-753882.2368	-890406.3645	-1944912.4660	-4306013.4260
Dipole moment	6.1629	6.8027	6.5482	6.5884
HOMO	-0.2415	-0.2398	-0.2402	-0.2412
LUMO	-0.0851	-0.0855	-0.0973	-0.0891
Chemical potential(μ)	-0.1633	-0.1627	-0.1688	-0.1651
Chemical hardness(η)	0.1563	0.1543	0.1429	0.1521
Electrophilicity(ω)	0.0853	0.0857	0.0997	0.0896
ΔN_{max}	1.0448	1.0544	1.1814	1.0859
HOMO-LUMO Gap	0.1564	0.1543	0.1429	0.1521
Electronegativity	0.1633	0.1627	0.1688	0.1651

Table 5. Thermal energy (Kcal/Mol), Heat capacity (Cal/Mo-Kelvin), Entropy (Cal/Mol-Kelvin), Total energy (Kcal/Mol), ZPVE (Kcal/Mol), Rotational constant(GHZ) for perfect and Al, Ga, In- doping in (5, 0) zigzag model of BNNTs

Method	**HF/6-31G for (N, O, B, Al, Ga and H) and LANL2DZ for In**			
Structure	**Perfect**	**Al Dope**	**Ga Dope**	**In Dope**
E (Thermal)	189.395	186.490	185.947	187.390
Heat capacity	75.365	78.697	79.733	79.443
Entropy				
Total	120.535	124.938	127.522	134.363
Translational	43.738	43.860	44.156	44.450
Rotational	34.227	34.416	34.628	34.740
Vibrational	42.569	46.663	48.738	55.173
Total energy	-748874.9735	-885167.8494	-1938933.192	-4299794.515
ZPVE	179.43262	175.86918	175.04241	176.00890
Rotational constant	0.30230	0.27939	0.25300	0.24366
	0.23421	0.22936	0.22391	0.21684
	0.23404	0.21386	0.19552	0.18722
Molecular mass	385.26394	401.23618	443.18022	489.15873

Doping different atoms on the nanotube surface is causing the significant change of vibrating parameter. As figure 4 shows the replacing bromine atom instead of Gallium, Aluminum and Indium atoms. The intensity and vibration parameters in different areas to be altered that represented the effect of doped atoms on the lengths and bond order.

Molecular Electrostatic Potential Map

The electrostatic potential represents charge distribution in the chemical structure and it is three-dimensional. In fact, this map enables readers to investigation charge distribution and prediction the behavior of atoms in chemical reactions in the different chemical structure [34]. Blue color represent the highest potential electrostatic of charge distribution and red color represent that it is lowest electrostatic potential. The average of parameters is shown yellow color. To measure electrostatic potential in the BNNT structure, first, relative structures optimized by density functional theory DFT at B3LYP and 6-31G (d) basis set and then the values of electrostatic potential was exanimated by Molekel package of program. All the relevant maps in three different states shown in figure 5.

As figure 5 shows when the structure is in perfect model the electrostatic potential is much more negative and appear in red color around the bromine atoms. However doping aluminum on BNNTstructure this section is almost green. The average of electrostatic potential appear on the surface of the nanotubes structure. After doping gallium on the BNNT structure, its area appears in yellow color that represented the values of negative electrostatic potential. But the most interesting part is when vanadium doping on nanotube structure surface. In this section vanadium causes the electrostatic potential completely has been blue and the electrostatic potential is negative.

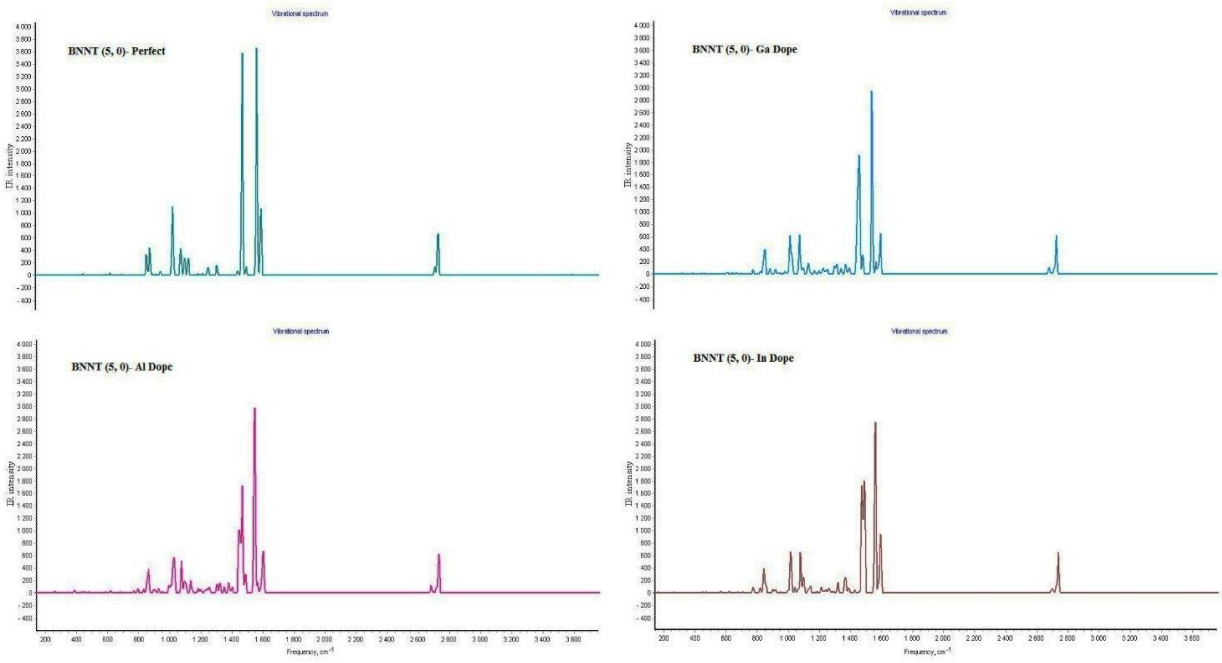


Fig. 4. The show of the vibrational spectrum for different zigzag BNNTs perfect (a), Al (b), Ga (c) and In (d) doped.

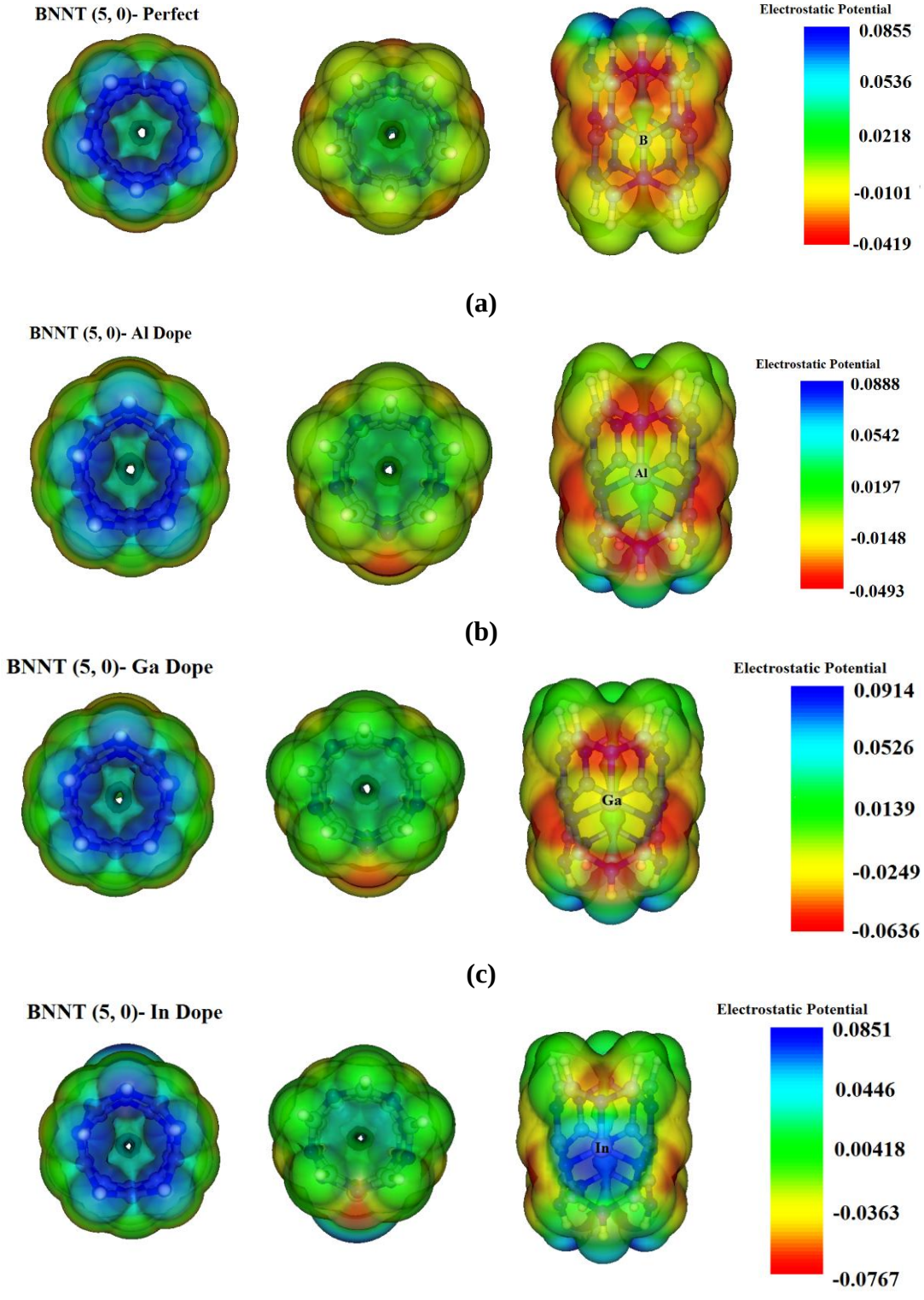


Fig 5. The view of the electrostatic potential maps for different zigzag BNNTs perfect (a), Al (b), Ga (c) and In (d) doped.

CONCLUSION

Four different states of zigzag BNNT (5, 0) structure to 8 Angstroms in Perfect model, and when Aluminum, Gallium, Indium-doping on the Zigzag (5, 0) BNNTs were discussed by density functional theory (DFT) at B3LYP level of theory and hartree fock (HF) method with 6-31 G(d), 6-31G basis set. The results showed that doping of Aluminum, Gallium, Indium atoms instead of boron atom to the nanotube surface change some structural parameter values, electrostatic potential, thermodynamic parameters, chemical hardness, chemical potentials, the maximum amount of electronic charge transfer, electrophilicity, electronegativity and dependent value of HOMO and LUMO. Atoms, bond length and bond angle that are closer to the doping atoms will have more affected and more changes and also stability process has been increased by doping different atoms on BNNT structure. Moreover doping atoms alter the electrical and chemical properties of BNNT structure that this change effects on the performance of boron nitride nanotubes structure. In fact, it can be expected. Doping atoms on the nanotube surface change and improve the application and properties of nanotubes as semiconductor compounds, resistant compounds to mechanical changes, degradation-resistant compounds, compounds used in fiber and also compound used in construction of solar panels.

ACKNOWLEDGEMENTS

This work was supported by Islamic Azad University Shahre-rey and Islamic Azad University Science and Research branch.

REFERENCES

[1] N. G. Chopra, R. J. Luyken, K. Cherrey et al., *Science*, 269 (1995) 966.
[2] D. Golberg, Y. Bando, M. Eremets, K. Takemura, K. Kurashima, and H. Yusa, Applied Physics Letters, 69 (1996) 2045.
[3] D. Goldberg, Y. Bando, M. Eremets1, K. Takemura, K. Kurashima, K. Tamiya, H. Yusa, Chemical Physics Letters, 279 (1997) 191.
[4] O. R. Lourie, C. R. Jones, B. M. Bartlett, P. C. Gibbons, R. S. Ruoff, and W. E. Buhro, Chemistry of Materials, 12 (2000) 1808.
[5] V. Nirmala, P. Kolandaivel, J. Mol. Struct. (THEOCHEM), 817 (2007) 137.
[6] A. Rubio, J. L. Corkill, L. Cohen, Phys. Rev. B, 21 (1994) 5081.
[7] T. Hirano, T. Oku, K. Sugannuma, Diamond Relat. Mater, 9 (2000) 625.
[8] R. Ma, Y. Bando, T. Sato, Chem. Phys. Lett, 337 (2001) 61.
[9] W. Han, Y. Bando, K. Kurashima, T. Sato, Appl. Phys. Lett, 73 (1998) 3085.
[10] S. Kalay, Z. Yilmaz, O. Sen, M. Emanet, E. Kazanc and M. Çulha, Beilstein J. Nanotechnol, 6 (2015) 84.
[11] R. Soleymani, M. K. C. Ali, N. Niakan, Oriental Journal of Chemistry, 28 (2012) 815.
[12] T. S. Ahmadi, A. Seif, G. M. Rozbahani, Arabian Journal of Chemistry, 3 (2010) 121.
[13] E. Zahedi, A. Bodaghi, A. Seif, A, Boshra, Superlattices and Microstructures, 49 (2011) 169.
[14] M. T. Baei, F. Kaveh, P. Torabi, S.Z.S. Alangi, E-Journal of Chemistry, 8 (2011) 609.
[15] R. Haubner, M. Wilhelm, R. Weissenbacher, B. Lux, High Performance Non-Oxide Ceramics II, Series Structure and Bonding, vol. 102, Springer/Heidelberg, Berlin/New

York, (2002).
[16] P.B. Mirkarimi, K.F. McCarty, D.L. Medlin, Mater. Sci. Eng. R, 21 (1997) 47.
[17] X. Blase, A. Rubio, S.G. Louie, M.L. Cohen, Europhys. Lett, 28 (1994) 335.
[18] A. Loiseau, F. Willaime, N. Demoncy, G. Hug, H. Pascard, Phys. Rev. Lett, 76 (1996) 4737.
[19] E. Bengu, L.D. Marks, Phys. Rev. Lett, 86 (2001) 2385.
[20] V. Nirmala, P. Kolandaivel, J. Mol. Struct. (THEOCHEM), 817 (2007) 137.
[21] K. B. Dhungana, R. Pati, Sensors, 14 (2014) 17655.
[22] C. Tang, Y. Bando, Y. Huang, Sh. Yue, C. Gu, F. F. Xu, and Dmitri Golberg, Journal of the American Chemical Society, 127 (2005) 6552.
[23] Y. Chen, L. T. Chadderton, J. F. Gerald, and J. S. Williams, Applied Physics Letters, 74 (1999) 2960.
[24] G. Leichtfried *et al.* "13.5 Properties of diamond and cubic boron nitride". In P. Beiss et al. Landolt-Börnstein-Group VIII Advanced Materials and Technologies: Powder Metallurgy Data. Refractory, Hard and Intermetallic Materials. 2A2. Berlin: Springer. pp. 118 (2002).
[25] J.H. Lan, J. Sh. Wang, Ch. K. Gan, and S. K. Chin, Physical Review B, 79 (2009) 115401.
[26] J. Hu, X. Ruan, Y.P. Chen, Nano Letters, 9 (2009) 2730.
[27] T. Ouyang, Y. Chen, Y. Xie, K. Yang, Z. Bao, J. Zhong, Nanotechnology, 21 (2010) 245701.
[28] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochter ski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian 03 Revision C.02, Gaussian Inc., Pittsburgh, PA, (1998).
[29] R.S. Drago, Physical Methods for Chemists, second ed, Saunders College Publishing, Florida, (1992).
[30] U. Haeberlen, in: J.S. Waugh (Ed.), Advances in Magnetic Resonance, Academic Press, New York, (1976).
[31] R. Dennington, T. Keith, J. Millam, K. Eppinnett, W.L. Hovell, R. Gilliland, GaussView, Version 3.07, Semichem, Inc., Shawnee Mission, KS, (2003).
[32] K. Wolinski, J.F. Hinton, P. Pulay, J. Am. Chem. Soc , 112 (1990) 8251.
[33] F.J. London, Phys. Radium, 8 (1937) 397.
[34] R. Ditchfield, Mol. Phys, 27 (1974) 789.
[35] R. Soleymani, Y. Mohammad Salehi, T. Yousofzad, M. Karimi-Cheshmeh Ali, Oriental Journal of Chemistry, 28 (2012) 627.
[36] R. Soleymani, S.F. Madan, Kh. G. Konandeh, Oriental Journal of Chemistry, 28 (2012) 703.

[37] [E. Fereyduni, M. Kamaee, R. Soleymani, R. Ahmadi, Journal of Theoretical and Computational Chemistry, 11 (2012) 1331.
[38] R. Ahmadi, R. Soleymani, T. Yousofzad, Oriental Journal of Chemistry, 28 (2012) 773.
[39] R. Soleymani, R. D. Dijvejin, A. F. Gozal Abad Hesa, 28 (2012) 1107.
[40] R. Soleymani, H. Rajabzadeh, Asian Journal of Chemistry, 24 (2012) 4614.
[41] R. Ahmadi, R. Soleymani, Oriental Journal of Chemistry, 30 (2014) 57.
[42] N.M. O'Boyle, A.L. Tenderholt and K.M. Langner. J. Comp. Chem, 29 (2008) 839.
[43] A. Seif, A. Boshra, Journal of Molecular Structure: THEOCHEM, 895 (2009) 96.
[44] A. Seif, A. Boshra, M. Seif, Journal of Molecular Structure: THEOCHEM, 895 (2009) 82.
[45] E. Chigo Anota, M. Salazar Villanueva, D. García Toral, L. Tepech Carrillo, M. del Rosario Melchor Martínez, Superlattices and Microstructures, 89 (2016) 319.
[46] S. Arshadi, A. Asghari, H. Raheimi, S. Abedini, Journal of Chemistry, 2013 (2013) 1.