

Adsorption ^{17}O , ^{15}N and CO molecules on the surface of SWCNT: A Computational NMR study

A.S. Ghasemi^{1,*}, F. Aashrafi¹

Dept. of Chem. Payame Noor University, Farhang Av., 15Khordad St.,
 Sari, Iran. Tel.: +98 9111570503; Fax: +98 1513258960;

*Corres.author : ashraf.ghasemi@gmail.com

Abstract: The results of adsorption of several gaseous molecules as nitrogen, oxygen and carbon monoxide, on external surface of H-capped zigzag (5, 0) semiconducting single-walled carbon nanotube (SWCNT) was studied, using density functional theory (DFT) calculations. Geometric optimizations were carried out at B3LYP/6-311G*level of theory using Gaussian 98 program. Structural models are optimized and adsorption energies are obtained to investigate the nuclear magnetic resonance (NMR) parameters for (N_2 -SWCNT), (O_2 -SWCNT) and (CO-SWCNT) model of zigzag (5, 0) SWCNT. The chemical-shielding (σ_{ii}) tensors were converted to isotropic chemical-shielding (σ_{iso}) and anisotropic chemical-shielding (σ_{aniso}) and asymmetrical (μ_i) parameters of ^{13}C , ^{15}N and ^{17}O nucleus for the optimized structures. NMR calculations were evinced that ^{13}C chemical shielding zigzag (5,0) external surface is more sensitive to nitrogen, oxygen and carbon monoxide molecules adsorption compared to zigzag (5,0) nanotube. However, NMR parameters vary with the tube diameter.

Keywords: single-walled carbon nanotube, DFT, NMR, chemical-shielding.

Introduction

Discovered carbon nanotubes, by Iijima in 1991, are members of the fullerene family¹⁻⁴. The study of the gas adsorption on SWCNT is nowadays the centre of interesting theoretical studies. Considering that the gases adsorption on SWCNT modifies sensibly of their electronic properties have proposed the use of SWCNT as gas sensors⁵⁻¹⁰. The adsorption behavior of gas molecules external surface of SWCNT has been studied extensively in the past decade by theoretical calculation¹¹⁻¹³. Reported the calculation results of to ^{13}C , ^{15}N and ^{17}O molecules attached external surface of SWCNT by density functional theory (DFT) based on B3LYP/6-311G*level and GIAO method and found that the interaction between nitrogen, oxygen and carbon monoxide molecules and SWCNT caused vigorous changes in the

electrical resistivity of SWCNTs and thus could be used to detect gas molecules. Because the derived well defined one dimensional structure of SWCNT has distinctive properties in mechanical, chemical and electronic aspects. Nuclear magnetic resonance (NMR) spectroscopy is among the most versatile techniques to study the electronic structure properties of matters¹⁴⁻¹⁶. The chemical-shielding (σ_{ii}) tensors originating at the sites of half-spin nuclei, magnetic nuclei, reveal important trends about the electronic properties at the sites of these nuclei. The (σ_{ii}) tensors are either measured experimentally or reliably reproduced by high-level quantum chemical calculations¹⁷.

Chemical shielding (σ_{ii}) tensors originating the sites of these nuclei are measured trusty, produced by high-level quantum chemical calculations. Band structure calculations, using

different quantum mechanical and semi-empirical methods have predicted electronic transport properties of SWCNT¹⁸. Interactions between nitrogen, oxygen and carbon monoxide molecules and SWCNT have been signified in modifying the intrinsic SWCNT electronic band gap. The tip gate changes the potential of localized defect states, so that the defect energy levels move in and out of resonance with the nanotube Fermi level¹⁹⁻²¹. There is a considerable anisotropy in structure of graphite. Such anisotropy in properties, particularly in electrical properties, can be wholly advantageous²²⁻²⁴. In connection with the size of the nanotube, it is useful mentioning at this stage that as will be seen from the studies verified in later sections, many computational studies involving standard nanotube have focused on the use of zigzag(5,0) nanotube, having a length and diameter of 7.09 Å and 4.17 Å, respectively.

Computational Method

In the present study, we investigate the effects of nitrogen, oxygen and carbon monoxide molecules adsorption on surface SWCNT of zigzag (5, 0). In order to investigate the electronic structure at the semiconductor SWCNT contacts of nitrogen, oxygen and carbon monoxide molecules, the computations were fully executed by Gaussian 98 Software package. Geometric optimizations were performed using 6-311G* basis set with DFT/B3LYP functional²⁵.

NMR ¹³C, ¹⁵N and ¹⁷O chemical shielding calculations were computed at B3LYP/6-311G* level of theory using gauge including atomic orbitals (GIAO) approach. The modeled zigzag (5, 0) consisted of 50 C atom with length of 7.09 Å was chosen for the purpose. In absence of periodic boundary conditions in molecular calculations, it is necessary to saturate the carbon dangling bonds with hydrogen atoms. Curvature of small tubes is a crucial characteristic responsible for intense interaction of atoms in tubes. Quantum chemical calculated tensors at the principal axes system (PAS) (\dagger_{11} \dagger_{22} \dagger_{33}) is converted to a diagonal matrix with \dagger_{11} , \dagger_{22} and \dagger_{33} components, measurable NMR parameters, chemical shielding isotropic (\dagger_{iso}) and chemical shielding anisotropic ($\Delta\dagger$) and asymmetrical (μ_j) using, respectively²⁶⁻²⁹. This shows a second order change in molecular energy, as was indicated in following equation.

$$E = E_0 + B_0 \dagger B_0 + \sum_{i=1}^N \mu_i \dagger B_0 + \dots \quad (1)$$

The summation is taken over the N nucleus in the system. We are not interested in the magnetic susceptibility, thus we have following equation³⁰⁻³²:

$$\dagger_{ij} = \left(\frac{\partial^2 E}{\partial B_i \partial B_j} \right)_{B_i = B_j = 0} \quad (2)$$

Where μ_j and B_i is the components of magnetic moment and external magnetic field, respectively.

The principal components for specification of shielding are defined by this coordinate system as following equations.

$$\dagger_{iso} = \frac{(\dagger_{11} + \dagger_{22} + \dagger_{33})}{3} \quad (3)$$

$$\Delta\dagger = \frac{3}{2}(\dagger_{33} - \dagger_{iso}) \quad (4)$$

$$y_{\dagger} = \frac{3}{2} \left(\frac{\dagger_{22} - \dagger_{11}}{\Delta\dagger} \right) \quad (5)$$

Where \dagger_{iso} , $\Delta\dagger$ and μ_j are isotropic, anisotropic and asymmetric parts of tensor, respectively and in certain cases vanishes³³⁻³⁵.

Results and Discussion

In present work, model of zigzag (5, 0) SWCNT with specified tube lengths are studied using quantum chemical calculations (fig1- 4). Chemical shielding model of zigzag (5, 0) SWCNT interacted with oxygen, nitrogen and carbon monoxide molecules were obtained. The calculated geometric parameters ¹³C, ¹⁵N and ¹⁷O nucleus chemical shielding are presented in Table. In the following sections, molecular geometries and NMR chemical shielding, adsorptions are discussed, separately.

The adsorption ¹⁷O, ¹⁵N and CO NMR parameter modeled of zigzag (5, 0) on external surface

Table exhibits the calculated ¹³C chemical shielding tensors for SWCNT. Nitrogen, oxygen and carbon monoxide molecules adsorption on external surface of SWCNT has a significant influence on ¹³C NMR tensors, which is in complete accordance with the facts mentioned above previously³⁷⁻³⁹. Consequently, it has been ¹⁷O, ¹⁵N and CO indicated that for the H-capped SWCNT, the calculated ¹³C chemical shielding values adsorption are different on the surface, if the carbon is directly bound to hydrogen, unless, it is larger⁴⁰⁻⁴³. To assess the dependence of

NMR results on carbon atom position, ^{13}C chemical shielding isotropy values of zigzag (5, 0) SWCNT have calculated on surface ^{15}N and ^{17}O of ^{13}C adsorption (Fig1- 4). Two different parts of surface tube axis are considered. Interesting surface are evidenced: for zigzag (5, 0) SWCNT, the isotropy adsorption SWCNT (5, 0) - CO (A_1) shielding tensor are larger compared to the adsorption ^{15}N and ^{17}O at the surface. It is also show that the chemical shielding components converge in a way similar to that of the chemical shifts when increasing the tube length even though not as smoothly as the isotropic shielding. Chemical shielding tensors and chemical shifts are efficient parameters for characterization of single walled carbon nanotubes. Calculation of these shielding tensors for oxygen and nitrogen carbon monoxide nucleus reveals that increasing length and diameter of zigzag (5, 0) SWCNT chemical shielding will cause oxygen, nitrogen and carbon monoxide nucleus converge on the single walled nano tube surface the results are consistent with strong interaction adsorption between the tube and carbon monoxide molecules in SWCNT (5,0) - CO(A_1) . This is consistent with previous results derived from band structure; calculations ⁴⁴. On the other hand, the calculated ^{17}O , ^{15}N and CO chemical shielding values in the middle of the surface zigzag (5, 0) SWCNT seem close to the values -93.43-102.48 ppm, 76.26-105.22. ppm and 67.55-115.96 ppm, respectively (Table). More recently, it is indicated that introduction of CO atoms is theoretically predicted to give rise to chiral current flow along the nanotube due to symmetry breaking. The results deduced from comparison of sites (A_1 and A_2), show that the carbon atoms included in oxygen and nitrogen and carbon monoxide molecular adsorption become more shielded. Among the six NMR principal components, intermediate shielding

component, σ_{22} , shows more change from SWCNT compared with surface the for N_2 -SWCNT, O_2 -SWCNT and CO-SWCNT systems. The interest of oxygen, nitrogen and carbon monoxide SWCNT in terms of application is the control of the type of charge carriers within the SWCNT. O_2 -SWCNT, N_2 -SWCNT and CO-SWCNT should show significant advantages over SWCNT for gas sensor applications, due to their reactive tube surfaces and the sensitivity of their transport characteristics in relation with the presence, distribution and chemistry of carbon monoxide. Peng et al (2003) first suggested O_2 -SWCNT, N_2 -SWCNT and CO-SWCNT for use in gas sensors, due to the ability of doped molecular oxygen, nitrogen and carbon monoxide to bind to incoming gas species. The molecular oxygen, nitrogen and carbon monoxide in the SWCNT can be seen as regular defects which change the adsorption behavior of the SWCNT.

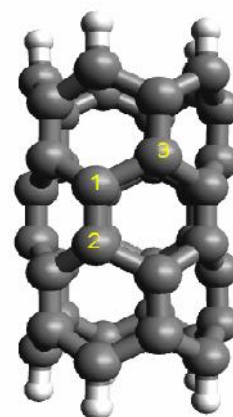


Fig. 1. Carbon nanotube zigzag (5,0) model.

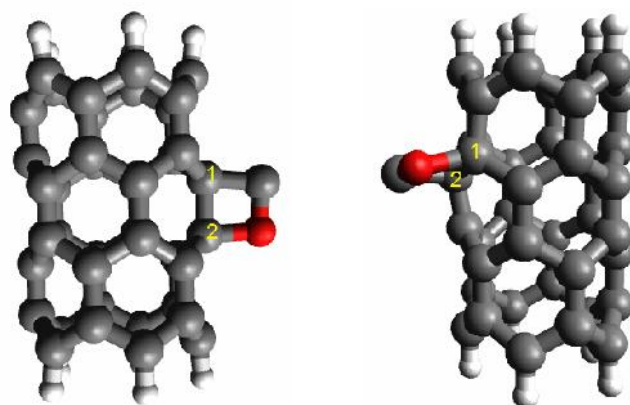


Fig. 2. CO molecule Adsorption on external surface of SWCNT of zigzag (5,0).

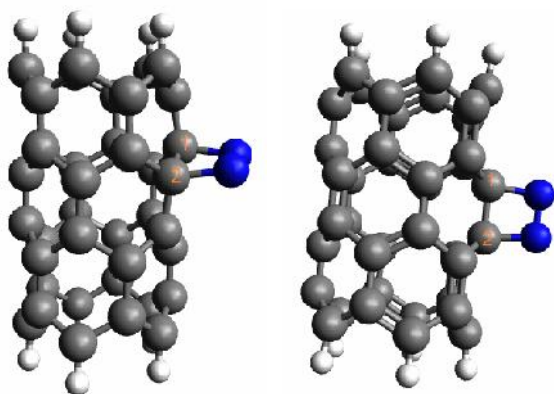


Fig. 3. N₂ molecule Adsorption on external surface of SWCNT of zigzag (5, 0).

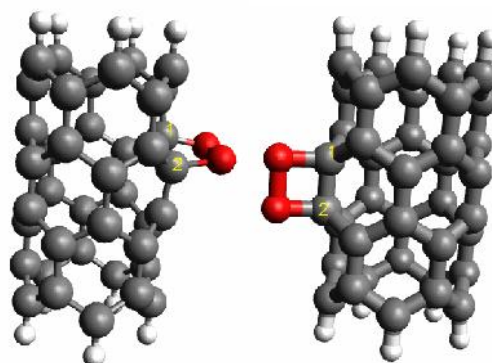


Fig. 4. O₂ molecule Adsorption on external surface of SWCNT of zigzag (5, 0).

Table: Calculated of chemical shielding and chemical shift tensors adsorption on the surface ¹⁵N, ¹⁷O and ¹³C parameters for CNT(5,0), CNT(5,0)–N₂, CNT(5,0)–O₂ and CNT(5,0)–CO system

Model	atoms	σ_{ii} (σ_{11} , σ_{22} , σ_{33}) ^b	σ_{iso}	$\Delta \sigma$	χ_T
CNT(5,0) (A)	C ₁	(27.4749; 155.3869; 319.6152)	149.1757	255.6593	1.0729
	C ₂	(-27.4737; 155.3875; 319.5851)	149.1663	255.6282	1.0730
	C ₃	(-166.2046; -4.1528; 153.1572)	-5.7334	238.3359	1.0199
CNT(5,0)-O ₂ (A ₁)	C ₁	(74.4312; 77.7044; 155.3112)	102.4823	79.2434	0.0620
	C ₂	(74.6323; 77.7154; 155.0228)	102.4568	79.2720	0.0637
CNT(5,0)-O ₂ (A ₂)	C ₁	(42.8507; 97.3469; 149.1738)	96.4571	79.0751	1.0338
	C ₂	(47.6078; 104.8761; 127.8227)	93.4355	51.5808	1.6654
CNT(5,0)-N ₂ (A ₁)	C ₁	(76.1071; 96.5323; 143.1071)	105.2245	56.8239	0.5411
	C ₂	(76.0659; 96.4950; 143.0751)	105.2120	56.7946	0.5396
CNT(5,0)-N ₂ (A ₂)	C ₁	(48.7700; 48.7700; 127.2600)	74.9305	78.4943	0.0000
	C ₂	(34.5201; 76.2487; 118.0313)	76.2667	62.6469	0.9991
CNT(5,0)-CO (A ₁)	C ₁	(69.6682; 130.0992; 148.1219)	115.9631	48.2382	1.8791
	C ₂	(40.6302; 72.3319; 147.0129)	86.6583	90.5319	0.5253
CNT(5,0)-CO (A ₂)	C ₁	(25.1718; 49.1976; 128.3019)	67.5571	91.1172	0.3955
	C ₂	(31.4237; 105.0031; 124.8031)	87.0766	56.5898	1.9503

^a Calculated σ_{ii} , σ_{iso} values in ppm

^b In each row, the first number is for σ_{11} , the second number is for σ_{22} , and the third number is for

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Conclusion

We have presented a systematic computational study on molecular oxygen, nitrogen and carbon monoxide interactions of SWCNT structure. Conformation and a quantum-

chemical calculation by the GIAO calculations at the B3LYP/6-311G* level using DFT optimized geometries provided isotropic shielding tensors that correlated well with the observed chemical

shift data. . The calculated NMR tensors at the sites of ^{13}C , ^{17}O and ^{15}N nucleus tensors in zigzag SWCNT (5, 0) model, put on evidence that isotropy of adsorption CO nucleus shielding tensor are larger at the surface compared to adsorption ^{17}O and ^{15}N nucleus. Calculation of chemical shielding tensors and chemical shifts for oxygen, nitrogen and carbon monoxide nucleus reveals that increasing length and diameter of SWCNT (5, 0) chemical shielding will cause oxygen, nitrogen and carbon monoxide nucleus on the single walled nanotube surface. The results are consistent with strong interaction adsorption

between the tube and CO molecules in SWCNT (5, 0) - CO(A₁). The results also show that the chemical shielding tensors and chemical shifts are efficient parameters for characterization of single walled carbon nanotube. While the NMR tensors at the sites of various nuclei are not similarly influenced by these interactions. Among other nucleuses of SWCNT, molecular nitrogen, oxygen and carbon monoxide molecules are those nucleuses which their NMR tensors are considerably influenced by SWCNT interactions.

References

1. S. Ijima, T. Ichihashi" *Single-shell carbon nanotubes of 1-nm diameter*", Nature, 363, (1993), 603–5.
2. Y.T. Jang, S.I. Moon, J.H. Ahn, Y.H. Lee, B.K. Ju, *A simple approach in fabricating chemical sensor using laterally grown multi-walled carbon nanotubes*, Sens. Actuators, B 99 (2004) 118.
3. L. Valentini, C. Cantalini, I. Armentano, J.M. Kenny, L. Lozzi, S. Santucci, *Highly Sensitive and Selective Sensors Based on carbon Nanotubes Thin films for Molecular Detection*, Diamond Relat. Mater. 13 (2004) 1301.
4. S.G. Wang, Q. Zhang, D.J. Yang, P.J. Sellin, G.F. Zhong, *Multi-walled carbon nanotube-based gas sensors for NH₃ detection*, Diamond Relat. Mater. 13 (2004) 327.
5. J. Kong, N.R. Franklin, C. Zhou, M.G. Chapline, S. Peng, K. Cho, H. Dai, *Nanotube molecular wire as chemical sensors*, Science, 287 (2000) 622.
6. S. Peng, K.J. Cho, *Chemical Control of Nanotube Electronics*, Nanotechnology, Vol. 11 (2000) 57.
7. S.A. Babanejad, F. Ashrafi, A. S. Ghasemi, *Optimization of adsorption of oxygen gas on Carbon nanotubes surface*, Archives of Applied Science Research, Vol. 2 (5), 2010, pp. 438 – 443.
8. F. Ashrafi, A.S. Ghasemi, S.A. Babanejad and M. Rahimova, *Optimization of Carbon Nanotubes for Nitrogen Gas Adsorption*, Research J. of Appl.Sci. Eng. Tech, Vol. 2 (6), 2010, pp. 547-551.
9. A. S. Ghasemi, F. Ashrafi, S. A. Babanejad, M. Rahimova, *A Computational NMR Study of Chemisorption of Nitrogen-Doped on the surface of Single-Walled Carbon Nanotubes*, Archives of Applied Science Research, 2 (4), (2010), 262.
10. X. Lu, Z.F. Chen, P.V. Schleyer, *Are the Stone-Wales Defects Always More Reactive than Perfect Sites in the Sidewalls of Single-Wall Carbon Nanotubes*, J. Am. Chem. Soc. 127 (2005) 20.
11. L.V. Liu, W.Q. Tian, Y.A. Wang, *Ozonization at the Vacancy Defect Site of the Single-Walled Carbon Nanotube*, J. Phys. Chem. B 110 (2006) 13037.
12. F. Ding, K. Bolton, A. Rosen, *Nucleation and growth of single-walled carbon nanotubes: A molecular dynamics study*, J. Phys. Chem. B 108 (2004) 17369.
13. J. Zhao, A. Martinez-Limia, P.B. Balbuena, *Understanding catalysed growth of single-wall carbon nanotubes*, Nanotechnology 16, (2005) S575.
14. M.J. Duer, *Solid State NMR Spectroscopy: Principles and Applications*, Blackwell Science Ltd., London,2001, ISBN: 9780632053513.
15. M. Mirzaei, N.L. Hadipour, *An investigation of hydrogen-bonding effects on the nitrogen and hydrogen electric field gradient and chemical shielding tensors in the 9-methyladenine real crystalline structure: a density functional theory study*, J. Phys. Chem. A, 110 (14), (2006), 4833.
16. G. Wu, S. Dong, R. Ida, N. Reen, *A solid-state ^{17}O nuclear magnetic resonance study of nucleic acid bases*, J. Am. Chem. Soc. 124 (2002) 1768.
17. J.W. Mintmire, B.I. Dunlap, C.T. White, *Are fullerene tubules metallic?* Phys. Rev. Lett. 68(1992) 631.
18. N. Hamada, S. Sawada, A. Oshiyama, *New one-dimensional conductors: Graphitic microtubules*, Phys. Rev. Lett. 68(1992) 1579.

19. X. Blase', L. Benedict, E.L. Shirley, S.G. Louie, *Are fullerene tubules metallic?* Phys. Rev. B57 (1994) 1878.
20. J.C. Charlier, Ph. Lambin, *Electronic structure of carbon nanotubes with chiral symmetry*, Phys. Rev. B 57(24), (1998), R15037.
21. W.C. Bailey, Chem., *DFT and HF-DFT Calculations of ¹⁴N Quadrupole coupling Constants in Molecules*, Phys. 252 (2000) 57-66.
22. M. Mirzaei, N.L. Hadipour, *An investigation of hydrogen-bonding effects on the nitrogen and hydrogen electric field gradient and chemical shielding tensors in the 9-methyladenine real crystalline structure: a density functional theory study*, J. Phys. Chem. A 110 (14), (2006), 4833.
23. M. Mirzaei, N.L. Hadipour, *Study of hydrogen bonds in 1-methyluracil by DFT calculations of oxygen, nitrogen, and hydrogen quadrupole coupling constants and isotropic chemical shifts*, Chem. Phys. Lett. 438 (4-6), (2007), 304.
24. Perdew P, Burke K, Wang Y. *Generalized gradient approximation for the exchange-correlation hole of a many-electron system*, Phys Rev B 54, (1996), 16533-16539.
25. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery Jr., R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, A.G. Baboul, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, M. Head-Gordon, E.S. Replogle, J.A. Pople, *Gaussian 98*, Gaussian Inc., Pittsburgh PA, 1998.
26. E.B. Barros, H. Son, Ge.G. Samsonidze, A.G. Souza Filho, R. Saito, Y.A. Kim, H. Muramatsu, T. Hayashi, M. Endo, J. Kong, M.S. Dresselhaus, *Raman spectroscopy of double-walled carbon nanotubes treated with H₂SO₄*, Phys. Rev. B 76 (4), (2007), 045425.
27. A.G. Souza Filho, V. Meunier, M. Terrones, B.G. Sumpter, E.B. Barros, F. Villalpando-Paez, J.M. Filho, Y.A. Kim, H. Muramatsu, T. Hayashi, M. Endo, M.S. Dresselhaus, *Selective tuning of the electronic properties of co-axial nanocables through exohedral doping*, Nano Lett. 7, (2007), 2383.
28. A.G. Souza Filho, M. Endo, H. Muramatsu, T. Hayashi, Y.A. Kim, E.B. Barros, N. Akuzawa, Ge.G. Samsonidze, R. Saito, M.S. Dresselhaus, *Resonance Raman scattering studies in Br₂-adsorbed double-wall carbon nanotubes*, Phys. Rev. B 73, 235413 (2006).
29. R.G. Parr, W. Yang, *Density Functional Theory of Atoms and Molecules*, Oxford University Press, (1994), ISBN13: 9780195092769.
30. S.A. Babanegad, F. Ashrafi, A.S. Ghasemi, M. Rahimova, *Influence of hydrogen doping on the ¹⁵N and ¹⁷O NMR parameters in zigzag and armchair single wall nanotube: A DFT study*, Der Chemica Sinica, 2012, 3(1):124-128.
31. K. Wolinski, J.F. Hilton, P. Pulay, *Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations*, J. Am. Chem. Soc. 112 (23), (1990), 8251.
32. M.J. Duer, *Solid State NMR Spectroscopy: Principles and Applications*, Blackwell Science Ltd., London, (2001), ISBN: 9780632053513.
33. C.M. Marian, M. Gastreich, *Structure-property relationships in boron nitrides: The ¹⁵N- and ¹¹B chemical shifts*, Solid State Nucl. Mag. 19, (2001), 29.
34. H.S. Kang, *Theoretical Study of Boron Nitride Nanotubes with Defects in Nitrogen-Rich Synthesis*, J. Phys. Chem. B 110 (10), (2006), 4621.
35. S. Hou, Z. Shen, J. Zhang, X. Zhao, Z. Xue, *Ab initio calculations on the open end of single-walled BN nanotubes*, Chem. Phys. Lett. 393 (1-3), (2004), 179.
36. A. Abragam, *Principles of Nuclear Magnetism*, Clarendon Press, Oxford, 1961, 599 p. OCLC Numbre: 242700.
36. E. A. C. Lucken, *Nuclear Quadrupole Coupling Constants*, Academic Press, London, (1969), ISBN-13: 978-0124584501.
38. H.J. Liu, J.P. Zhai, C.T. Chan, Z.K. Tang, *Density functional theory study of atomic oxygen, O₂ and O₃ adsorptions on the H-capped (5,0) single-walled carbon nanotube*, Nanotechnology 18, (2007) 65704.

39. A. Rubio, J.L. Corkill, M.L. Cohen, *Theory of graphitic boron nitride nanotubes*, Phys. Rev. B 49 (7), (1994), 5081.
40. X. Balase, A. Rubio, S.G. Louie, M.L. Cohen, *Stability and Band Gap Constancy of Boron-Nitride Nanotubes*, Europhys. Lett. 28 (1994) 335.
41. E. Zurek, C.J. Pickard, B.J. Autschbach, *Determining the Diameter of Functionalized Single-Walled Carbon Nanotubes with ¹³C NMR: A Theoretical Study*, J. Phys. Chem. C 112 (2008) 9267.
42. Y. Liu, H.Guo, *Current distributions in B- and N-doped carbon nanotubes*, Phys. Rev. B, 69, (2004), 115401.
43. Y. Miyamoto, *Mechanically stretched carbon nanotubes: Induction of chiral current*, Phys. Rev. B, 54 (14), (1996), R11149.
44. S. Peng, K. Cho, *Ab Initio Study of Doped Carbon Nanotube Sensors*, Nano Lett., 3(4), (2003), 513-517.
