Fullerenes, Nanotubes and Carbon Nanostructures. 2009;17(1):26-37.

Structural Relationship Between Degree of Unsaturation with Fermi Energy, Chemical Hardness, and The HOMO-LUMO Gap of (5,5) Armchair Single-Walled Carbon Nanotubes

Avat (Arman) TAHERPOUR
Chemistry Department, Graduate Faculty, Islamic Azad University, Arak, Iran

Abstract
Carbon nanostructure compounds in an attractive variation of structures and wonderful forms have been synthesized and identified. One of these structures is the carbon nanotubes. These structures have several rings that share number of carbons. Study about properties of *nanotubes* with medicinal and electronic applications have been made the highly useful and effective results for applications in different areas of science. One of the main recognized structures of nanotubes is (5,5) single-walled tube (SWCN). Topological indices are the digital value combined with chemical constitution purporting for correlation of chemical structures with various chemical and physical properties that have constructed the effective and useful mathematical methods for finding good relationship between several data of the properties in these materials. One of the useful numerical and structural items in unsaturated compounds is degree of unsaturation (D_U) which is illustrated here. In this study, the relationship between this index (D_U), Fermi energy (E_f), chemical hardness, and relative energetic stability all show the length periodicity seen in the HOMO-LUMO gap, in contrast to the optical "charge transfer" transition are represented as some of the important properties of nanotubes (5,5) armchair SWCN. By the simple model presented here, in good approximation can calculate the structural and electronic properties of these nanotubes and can be used the approximated values in electronic structures and electrical properties studies of this type of nanotubes. The interesting results of relationship among D_U and the properties of these nanotubes are presented.

References
1. Zhou, Z., Steigerwald, M., Hybertsen, M., Brus, L., Friesner, R.A. Electronic Structure of Tubular Aromatic Molecules Derived from the Metallic (5,5) Armchair Single Wall Carbon Nanotube (2004) Journal of the American Chemical Society, 126 (11), pp. 3597-3607. doi: 10.1021/ja039294p
2. Srivastava, D., Menon, M., Cho, K. (2001) Compu. Sci. & Eng, pp. 42-55. and the literature cited therein
3. Arellano, J.S., Molina, L.M., Rubio, A., Lo´pez, M.J., Alonso, J.A. Interaction of molecular and atomic hydrogen with (5,5) and (6,6) single-wall carbon nanotubes (2002) Journal of Chemical Physics, 117 (5), pp. 2281-2288. doi: 10.1063/1.1488595
4. Srivastava, D., Barnard, S. Molecular dynamics simulation of large-scale carbon nanotubes on a shared memory architecture (1997) Proc. IEEE Super computing '97. IEEE Computer Soc. Press, Los Alamitos, Calif
5. Yakobson, B.I., Brabec, C.J., Bernholc, J. Nanomechanics of carbon tubes: Instabilities beyond linear pesponse (1996) Physical Rev. Letters, 76, p. 2511.
6. Srivastava, D., Menon, M., Cho, K. Nanoplasticity of single-wall carbon nanotubes under uniaxial compression (1999) Physical Review Letters, 83 (15), pp. 2973-2976.
7. Yakobson, B.I., Avouris, P. Mechanical properties of carbon nanotubes (2001) Carbon Nanotubes, p. 293. Springer-Verlag: Berlin
8. Lourie, O., Cox, D.M., Wagner, H.D. Buckling and collapse of embedded carbon nanotubes (1998) Physical Review Letters, 81 (8), pp. 1638-1641.
9. Dresselhaus, M.S., Dresselhaus, G., Eklund, P.C. (1996) Science of Fullerenes and Carbon Nanotubes. Academic Press: New York

10. Avouris, P. Molecular electronics with carbon nanotubes (2002) Accounts of Chemical Research, 35 (12), pp. 1026-1034. doi: 10.1021/ar010152e
11. Dresselhaus, M.S., Dresselhaus, G. Ph. Avouris (2001) Carbon Nanotubes: Synthesis, Structure Properties and Applications Springer-Verlag: Berlin
12. Special issue on carbon nanotubes, Physics World, 13(6), June 2000. (Cross ref.)
13. Collins, P.G., Avouris, P. (2000) Nanotubes for Electronics. Sci. Am, 283, pp. 38-45.
14. Dresselhaus, M.S., Dresselhaus, G., Saito, R. Carbon fibers based on C60 and their symmetry (1992) Physical Review B, 45 (11), pp. 6234-6242. doi: 10.1103/PhysRevB.45.6234
15. Mintmire, J.W., Dunlap, B.I., White, C.T. Are fullerene tubules metallic? (1992) Physical Review Letters, 68 (5), pp. 631-634. doi: 10.1103/PhysRevLett.68.631
16. Barnett, R., Demler, E., Kaxiras, E. Superconducting and charge-density wave instabilities in ultrasmall-radius carbon nanotubes (2005) Solid State Communications, 135 (5), pp. 335-339. doi: 10.1016/j.ssc.2005.04.049
17. Hansen, P.J., Jurs, P.C. Chemical applications of graph theory: Part I. Fundamentals and toplogical indices (1988) Journal of Chemical Education, 65 (7), pp. 574-580.
18. Hosoya, H. (1971) Bull. Chem. Soc. Jpn, 44, pp. 2332-2339.
19. Randic, M. On characterization of molecular attributes (1998) Acta Chimica Slovenica, 45 (3), pp. 239-252.
20. Rucker, G., Rucker, C. On topological indices, boiling points, and cycloalkanes (1999) Journal of Chemical Information and Computer Sciences, 39 (5), pp. 788-802.
21. Wiener, H. Structural determination of paraffin boiling points (1947) Journal of the American Chemical Society, 69 (1), pp. 17-20.
22. Du, Y.P., Liang, Y.Z., Li, B.Y., Xu, C.J. (2002) J. Chem. Inf. Cmput. Sci, 42, pp. 1128-1138.
23. Randic, M. On characterization of molecular branching (1975) Journal of the American Chemical Society, 97 (23), pp. 6609-6615.
24. Taherpour, A., Shafiei, F. The structural relationship between Randic´ indices, adjacency matrixes, distance matrixes and maximum wave length of linear simple conjugated polyene compounds (2005) Journal of Molecular Structure: THEOCHEM, 726 (1-3), pp. 183-188. doi: 10.1016/j.theochem.2005.03.053
25. Bolboaca, S.D., Jantschi, L. How good can the characteristic polynomial be for correlations? (2007) International Journal of Molecular Sciences, 8 (4), pp. 335-345. http://www.mdpi.net/ijms/papers/i8040335.pdf
26. Slanina, Z., Uhlk, F., Lee, S.-L., Osawa, E. Geometrical and thermodynamic approaches to the relative stabilities of fullerene isomers (2001) Match, 44, pp. 335-348.
27. Taherpour, A.A. (2005) Aust. J. Ed. Chem., 65: 37.
28. Taherpour A. A. A Simple Method for Determining the Number of Rings in Polycyclic Compounds, 2nd International Conf. Chem. Edu. & & Sustainable Development, Moscow, Russia, 16-18 Nov. 2004, Proc. P. 103.
29. Taherpour, A. Structural relationship between degree of unsaturation with polarizability of (5,5) armchair single-wall carbon nanotubes (2007) Fullerenes Nanotubes and Carbon Nanostructures, 15 (4), pp. 279-289. doi: 10.1080/15363830701423674
30. Brus, L.E. A simple model for the ionization potential, electron affinity, and aqueous redox potentials of small semiconductor crystallites (1983) The Journal of Chemical Physics, 79 (11), pp. 5566-5571.
31. Makov, G., Nitzan, A., Brus, L.E. On the ionization potential of small metal and dielectric particles (1988) The Journal of Chemical Physics, 88 (8), pp. 5076-5085.