Research Article **CODEN: IJRPJK** **ISSN: 2319 – 9563**

International Journal of Research in Pharmaceutical and Nano Sciences

Journal homepage: **www.ijrpns.com**

HETEROGENEOUS NANOTUBES: THEORETICAL CALCULATION OF ENERGY GAP INFLUENCE BY BOND LENGTH AND GEOMETRY

V. Uma[*1], N. Pradeep[1], V. Chaitra[1]

[1*]Department of Electronics, Mount Carmel College, Bengaluru, Karnataka, India.
[2]Department of Nanoscience and Technology, Mount Carmel College, Bengaluru, Karnataka, India.

ABSTRACT

This paper, we present the systematic calculation of the Heterogeneous nanotubes band gap based on its bond length and geometry's of nanotubes we used selected heterogeneous nanotubes and integers for Zig Zag, Armchair, Chiral geometries for calculation. Energy gap variation is not large and it varies inversely with nanotubes diameter, as predicted by theory. The band gap is calculated with the all three geometries using integers and it's compared with the each geometries. Possible explanation for the band gap variation in heterogeneous nanotubes is given using a mathematical calculation.

KEYWORDS

Heterogeneous Nanotubes, Zinc Oxide Nanotube, Band gap, Bond length and Geometry.

Author for Correspondence:

Uma V,

Department of Electronics,

Mount Carmel College,

Bengaluru, Karnataka, India.

Email: umamcciyer@gmail.com

INTRODUCTION

Nanotubes are current tremble in research community. In 1991 Sumio Iijima reported about carbon nanotubes in Nature[1], Followed by many researchers persist the nanotubes research for past two decades. For attractive physical and chemical property of carbon nanotubes draw the attention of industries and scientists. Consequently nanotubes were prepared or designed by different material such as Nitride nanotubes, phosphide nanotubes, oxide nanotubes, sulfide nanotubes etc. Generally these nanotubes called as heterogeneous nanotubes (HGNT). The potential application of carbon nanotubes is huge in many areas, especially the

electrical properties of carbon nanotubes leads application to the sensor, electronics etc. Many research groups are reported the study of electrical properties of carbon nanotubes by experimentally and theoretically but research and theoretical attention has not been paid for Heterogeneous nanotubes so far. Exceptional property and application is expected from heterogeneous nanotubes, so the demands for HGNT tubes are more. Many properties of heterogeneous nanotubes still yet to be discover. Theoretical calculation carbon nanotubes electrical properties are reported, but there are no literature for theoretical calculation of heterogeneous nanotubes electrical properties (band gap) based on the bond length and its geometry. In this report we calculate and study the effect of bond length and geometry. Heterogeneous nanotubes varieties are more from these we used for calculation selected heterogeneous nanotubes and selected integers.

CALCULATION METHOD

Widely used to approach to find the geometry is r= na + mb[1] where r is rolled vector, n and m are integers. The relations between n, m also defines the three categories of CNT. The way the graphene sheet is rolled is represented by chiral vector or chirality (n, m). If n = m = l where l is an integer then nanotube formed is known as armchair, if n = l and m = 0, then nanotube formed is known as zigzag and if n = 2l and m = l, then nanotube formed is known as chiral[2].Length of unit vector is $a= \sqrt{3}\ a_{x-y}$, x and y are bond length between two different atoms. Length of Chiral vector $L= a\sqrt{n2+m2+nm}$[3]. Diameter of the tube is $d_t = L/\pi$[3]. Eg ~ 1/dt[4] For this calculation we take selected nanotubes (Table No. 1) and Selected integers , they are (2,0)(3,0)(4,0)(5,0)(6,0) for Zig Zag, (2,2)(3,3)(4,4)(5,5)(6,6) for Arm chair, (2,1)(3,1)(4,1)(5,1)(6,1) for Chiral geometry.

RESULTS AND DISCUSSION

We have used above mentioned equations to calculate the Energy gap (Eg), for each nanotube from respective integers we found circumference and the diameter. Using diameter approximate energy gap we calculated, that is plotted for three different geometry types of Zig zag, Armchair, Chiral with the bond length of different nanotubes. Graph shows the Energy gap for respective bond length for zig zag nanotubes, Arm chair, Chiral shown in (Figure No. 1(a), 1(b), 1(c)). For interpretation Convenience ZnO nanotubes graph plot separately. We observed from graph (Figure No.1(a), 1(b), 1(c)) for lower integer value such as Zig Zag (2, 0), (5,1) and (6,1) integers, respective band gap Arm Chair (2,2) Chiral (2,1) have higher band gap than the high integer value of (6,0), (6,1), (6,6) for all type of heterogeneous nanotubes and geometry's. The lower bond length of Boron nitride (BN) Nanotubes has high energy gap than rest of the nanotubes, for all three geometry's nanotubes. It indicates that from our calculation smaller bond length leads to semi metallic nanotubes from 0.6169eV to 0.2056 eV for BNNT for Zig Zag, higher bond length leads towards metallic nanotubes 0.3977 to 0.1325 eV for Ga-P NT for Zig Zag.

The distance between graph lines are closer and closer from lower integers to higher integers that is indicating the difference in band gap is decreasing in higher integers values this we can clearly seen form all three geometry graph plots, for charily nanotubes plot of BNNT band gap for (2,1) is 0.4664 eV, (3,1) is 0.3422 eV difference is 0.1242 eV consequently are 0.2216eV, 0.1881eV, the difference is 0.0335eV, which is lower than a (2,1),(3,1) integers. This decrease in band gap energy irrespective of all geometry and all bond lengths HGNT were occurred. From that we got know the integers becoming higher value there are no much difference in band gap. Literally same band gap higher integers which is not taken for valuation here. The semimetal to metallic band gap shift is occurring in all type of geometry's in heterogeneous nanotubes irrespective of bond length and geometry's. From (Figure No. 1(d)) shows the ZnO nanotubes merged graph of Armchair, Chiral, Zig Zag geometries. Zig Zag type nanotubes shows higher band gap as 0.4847 eV than chiral and Armchair. Armchair shows the lowest band gap as 0.0932 eV. Interestingly Arm chair and

Zig zag nanotubes band gaps are merge together and increase simultaneously, may this happen because of the integers are closer values of armchair and zig zag. There is linear shift in zig zag and chiral nanotubes. In ZnO nanotubes Armchair tubes are become metallic for higher integer as 0.0932 eV for (6, 6).

Table No.1: HGNT and its bond length

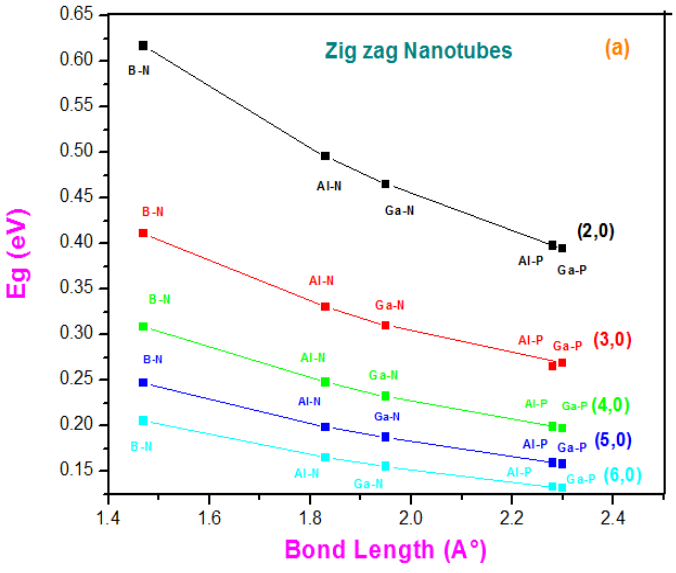
S.No	Heterogeneous Nanotubes	Bond length (A°)
1	Boron Nitride Nanotubes (B-N)	1.47[5]
2	Gallium Nitride Nanotubes (Ga-N)	1.95[6]
3	Aluminum Nitride Nanotubes (Al-N)	1.83[7]
4	Aluminum Phosphide Nanotubes (Al-P)	2.3[8]
5	Gallium Phosphide Nanotubes (Ga-P)	2.28[8]
6	Zinc oxide Nanotubes (ZnO)	1.87[9]

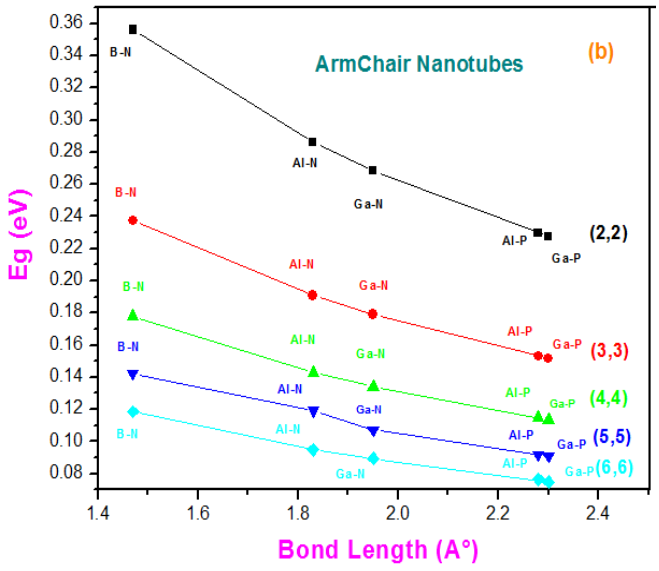
Table No.2: Diameter and Bandgap of Boron Nitride Nanotubes (BN-NT), Gallium Nitride Nanotubes (GaN-NT), Aluminum Nitride Nanotubes (AlN-NT)

S.No	Integers	BN-NT		AlN-NT		GaN-NT	
		Diameter (nm)	Band gap(eV)	Diameter(nm)	Band gap(eV)	Diameter(nm)	Band gap(eV)
1	(2,0)	1.621	0.6169	2.018	0.4955	2.150	0.4651
2	(3,0)	2.431	0.4112	3.027	0.3306	3.225	0.3100
3	(4,0)	3.242	0.3084	4.036	0.2477	4.300	0.2325
4	(5,0)	4.052	0.2467	5.045	0.1982	5.335	0.1874
5	(6,0)	4.863	0.2056	6.054	0.1651	6.451	0.1550
6	(2,2)	2.807	0.3562	3.495	0.2861	3.724	0.2865
7	(3,3)	4.211	0.2374	5.243	0.1907	5.586	0.1790
8	(4,4)	5.615	0.1780	6.990	0.1430	7.448	0.1342
9	(5,5)	7.019	0.1424	8.378	0.1193	9.311	0.1073
10	(6,6)	8.422	0.1187	10.485	0.0950	11.713	0.0895
11	(2,1)	2.144	0.4664	2.669	0.3746	2.844	0.3516
12	(3,1)	2.922	0.3422	3.638	0.2748	3.876	0.2579
13	(4,1)	3.714	0.2692	4.624	0.2162	4.927	0.2029
14	(5,1)	4.512	0.2216	5.617	0.1780	5.986	0.1670
15	(6,1)	5.314	0.1881	6.616	0.1514	7.050	0.1418

Table No.3: Diameter and Band gap for Aluminum Phosphide Nanotubes (Al-P NT), Gallium Phosphide Nanotubes (GaP-NT), ZnO nanotubes.

S.No	Integers	AlP-NT		GaP-NT		ZnO NT	
		Diameter (nm)	Band gap(eV)	Diameter(nm)	Band gap(eV)	Diameter(nm)	Band gap(eV)
1	(2,0)	2.536	0.3943	2.514	0.3977	2.062	0.4847
2	(3,0)	3.084	0.2628	3.771	0.2651	3.094	0.3231
3	(4,0)	5.072	0.1971	5.028	0.1988	4.125	0.2423
4	(5,0)	6.340	0.1577	6.285	0.1591	5.157	0.1938
5	(6,0)	7.068	0.1314	7.542	0.1325	6.188	0.1615
6	(2,2)	4.393	0.2276	4.354	0.2296	3.573	0.279
7	(3,3)	6.589	0.1517	6.532	0.1530	2.359	0.1865
8	(4,4)	8.785	0.1138	80709	0.1148	7.146	0.1399
9	(5,5)	10.982	0.0910	10.886	0.0918	8.932	0.1119
10	(6,6)	13.178	0.0750	13.063	0.0765	10.719	0.0932
11	(2,1)	3.326	0.3006	3.355	0.2980	2.728	0.3593
12	(3,1)	4.532	0.2206	4.572	0.2187	3.718	0.2688
13	(4,1)	5.760	0.1736	5.811	0.1720	4.726	0.2115
14	(5,1)	6.999	0.1428	7.060	0.1416	5.742	0.1741
15	(6,1)	8.243	0.1213	8.315	0.1202	6.7637	0.1478





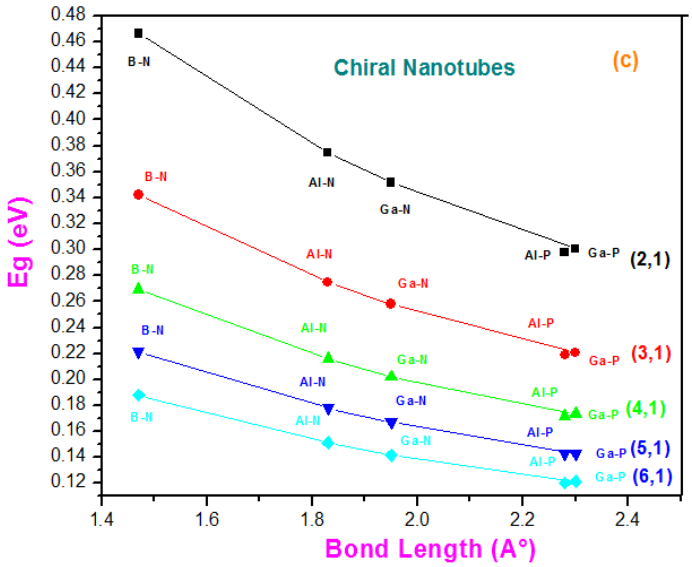


Figure No.1: Graph between Bond lengths vs. Energy gap of Heterogeneous Nanotubes

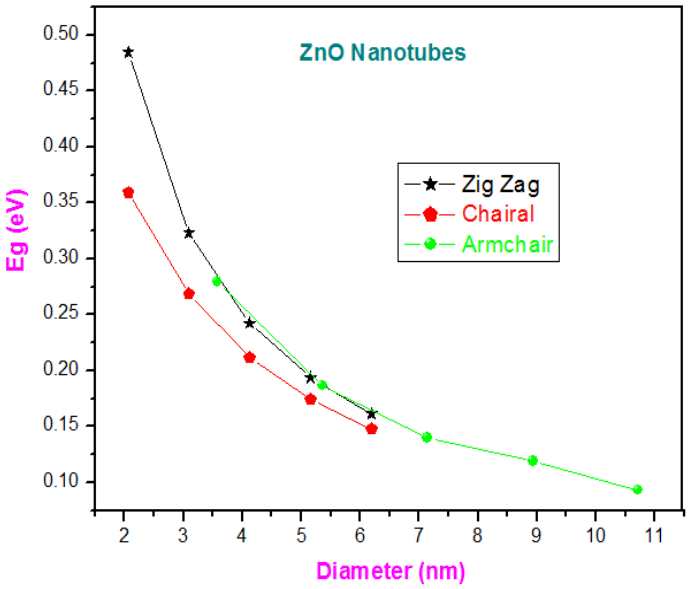


Figure No.2: Graph between Diameters vs. Band gap of Zinc Oxide (ZnO) nanotubes

CONCLUSION

In this paper the Energy gap calculated by using the Integers of Armchair, Zig Zag, Chiral geometry for different heterogeneous nanotubes and results are showed. The results indicate that the influence of bond length is mainly affect the band gap specifically the result determines by the integers of nanotubes irrespective of nanotubes and its geometry's. These above mentioned band gaps are approximately close with the ideal band gaps; however future work is needed for practical way to confirm these band gaps results to experimental results. Also future work is required for higher integer's numbers for theoretical and practical determinations of band gaps.

ACKNOWLEDGEMENT

The authors are highly thankful to Mount Carmel College, Bengaluru, India for providing all the facilities to carry out this work.

CONFLICT OF INTEREST

We declare that we have no conflict of interest.

REFERENCES

1. Sumio iijima. Helical microtubules of graphitic carbon, *Nature* 354(7), 1991, 56-58.
2. Rodney S, Ruoff, Dong Qian, Wing Kam Liu. Mechanical properties of carbon nanotubes, theoretical predictions and experimental measurements, *Comptes Rendus Physique*, 4(9), 2003, 993-1008.
3. Devi Dass, Rakesh Prasher, Rakesh, Vaid. Analytical Study of Unit Cell and Molecular Structures of Single Walled Carbon Nanotubes, *International Journal of Computational Engineering Research*, 2(5), 2012, 1447-1457.
4. Ganesh E N. Single Walled and Multi Walled Carbon Nanotube Structure, Synthesis and Applications, *International Journal of Innovative Technology and Exploring Engineering*, 2(4), 2013, 311-320.
5. Michael J, Biercuk, ShahalIlan, Charles M, Marcus and Paul L, McEuen. Electrical Transport in Single-Wall Carbon nanotubes, *A. Jorio, G. Dresselhaus, M. S. Dresselhaus* (Eds.), Carbon Nanotubes, Topics Appl. Physics, *Springer-Verlag Berlin Heidelberg*, 111(3), 2008, 455-493.
6. Traian Dumitrica, Holger F, Bettinger, Gustavo E, Scuseria and Boris I, Yakobson. Thermodynamics of yield in boron nitride nanotubes, *Physical Review B*, 68(2), 2003, 0854121-8.
7. Rezouali K and Belkhir M A. An abinitio Study of a Model of Single Wall GaN Nanotubes with Oxygen and Zinc as Impurities: Structural and Electronic Properties, *Acta Physica Polonica A*, 113(2), 2008, 713-722.
8. Seif A, Aghaie H, Majlesi. Influences of Si and C- Doping on the Al-27 and N-14 Quardrupole Coupling Constants in AlN Nanotubes, A DFT Study, World Academy of Science, Engineering and Technology, *International Journal of Chemical, Molecular, Nuclear, Materials and Metallurgical Engineering*, 1(5), 2007, 54-58.
9. Chowdhury R, Adhikari S, Scarpa F. Vibration of ZnO nanotubes, a molecular mechanics approach, *Appl Phys* A, 102(3), 2011, 301-308.

Please cite this article in press as: Uma V *et al*. Heterogeneous nanotubes: theoretical calculation of energy gap influence by bond length and geometry, *International Journal* of *Research in Pharmaceutical and Nano Sciences*, 5(1), 2016, 20-25.