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MATERIALS SCIENCE | RESEARCH ARTICLE

Empirical prediction of optical transitions in metallic armchair SWCNTs

G. R. Ahmed Jamal^{1*} and S. M. Mominuzzaman¹

Abstract: In this work, a quick and effective method to calculate the second and third optical transition energies of metallic armchair single-wall carbon nanotubes (SWCNT) is presented. In this proposed method, the transition energy of any armchair SWCNT can be predicted directly by knowing its one chiral index as both of its chiral indices are same. The predicted results are compared with recent experimental data and found to be accurate over a wide diameter range from 2 to 4.8 nm. The empirical equation proposed here is also compared with that proposed in earlier works. The proposed way may help the research works or applications where information of optical transitions of armchair metallic nanotubes is needed.

Subjects: Science; Technology; Physics

Keywords: SWCNT; chiral index; metallic; optical transition energy

1. Introduction

Electronic and optical properties of single-wall carbon nanotubes (SWCNT) are directly associated with their geometrical structures (Odom, Huang, Kim, & Lieber, 2000; Popov, 2004a) which are uniquely specified by a pair of chiral index (n, m) . A SWCNT (n, m) will be metallic if its $n-m = 3k$ (k is integer), i.e. $\text{mod}(n-m, 3) = 0$ and it will be semiconducting if its $n-m \neq 3k$, i.e. $\text{mod}(n-m, 3) = 1$ or 2 (Hamada, Sawada, & Oshiyama, 1992). This relation is always found true except for SWCNT with very small diameter, where curvature effect dominates its properties (Zólyomi & Kürti, 2004). This relation indicates that theoretically two-third of the total SWCNTs are semiconducting and one-third are

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PUBLIC INTEREST STATEMENT

Metallic single-wall carbon nanotubes, a special carbon material, is a potential choice for nanoscale electrodes, 1D quantum wires, transparent conductors, semi-transparent conductive coating and many similar nanodevice applications. In this work, a quick method to calculate optical transition energies of metallic armchair single-wall carbon nanotubes (SWCNT) is presented. It is showed here that the transition energy of any armchair SWCNT can be predicted directly from a structural parameter that uniquely defines that particular armchair SWCNT. The predicted results are compared with recent experimental data and found to be accurate over a wide diameter range. The empirical equation proposed here is also compared with that proposed in earlier works. The proposed way may help the research works or applications where information of optical transitions of armchair metallic nanotubes is needed.

metallic. Metallic nanotubes are a potential choice for nanoscale electrodes and 1D quantum wires (Tans et al., 1997), transparent conductors and semi-transparent conductive coating (Green & Hersam, 2008; Kociak et al., 2001) and many similar nanodevice applications.

The one-dimensionality of the nanotubes gives rise to a discrete set of singularities (splitting into 1D subbands instead of one wide electronic energy band), the so-called *van Hove singularities* (vHS) in the nanotube density of states (DOS) (Mintmire & White, 1998; Odom et al., 2000; Reich & Thomsen, 2000). Each SWCNT (n, m) has a unique set of interband energies E_{ii} denoting the energy differences between the i th van Hove singularities in the conduction, and valence bands and optical transitions associated with the vHS can only occur between these mirror subbands (Odom et al., 2000). This vHS is a unique feature of nanotubes and also primarily responsible for many distinguished optical and electronic properties of SWCNTs.

According to the electronic band theory, the vertical interband transition energy (E_{ii}) between the i -th pair of vHS in both the valence and the conduction bands of a semiconducting (S) or metallic (M) nanotube is represented by E_{ii} , which is inversely proportional to nanotube diameter and corresponds to the first, second, third, ... interband transitions ($E_{11}^S, E_{22}^S, E_{44}^S, \dots$) of semiconducting SWCNTs when $i = 1, 2, 4, \dots$ and to the first, second, third interband transitions ($E_{33}^M, E_{66}^M, E_{99}^M, \dots$) of metallic SWCNTs when $i = 3, 6, 9, \dots$, respectively (Odom et al., 2000). This inverse proportional trend of transition energy with SWCNTs diameter is also observed from well-known Kataura plot (Kataura et al., 1999).

Theoretical model derived from electronic band theory fails quantitatively to predict experimentally observed values of optical transitions for both semiconducting and metallic SWCNTs. Nanotube's "curvature effect" (Gülseren, Yildirim, & Ciraci, 2002; Popov, 2004b; Zeng et al., 2007; Zólyomi & Kürti, 2004) and "trigonal warping effect" (Saito, Dresselhaus, & Dresselhaus, 2000) cause deviations in the electronic properties of nanotubes derived from the simple π -orbital graphene picture. Curvature causes π and σ states of nanotube's chemical bond to mix. This leads to increased hybridization between σ and π orbitals as the diameter of a SWCNT gets smaller (Zeng et al., 2007). The σ - π hybridization effect has been considered and calculated in the literature (Gülseren et al., 2002; Popov, 2004b; Zeng et al., 2007). The main result is that nanotubes satisfying $|n-m| = 3k$ ($k = 0, 1, 2, \dots$) develop a small curvature-induced bandgap, and hence become quasi-metallic or small gap semiconductor (Leonard, 2009). Armchair nanotubes (n, n) are an exception because of their special symmetry, and only they remain truly metallic for all diameters (Leonard, 2009). Saito et al. (2000) investigated the "trigonal warping effect" analytically and derived expressions to estimate the corresponding deviation in optical transitions of metallic and semiconducting SWCNTs. They showed that trigonal warping causes splitting of the DOS peaks of metallic SWCNTs except for armchair tubes. Thus, only armchair SWCNTs are unaffected due to curvature and trigonal warping and remain truly metallic.

As armchair nanotubes are the most pure kind of metallic SWCNTs, we concentrate on armchair tubes. Sometimes, researchers need to find or measure the optical transitions in metallic nanotubes. Many authors (Fantini et al., 2004; Liu et al., 2012; Maultzsch, Telg, Reich, & Thomsen, 2005; Strano et al., 2003) studied the properties of metallic SWCNTs and discussed the first, second and third optical transition energies of metallic SWCNTs. From these works, Liu et al. (2012) studied the matter more recently and more extensively than anyone before. They carried out a series of optical experiments and measured optical transition energies of numerous semiconducting and metallic SWCNTs. The experimental data of optical transitions of metallic armchair SWCNTs used in this work are primarily based on the work of Liu et al. (2012). Though sometimes researchers need the value of optical transitions in metallic nanotubes, but there is no easy way to calculate or predict those transitions and one has to rely solely on experiment. Some complex empirical relations have been proposed (Fantini et al., 2004; Maultzsch et al., 2005; Strano et al., 2003) but they are not simple to calculate and involve many parameters. Here, in this work, a concise empirical relation is devised to predict the second and third optical transitions in armchair metallic nanotubes which directly relates

the optical transition value with any of the chiral index of armchair tubes. The proposed relation can give a quick as well as highly accurate prediction of the second and third optical transitions in armchair metallic SWCNTs.

2. Method and results

Optical transition energies for metallic armchair (n, n) SWCNTs with chiral index (15, 15) to (35, 35) were closely studied here. There are total 21 armchair SWCNTs within these two chiral index range having diameter from 2 to 4.8 nm. The main reason for using this chiral indices range is experimental data of the second and third optical transition energies are available only for these diameter range till now. Values of optical transition energies of these tubes were recorded from various experimental reports (Fantini et al., 2004; Liu et al., 2012; Maultzsch et al., 2005; Strano et al., 2003) with a special focus on the work of Liu et al. (2012) which is most recent and provides most comprehensive data. From these experimental reports, the second optical transition energy of 16 armchair tubes ranging from chiral index (15, 15) to (30, 30) and the third optical transition energy of 13 armchair tubes ranging from chiral index (23, 23) to (35, 35) were found.

In their work, Liu et al. (2012) proposed the following empirical equation to fit their experimental values of different optical transitions of a number of semiconducting and metallic nanotubes:

$$E_p(k) = 2\hbar v_f(p) \times k + \beta \times k^2 + \eta(p) \times k^2 \cos(3\theta)$$

Here, p is the transition index, k is the magnitude of wave vector in the graphene Brillouin zone that varies with nanotube chirality (n, m) and transition index p . The magnitude of k is given by $p \times 2/(3d)$, where d is the nanotube diameter. $E_p(k)$ is the effective dispersion for transition p , \hbar is the reduced Planck constant = 6.582×10^{-16} eV s and $\beta = -0.173$ eV nm². Rest two parameters v_f and η have different values for different transition index p .

For the second optical transition energy (E_{66}) of metallic tubes, $p = 6$, so, $k = 4/d$. Liu et al. (2012) proposed $v_f(p) = 1.236 \times 10^6$ m/s and $\eta(p) = 0.058$ eV nm² for $p = 6$. Using their proposed values and using the fact that $\theta = 30^\circ$ for armchair tubes, the expression for the second optical transition energy (E_{66}) of metallic armchair tubes reduces to,

$$E_{66} = \frac{6.5083}{d} - \frac{2.768}{d^2} \quad (1)$$

For the third optical transition energy (E_{99}) of metallic tubes, $p = 9$, so, $k = 6/d$. Liu et al. (2012) proposed $v_f(p) = 1.248 \times 10^6$ m/s and $\eta(p) = 0.047$ eV nm² for $p = 9$. Using their proposed values and using the fact that $\theta = 30^\circ$ for armchair tubes, the expression for the third optical transition energy (E_{99}) of metallic armchair tubes reduces to,

$$E_{99} = \frac{9.8572}{d} - \frac{6.228}{d^2} \quad (2)$$

So, these are the empirical expression of E_{66} and E_{99} , simplified from the work of Liu et al. (2012). One can easily note that a lot of parameters are involved in the overall calculation of the empirical values of E_{66} and E_{99} from their parent equation which increases the computational efforts. Hence, an attempt will be made here to devise a simple empirical relation between the chirality and optical transition of armchair metallic tubes so that the value of the second or third optical transition of these tubes can be predicted directly from its chiral index (n, n).

After a careful study of the symmetry in the structure of armchair tubes, their optical transitions and their relation with corresponding chiral index, we devised the following empirical formula to predict the optical transitions from corresponding chiral index n of any armchair nanotube (n, n).

For the second optical transition energy (E_{66}) of armchair SWCNTs:

$$E_{66} = \left(\frac{50}{n}\right) e^{\left(-\frac{4.3}{n}\right)} \quad (3)$$

For the third optical transition energy (E_{99}) of armchair SWCNTs:

$$E_{99} = \left(\frac{75}{n}\right) e^{\left(-\frac{6}{n}\right)} \quad (4)$$

The empirical values of the second and third optical transition energies of these armchair SWCNTs with chiral index (15, 15) to (35, 35) were calculated using the empirical Equations 1 and 2 as well as using the empirical Equations 3 and 4. Both results agree well with experimental values of the second and third optical transitions of corresponding metallic armchair SWCNTs. Nevertheless, it was observed that the overall prediction accuracy of Equations 3 and 4 as proposed in this work is much better than that of Equations 1 and 2 as simplified from the parent equation proposed by Liu et al. (2012). To clarify this point, we can mathematically compare Equations 3 and 4 with Equations 1 and 2 in following way:

The diameter of a SWCNT (n, m) is expressed by, $d = \sqrt{3(n^2 + nm + m^2)} a_{cc} / \pi$, where, a_{cc} = carbon-carbon bond length = 0.142 nm. For armchair SWCNTs, $n = m$, which gives, $d = 0.1356 n$ nm or, $n = 7.375 d$ nm. If the exponential term of Equations 3 and 4 are expanded using this trivial relation between n and d , the expressions for the second and third optical transitions become,

$$E_{66} = \frac{6.78}{d} - \frac{3.95}{d^2} + \frac{1.15}{d^3} - \frac{0.224}{d^4} + \dots \quad (5)$$

$$E_{99} = \frac{10.17}{d} - \frac{8.27}{d^2} + \frac{3.36}{d^3} - \frac{0.91}{d^4} + \dots \quad (6)$$

Now, if Equations 5 and 6 are compared with Equations 1 and 2, respectively, then it can be clearly observed that first two terms of both sets of equations are almost identical except slight difference in constant parameters. Thus, it can be said that Equations 3 and 4 are simple but more general and compact form of the relation between optical transition and diameter, or chiral index; whereas, Equations 1 and 2 are in fact an approximated or truncated forms of Equations 3 and 4 ignoring their higher order terms.

Another observation is, Equations 1 and 2 use diameter d which is a fractional number usually taken up to three decimal points at least. Numerical parameters used in Equations 1 and 2 are also taken up to three or four decimal points to reduce prediction error. But, proposed Equations 3 and 4 use chiral index n which is always an integer and the numerical parameters used in these equations take only one decimal point. Moreover, it has to be noted that the simplified expression of Equations 1 and 2 results from its parent equation only after knowing the values of a number of parameters. Hence, the empirical equations 3 and 4 proposed in this work are simpler and better in predicting experimental values than empirical Equations 1 and 2 simplified from the work of Liu et al. (2012).

Experimental (Liu et al., 2012) and the empirical values of optical transition energies along with chiral index (n, n) and diameter of these armchair tubes are shown in Table 1 and Table 2. In Table 1, the empirical result for the second optical transition (E_{66}) from this work using Equation 3 and the empirical result from the work of Liu et al. (2012) using Equation 1, both are provided so as to compare them. Similarly, in Table 2, the empirical result for the third optical transition (E_{99}) from this work using Equation 4 and the empirical result from the work of Liu et al. (2012) using Equation 2, both are

Table 1. Experimental (Liu et al., 2012) and the empirical values of the second optical transition energy of 16 armchair SWCNTs

<i>n</i>	<i>m</i>	Diameter d_t (nm)	Experimental E_{66} (ev)	Empirical E_{66} (ev) from Equation 3	Empirical E_{66} (ev) from Equation 1
15	15	2.063	2.52	2.503	2.505
16	16	2.200	2.38	2.389	2.386
17	17	2.338	2.30	2.284	2.277
18	18	2.475	2.19	2.188	2.177
19	19	2.613	2.11	2.099	2.085
20	20	2.750	2.02	2.016	2.000
21	21	2.888	1.94	1.940	1.922
22	22	3.026	1.87	1.869	1.849
23	23	3.163	1.80	1.803	1.781
24	24	3.301	1.74	1.742	1.718
25	25	3.438	1.68	1.684	1.659
26	26	3.576	1.62	1.630	1.604
27	27	3.713	1.57	1.579	1.552
28	28	3.851	1.49	1.531	1.503
29	29	3.988	1.48	1.487	1.458
30	30	4.126	1.43	1.444	1.415

Table 2. Experimental (Liu et al., 2012) and the empirical values of the third optical transition energy of 13 armchair SWCNTs

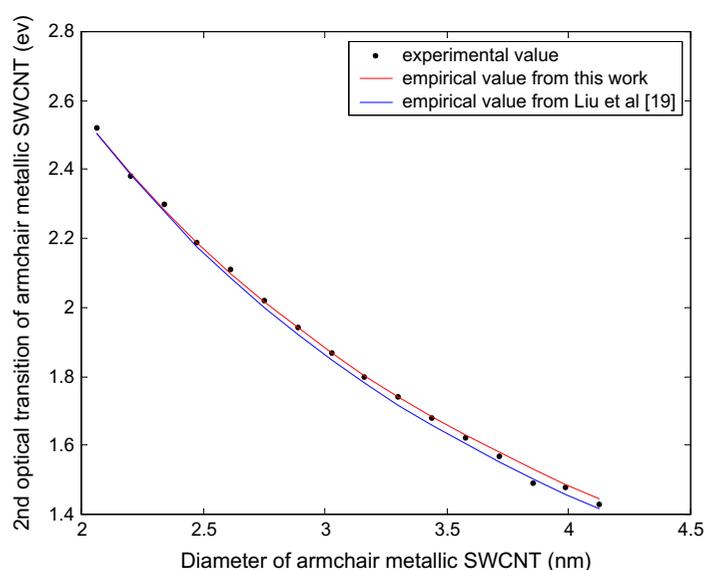
<i>n</i>	<i>m</i>	Diameter d_t (nm)	Experimental E_{99} (ev)	Empirical E_{99} (ev) from Equation 4	Empirical E_{99} (ev) from Equation 2
23	23	3.163	2.52	2.512	2.494
24	24	3.301	2.44	2.434	2.415
25	25	3.438	2.36	2.360	2.34
26	26	3.576	2.29	2.290	2.27
27	27	3.713	2.23	2.224	2.203
28	28	3.851	2.14	2.162	2.14
29	29	3.988	2.10	2.103	2.08
30	30	4.126	2.05	2.047	2.023
31	31	4.263	1.99	1.994	1.969
32	32	4.401	1.94	1.943	1.918
33	33	4.538	1.89	1.895	1.87
34	34	4.676	1.84	1.849	1.823
35	35	4.813	1.80	1.805	1.779

provided so as to compare them. From these two tables, it can be observed clearly that the predicted values from Equations 3 and 4 are much closer to the experimental values than those predicted by Equations 1 and 2. For the second optical transition (E_{66}), the average absolute error in prediction using Equation 3 was found to be only 0.009 ev and corresponding per cent average absolute error is only 0.53%. Similarly, for the third optical transition (E_{99}) the average absolute error in prediction

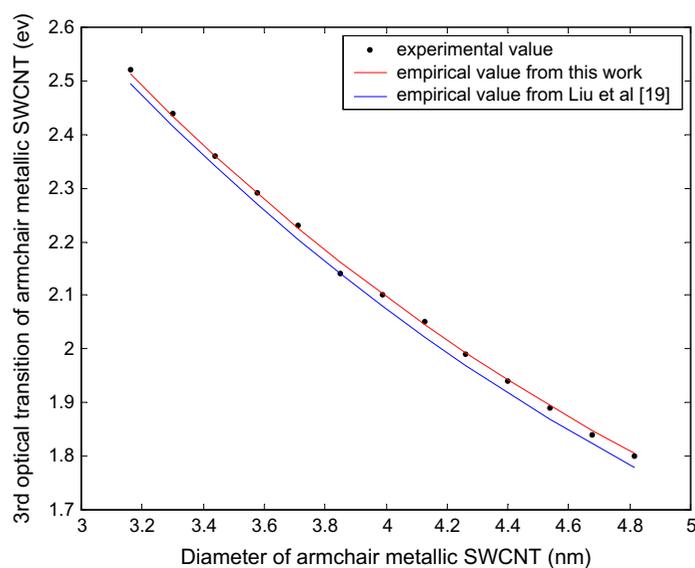
using Equation 4 was found to be only 0.006 eV and corresponding per cent average absolute error is only 0.27%. Thus, the empirical equations proposed here can predict the value of optical transition energies of armchair tubes with higher accuracy.

Figure 1 (a) and (b) shows the plot of experimental and the empirical values of the second and third optical transition energies, respectively, of metallic armchair SWCNTs with respect to their diameters. Here also, the empirical results for the second and third optical transition (E_{66} and E_{99}) from this work using Equations 3 and 4 and the empirical result from the work of Liu et al. (2012) using Equations 1 and 2, both are plotted so as to compare them. Again it can be observed from these two plots that, for both optical transitions, the empirical values predicted by Equations 3 and 4 are closer to the experimental values in comparison to those predicted by Equations 1 and 2 over the full diameter range under consideration. This curve can be extrapolated using the two empirical relations from above to predict other armchair tubes beyond this diameter range.

Figure 1. Experimental value (black), the empirical value from this work (red) and the empirical value from earlier work (blue) of optical transition vs. diameter of armchair SWCNTs, (a) the second optical transition, (b) the third optical transition.



(a)



(b)

Another interesting observation from the second and third optical transition energies of armchair SWCNTs is, the ratio of the third transition to the second transition of same armchair tubes are equal to a constant whose value around 1.4. This observation further facilitate the calculation of higher optical transitions in metallic armchair tubes as one can know the third transition energy value of a tube by knowing the value of the second transition multiplied by that constant. This relation also indicates the built in high symmetry in armchair SWCNTs which causes their higher optical transition energy values to grow in a systematic order. This relation may also help to study the behaviour of metallic armchair tubes in a more systematic way.

3. Conclusions

In this work, an effective method to calculate the second and third optical transition energies of metallic armchair single-wall carbon nanotubes (SWCNTs) is presented. The second and third optical transitions of metallic armchair (n, n) SWCNTs are expressed through a concise empirical formula that directly relates the transition energy with chiral index n . Thus, in this method, the transition energy of any armchair SWCNT can be predicted quickly and directly by knowing its one chiral index as both of the chiral indices of armchair tubes are equal. The predicted or calculated results are compared with recent experimental data and found to be accurate over a wide diameter range. The empirical equations and corresponding result found in this work are also compared with the empirical works proposed by others. It was found that the empirical expression proposed here is much simpler than earlier works and corresponding result provides better accuracy for armchair metallic SWCNTs than earlier works. Based on this accuracy, it can be expected that the proposed empirical equations are also capable to predict the second and third optical transitions beyond this diameter range. New experimental works are needed to confirm this. Nevertheless, the proposed way will help the research works or applications where information of optical transitions of armchair metallic SWCNTs is needed.

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