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Double Walled Carbon Nanotube Simulator to Achieve Higher Accuracy in Finding Optical and Electrical Properties of the Tubes

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Abstract

Many Software have been made to predict the optical transition energy of Single Walled Carbon Nanotube. Predicting the Radial Breathing Mode frequency for Double Walled Carbon Nanotube has been really tough due to inter tube interaction. Experimental values show clear indication that these frequencies and Transition energies depends heavily on inter tube interaction and chirality of the Nanotube. All the previous software to predict any kinds of Band structure of CNT failed to take this effects into account. Moreover most of them gives fairly accurate value for Single Walled Carbon Nanotube. Here for the first time a software was built to predict different kinds of Parameter for Double Walled Carbon Nanotube. This software can be significant in simulating Resonant Raman Spectroscopy for DWNT. The equations used to predict the Band Structure of DWNT in this software is also the most accurate one till date.

Keywords: Radial Breathing Mode; Double Walled Carbon Nanotube Simulator; Interaction.

1. Introduction

Carbon Nanotube is undoubtedly one of the most intense research topic of modern day. Its potential to change Electrical devices and make its application visible in Nano electronics and Optical devices is really fascinating.

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It will open new fields of exciting implications, ranging from bio electronics and computation at quantum level to science of materials and photonics are the characteristics that sets carbon nanotube above the rest. Among all the available tools that is used for the characterization of nanotube Raman Spectroscopy is found to give more accurate Information as it is more robust to environmental changes.

The RBM frequency and diameter relationship is more complex in double walled carbon nanotube than in Single Walled Nanotube because of factors like wall to wall stresses and charge transfer [1]. Previous investigation indicated that RBM frequencies have a systematic upward shift for the SWCNTs in the bundles compared with the isolated ones due to the van der Waals interaction [2, 3]. Typical improvement from this simple relation however was found in some of the previous works [4, 5, 6]. However, this equation fails to take into account the chirality, curvature and inter tube interaction affect into consideration. Thus it can be concluded that there might be an error leading to the diameter found from this equations. However, there is not a single software at the moment that could solve this complex phenomenon to find the Radial Breathing Mode frequency of resonant Raman Spectroscopy neither for single nor for double walled carbon nanotube.

Secondly, typical electronic Band structure relations for SWNT was found using the tight binding model of grapheme [7, 8]. However this relation was improved by Jamal, G. R. A. and his colleagues who modified the value of γ showing that it has a relation with chirality [9]. Most of the software that predicts the Band structure of Single walled carbon Nanotube usually goes in accordance with the values found by them. However, those software usually predicts the mechanical structure of nanotube and hardly gives any optical or electronic information for multi wall tube [10, 11].

Looking at its prospect as a future changing materials for electronic devices and optics a complete and accurate simulator was required to predict its necessary electronic and optical properties to carry the work done by researcher previously forward. Here for the first time a complete Raman RBM mode and Optical transition energy for Double Walled Carbon Nanotube simulator is presented which would give data exactly in accordance with experimental values

2. Developing the Software

2.1. Software building medium

Microsoft Visual Studio was used as a platform to build the software. Coding language was C sharp. Using the tools of Visual studio the software was designed to perform the required tasks. Relevant equations for simulation was taken by our previous work [12] and other necessary equation was generated from experimental data using curve fitting in MATLAB. In this software both double and single nanotube can be simulated. Only by giving the chirality as input one would get important data such as RBM frequency, diameter, transition energy and nanotube type etc. using this software. All the data generated are perfectly matched with experimental data found by others [13, 14].

2.2. Observations

After opening the software it will give an interface to show the welcome message:

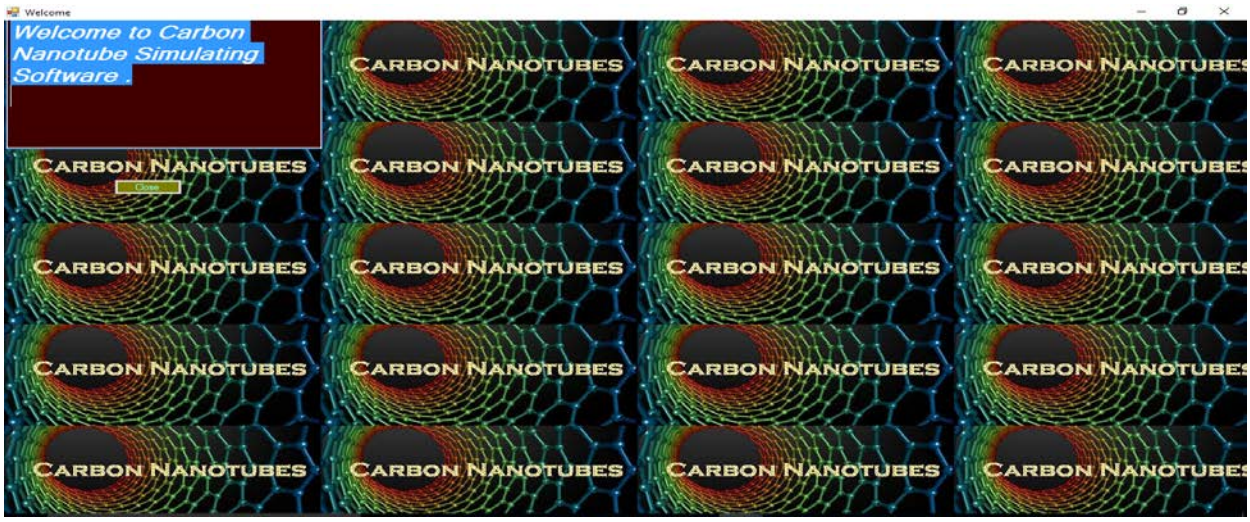

Figure 1: Opening interface of the software.

By selecting the close option it will take to the new menu option where it has to be chosen as what type of CNT one would like to simulate.

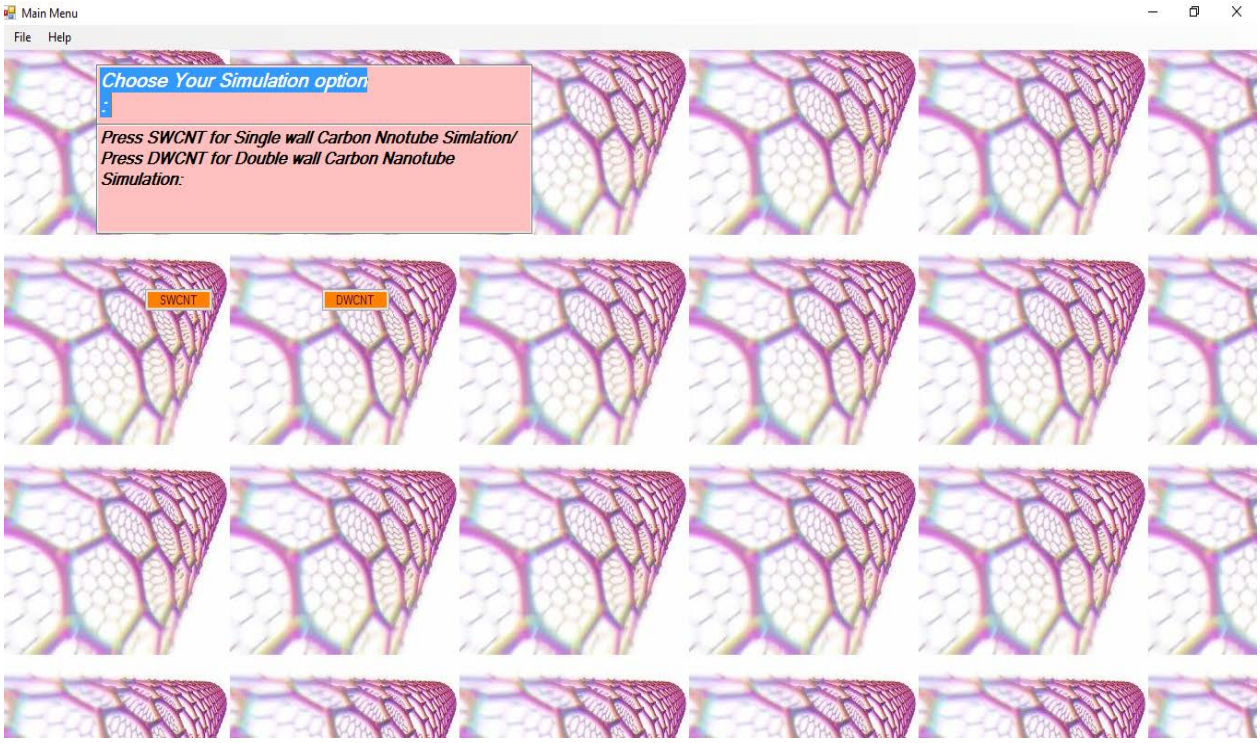

Figure 2: Opening interface of the software.

If SWNT is selected then the following window will pop up where values of n and m has to be given as input:

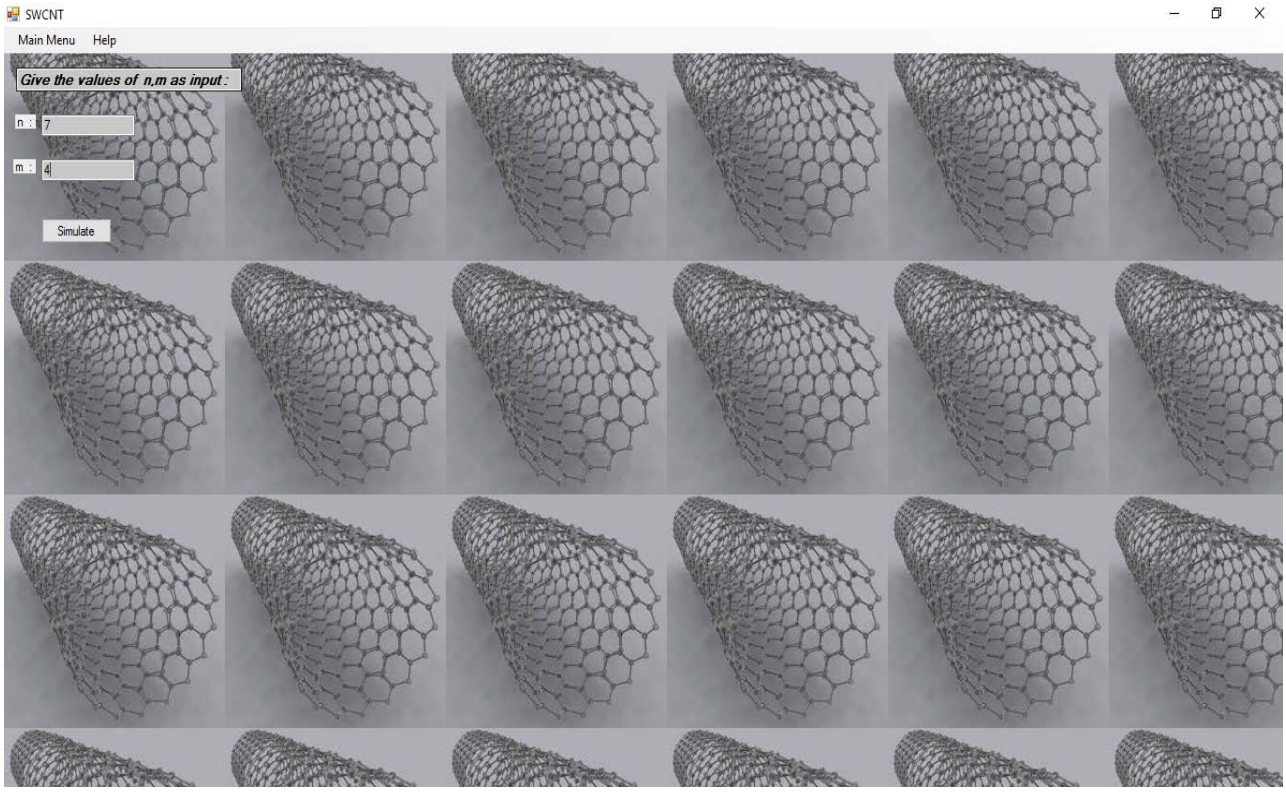

Figure 3: SWNT input.

After selecting simulate option we would get the result of the simulation. One would notice that for metallic tube values of E33 and E66 will be obtained. On the other hand for Semiconducting tube values of E11 and E22 will be obtained. All these values are perfectly matched with the experimental data [9, 15].

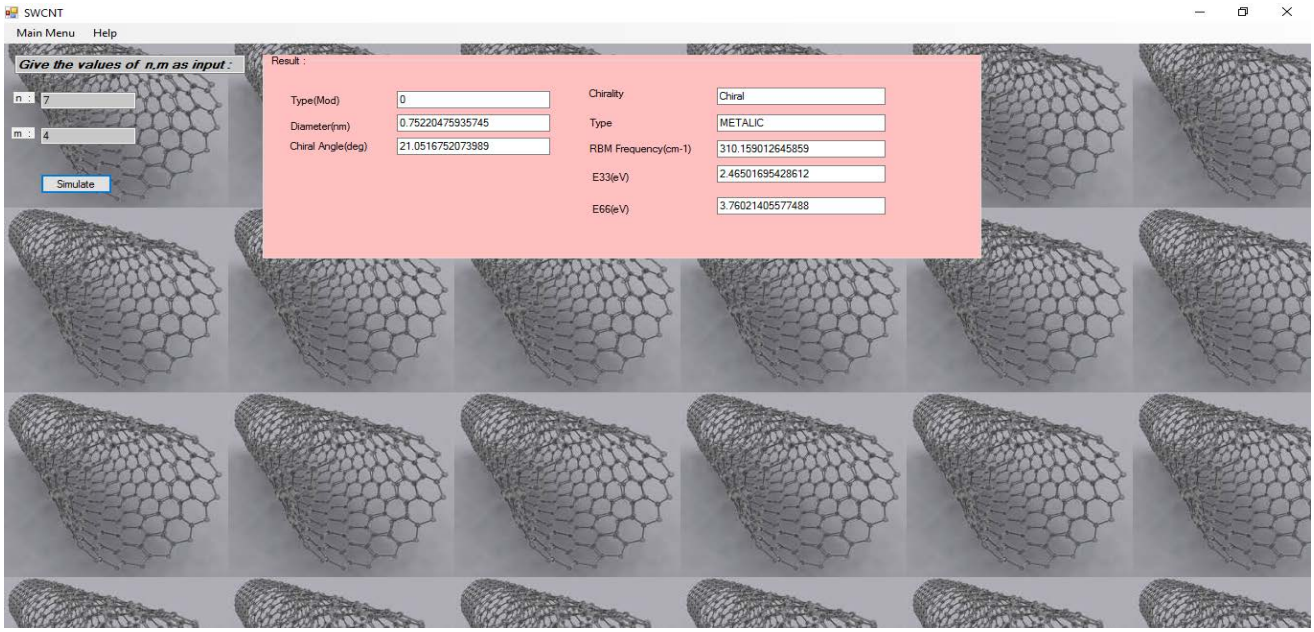

Figure 4: Simulation for metallic tube.

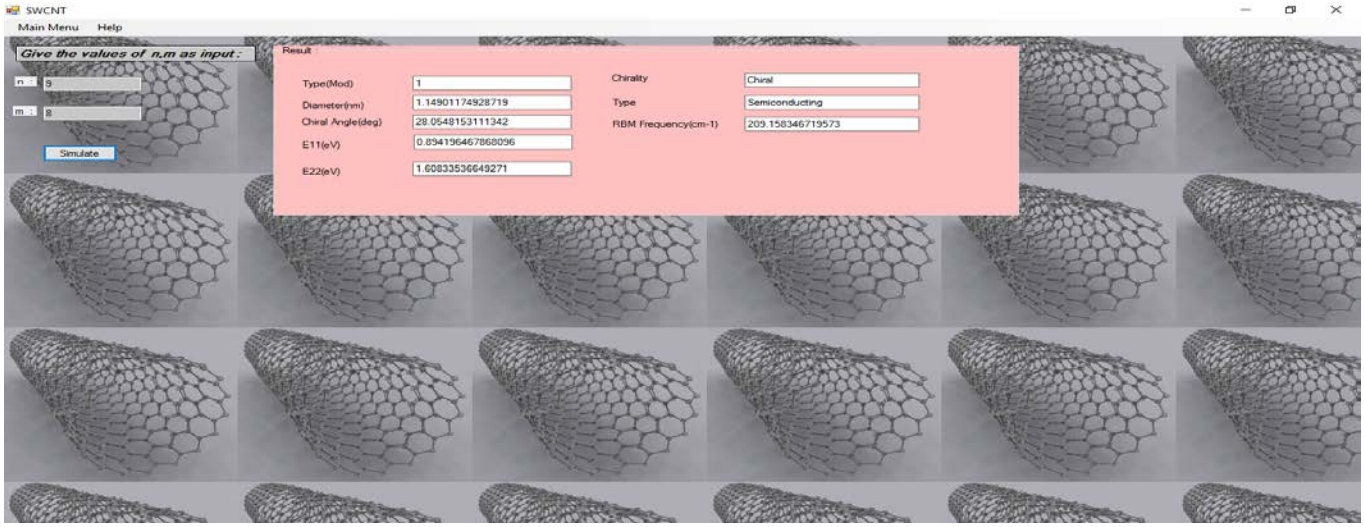

Figure 5: Simulation for semiconducting tube.

Now to simulate DWNT from this window Main Menu bar has to be selected to go back to the menu. Now DWNT will be selected where two pairs of (n,m) will be given as input for both inner and outer tube.

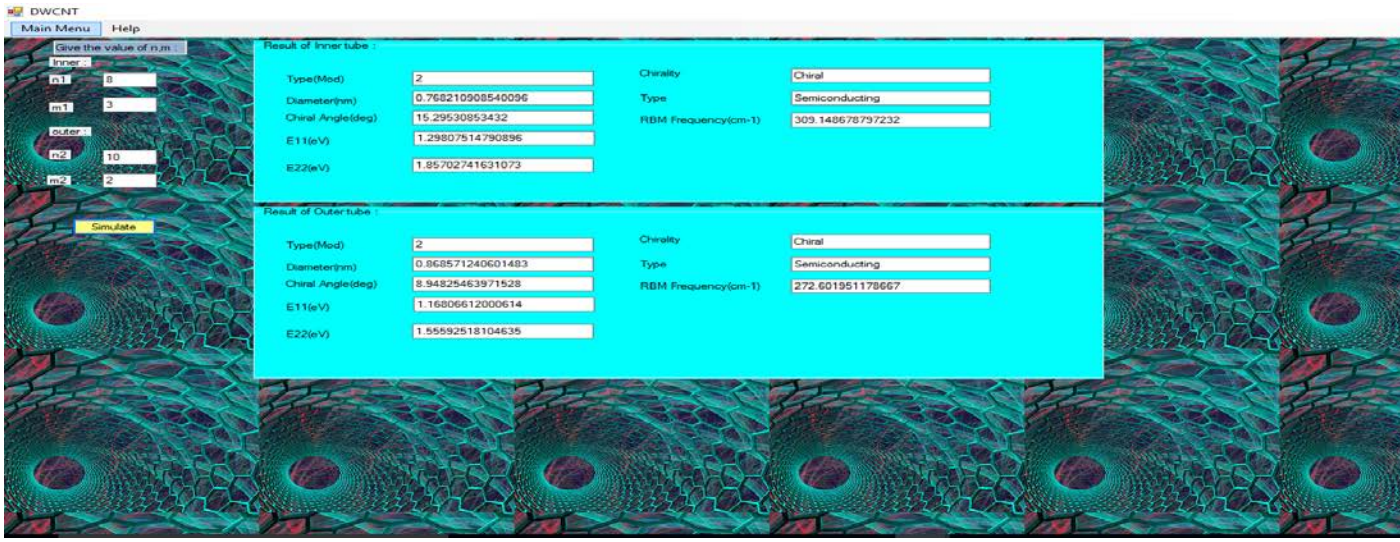

TABLE I. Experimental transition energies and PL intensities of SDBS-wrapped DWNTs and SWNTs.

				SWNT			Inner-DWNT			DWNT-SWNT		Possible outer-DWNT		
(n,m)	$2n+m$, type I/II	d_t (nm)	θ	E_{11} (eV)	E_{22} (eV)	I_{PL} [a]	E_{11} (eV)	E_{22} (eV)	I_{PL} [a]	ΔE_{11} [b] (meV)	ΔE_{22} [b] (meV)	(n,m)	Δd_t [c] (nm)	ΔE [d] (meV)
(8,3)	19, I	0.77	15.3	1.302	1.860	50	1.298	1.859	331	−4	−2	(14,6)	0.62	29
(7,5)	19, I	0.82	24.5	1.211	1.919	96	1.209	1.916	351	−2	−3	(18,1)	0.61	18
(10,2)	22, I	0.87	9.0	1.174	1.689	120	1.169	1.685	450	−5	−4	(15,7)	0.63	59
(7,6)	20,II	0.88	27.5	1.106	1.916	157	1.103	1.911	219	−3	−5	(17,4)	0.62	192
(9,4)	22, I	0.90	17.5	1.123	1.718	189	1.119	1.714	267	−4	−4	(16,6)	0.62	140
(8,6)	22, I	0.95	25.3	1.057	1.734	242	1.051	1.728	221	−6	−6	(15,8)	0.62	173

Figure 6: Simulation for Double walled carbon nanotube and its predicting accuracy with experimental data [14] in finding the optical transition energy.

For the inner tube (8,3) the first optical transition energy was 1.298 for both the software and in PL experiments which would give an error of Zero. Again for the outer tube (10,2) the experimental value is 1.169 where the software gives 1.168 which would give and error of .08 percent. Equations used to find first optical transition energy was found from our previous work [12] and second transition energy equation was developed using curve fitting in MATLAB.

Again the values of RBM frequencies was also obtained with a certain degree of accuracy and equations used to find that would be available in our previous work [12].

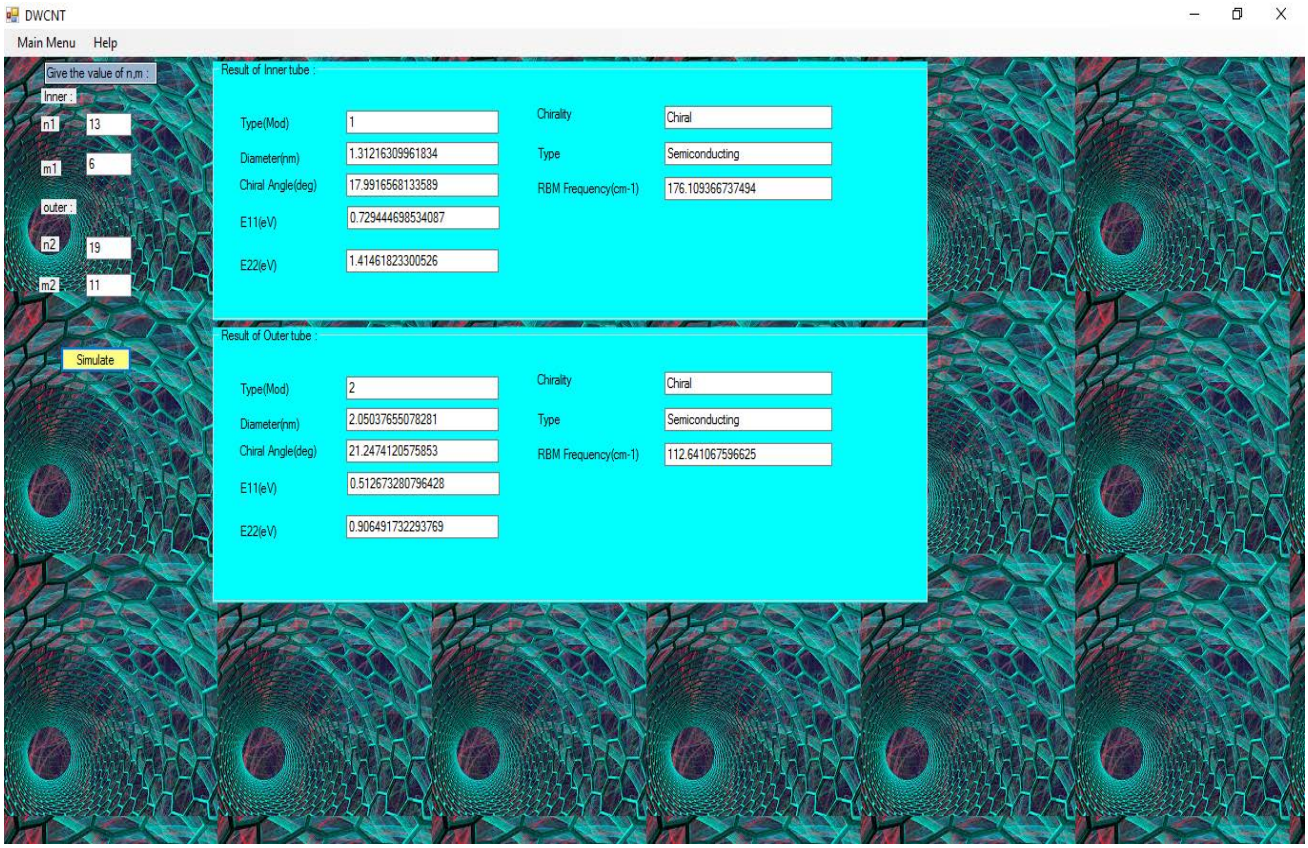

TABLE III. The first and second columns are experiment data,[11] in which the data in brackets are evaluated from the BMs formula of the SWNTs. The other columns are derived from our calculations.

$^{expt.}\omega_{B2}$(cm^{-1}) D (nm)	$^{expt.}\omega_{B1}$(cm^{-1}) d (nm)	ω_{B2}(cm^{-1}) D (nm)	outer (n',m')	ω_{B1}(cm^{-1}) d (nm)	inner (n,m)	b (Å)
108.0(2.29)[a]	159.2(1.50)	108.7(2.205)	(11,21)	159.3(1.494)	(10,12)	3.56
	163.5(1.46)	108.3(2.205)	(7,24)	163.5(1.450)	(1,18)	3.78
112.7(2.18)	169.5(1.40)	112.6(2.120)	(12,19)	170.2(1.392)	(6,14)	3.64
115.7(2.12)	179.3(1.32)	115.6(2.058)	(11,19)	179.3(1.317)	(6,13)	3.71
119.0(2.06)	192.0(1.23)	118.6(1.998)	(10,19)	192.2(1.223)	(8,10)	3.88
124.2(1.96)	211.3(1.11)	124.3(1.90)	(7,20)	211.2(1.110)	(5,11)	3.95
131.9(1.84)	215.0(1.09)	131.4(1.806)	(2,22)	214.7(1.096)	(6,10)	3.55
135.7(1.78)[a]	240.8(0.97)	135.3(1.744)	(4,20)	239.4(0.978)	(4,10)	3.83
	249.8(0.93)	136.0(1.731)	(8,17)	248.8(0.940)	(0,12)	3.96
147.0(1.64)[a]	260.6(0.89)	147.0(1.606)	(1,20)	259.5(0.903)	(4,9)	3.52
	280.6(0.83)	146.9(1.599)[b]	(7,16)	281.7(0.829)	(4,8)	3.85
	294.4(0.79)	146.7(1.599)[b]	(7,16)	293.4(0.795)	(2,9)	4.02
163.5(1.46)	359.8(0.64)	163.0(1.435)	(4,16)	363.1(0.641)[c]	(2,7)	3.97
169.5(1.40)	385.5(0.60)	169.0(1.385)	(3,16)	380.6(0.612)[c]	(4,5)	3.87

Figure 7: RBM frequency of Double walled carbon nanotube predicted by the software is almost equal to the experimental values [13].

The values are almost similar with experimental values with an error of 2 percent and 1.6 percent for outer and inner tube respectively. Thus it can be safely said that this software will predict experimental results of both optical transition energy and RBM frequency of RRS fairly accurately.

3. Conclusion

From that observation of experimental data and values obtained from this software it is clear that this software will create new opportunities for researcher to explore different fascinating properties of DWNT successfully in future. Even though works related to graphics was not done during this work but it remains something to work on in future. With proper graphics and designing it is possible to make this software available for all researcher. Other than being accurate this software is user friendly as well and options like help will always guide the user in a proper manner. It highly desired that the future Nanotube explorer will be benefited from this software and its results.

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