Original Article

Simulation of Carbon Nanotubes Using CNT Band Based on Extended Huckel Theory and Number of P_z Orbital theory to predict its density of state

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Abstract

Aim: The aim of this research work is to simulate a carbon nanotube (CNT Band Tool) to predict its density of state by comparing the band gap using P_z orbital theory and extended huckel theory from 4nm to 22nm.

Materials and Methods: The data for this study was collected using nanohub.org, Samples were considered as (N=20) for extended huckel theory and (N=20) for number of P_z orbital theory according to clinical.com by keeping alpha error-threshold by 0.05, enrollment ratio as 0:1, 95% confidence interval, power at 80% in the NanoHub tool simulation environment. The comparison of P_z orbital theory and Extended Huckel theory is done by independent sample t-test SPSS software. The CNT length was studied from 4 to 22nm in the NanoHub tool simulation environment.

Result: Comparison of data is done by independent sample test using SPSS software. There is a statistical significant difference between Extended Huckel theory and the number of P_z Orbital theory. Extended Huckel theory (77.4%) showed better results in comparison to P_z orbital theory (51.6%). Here the p value was predicted to be insignificant ($p=0.423$, $p>0.05$).

Conclusion: The Extended huckel theory based on carbon nanotubes showed the best conductivity compared to P_z orbital theory to predict its density of state using a novel CNT band tool.

Keywords: Carbon nanotube, Extended huckel theory, Density of state, P_z Orbital theory, Nanohub, Novel CNT band tool.

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INTRODUCTION

Extended huckel theory is defined as a well established method for studying the electronic structure of electrons and molecules, commonly used to determine the molecular orbital (Cuevas and Scheer 2010). The density of states in the Fermi level of single-wall carbon nanotubes can be expressed in terms of a universal relationship that depends only on whether the nanotube is metallic or semiconductingand carbon nanotube is formed when a single walled carbon nanotube is increased in a tube length (Orellana and Vásquez 2006). The importance of this work is to determine the density of state for carbon nanotubes by varying the size and position by two given comparisons (Wong and Akinwande 2011). The application of extended Huckel theory is that only valence electrons are considered; the core electron energies and functions are supposed to be more or less constant between atoms of the same type(Ali, Öchsner, and Ahmed 2010). Carbon nanotubes were synthesized by combining one or more molecules to form a large sheet-like structure (Yoosefian and Etminan 2016).

About 135 Google Scholar and 15 ScienceDirect articles were seen related to this work carried out in the last five years reporting the development of structural parametric and molecular orbital based on density of state forstructural geometry of organic molecules (Dass 2018). This article deals with predicting the density of the state of CNT using the novel CNT band. There are works regarding electrical doping in the Novel CNT band and also predicting the properties of optical carbon nanotubes (Parvaiz et al. 2020). This work is based on improving the performance of density of state of carbon nanotubes. There are few reports on the synthesis of CNT, characterization and simulation based on CNT band (Mayo 2015). It explains about the process, function and also the steps involved in the modification of carbon nanotubes. It gives a clear explanation about the structural properties of carbon material that has a strength 100-200 GPa range. This method is best in the present, due to the fact that an increase in current with increased electrical doping by using extended huckel theory is well investigated. They are reports on research that explains about the effective density of state in carbon nanotubes (Jones and Lee 2011). Our team has extensive knowledge and research experience that has translate into high quality publications(Bhansali et al. 2021; Jayanth et al. 2021; Sudhakar, Ravel, and Perumal 2021; Sathiyamoorthi et al. 2021; Deepanraj et al. 2021; Raju et al. 2021; Arun Prakash et al. 2020; Kamath et al. 2020; Shanmugam et al. 2021; Rajasekaran et al. 2020; Adhinarayanan et al. 2020; Rajesh et al. 2020; Aurtherson et al. 2021)

The unanswered problem in the simulation of a carbon nanotube to predict its density of state is whether it is semiconductor or metallic based on changing its position, size along with different (n,m) to check the property. Therefore optimizing the chirality of CNT is nessesary to determine its density of state. The aim of the proposed study is to compare the extended Huckel theory and P_z orbital theory of carbon nanotube with the novel CNT band tool to calculate the band gap by varying its tube length from 4 to 22 nm .

MATERIALS AND METHODS

This study was carried out at the simulation lab, Saveetha School of Engineering at the biomedical department, Chennai using Novel CNT band tool, and ethical approval is not necessary for our proposal study. There are two groups included in this study are extended Huckel theory and number of P_z orbital theory. Group 1 refers to extended Huckel theory based on carbon nanotube and other group is based on Pz Orbital theory based on carbon nanotube. The sample size calculation was done using previous study results (Bachour, Ali, and Alabboud 2020) using clinical.com by keeping alpha error-threshold by 0.05, enrollment ratio as 0:1, 95% confidence interval, power at 80%.

In sample preparation for two groups is done by collectively 40 dataset. 20 for each group for each category of the parameters from standard database (Nanohub.org). The proposed parameters are carbon-carbon spacing and CNT tube length. Huckel theory and number of P_z orbital theory was done to estimate the band gap; thereby evaluating the density of states.

Testing setup is done by installing a novel CNT band tool from Nanohub.org. Select the type of theory (Huckel theory or number of P_z orbital theory) in the CNT band tool. Next, select the type of simulation method. Apply the chirality like (n,m) by keeping model parameters as a constant, select the parametric and run the simulation to get the graph.

Statistical Analysis

To validate the result of both parameters, statistical analysis was done using IBM-SPSS software. The density of state was measured by using chirality (n,m) as dependent variables and model parameters as independent variables.

RESULTS

In this research work of predicting its density of state, both the techniques appear to produce the same variable results with accuracy ranging from 51.6% to 77.4%. It is observed in Fig. 1, the mean density of states of P_z orbital theory is less compared to extended Huckel theory. Figure 2 represents the outcome of Extended huckel theory and P_z orbital theory of carbon nanotube.Extended huckel theory had the highest accuracy 77.4% in comparison to the number of P_z orbital theory 51.6%. The descriptive statistics in Table 1 demonstrate band gap magnitude for extended Huckel theory based carbon nanotubes. Table 2 demonstrates band gap magnitude for P_z orbital theory based carbon nanotube. Table 3 demonstrated that extended Huckel theory had less error rate than the P_z orbital theory. Table 4 represents the mean different, accuracy, significant and std error different.There appears to

be a statistically insignificant difference (p=0.423, p>0.05) using independent sample T tests. These results showed that the extended Huckel theory can be used to predict the density of state of carbon nanotube comparison with the number of P_z orbital theory.

DISCUSSION

To simulate the carbon nanotube for predicting its density of state we need to determine the changes in the Extended huckel theory and Number of P_z orbital. Extended huckel theory had highest accuracy (77.4%) in comparison to P_z orbital theory (51.6%). From obtaining the density of state for both Extended huckel theory and P_z orbital theory p=0.423, (p>0.05). Hence it is an insignificant and independent sample T-test.

Extended huckel theory is used to calculate bulk band structure, surface density of state, electronic transmission, and interfacial chemistry of various materials within the same platform (Zienert, Schuster, and Gessner 2013). The parameter of different environments is demonstrated by comparing the surface band structure with density functional theory (Kienle et al. 2006). The transfer of the parameters investigate by applying different chemical and physical environments by calculating the band structure of two reconstructed surfaces with different orientation. It has a disadvantage that if there is any low energy consumption sometimes it may fail to determine its property (Tang, Tang, and Gong 2012). It explains the effects, electronics arrangement and aromaticity patterns of finite length carbon nanotubes. Long carbon nanotubes retain bond patterns that are characterized by the localization of carbon nanotubes with 10 nm length (Dresselhaus, Dresselhaus, and Avouris 2003). It explains the atomistic model for graphene nanoelectronics by varying the position and size of the given electron (Raza and Kan 2008). Factor affecting carbon nanotubes based on the density of state is difficult whether it is metallic or semiconductor because of low energy consumption it may fail to identify it. This study demonstrated several advantages over the other algorithms that attempted to predict and differentiate other density of state.

Extended huckel theory is expected to identify the structure and application for the carbon nanotube. It mainly depends on the molecular structure. It established a semi-empirical quantum method for the study of band structure, chemistry and transport properties of low dimensional carbon material.

CONCLUSION

In this paper the prediction of density of state, the novel extended huckel theory (77.4%) that operates using nanohub appeared to give better results when compared to P_z orbital theory (51.6%). The performance also continuously increased with increase in data which is not seen in other variables. This model is very efficient and holds a good potential to improve the prediction of the efficacy of density of state.

DECLARATIONS

Conflict of interests

No conflict of interests in this manuscript

Authors Contributions

Author MD was involved in data collection, data analysis and manuscript writing. Author SCK was involved in conceptualization, data validation, and critical review of manuscript.

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TABLES AND FIGURES

Table 1: Band Gap magnitude for extended Huckel theory based carbon nanotube.

TUBE LENGTH(nm)	CARBON-CARBON SPACING (Å)	BANDGAP MAGNITUDE(eV)
4	1.32	0.3772
5	1.42	0.3872
6	1.52	0.3712
7	1.32	0.2478
8	1.43	0.9581
9	1.52	0.7353
10	1.32	0.5963
11	1.42	0.5014
12	1.32	0.8547
13	1.42	0.6490
14	1.52	0.1962
15	1.32	0.2469
16	1.42	0.2542
17	1.52	0.5709
18	1.32	0.5613
19	1.42	0.3654
20	1.52	0.0108
21	1.32	0.5476
22	1.42	0.0458

Table 2: Band Gap magnitude for P_z orbital theory based carbon nanotube.

TUBE LENGTH(nm)	CARBON-CARBON SPACING (Å)	BANDGAP MAGNITUDE(eV)
4	1.42	0.6490
5	1.52	0.3580
6	1.32	0.2469
7	1.42	0.1080
8	1.52	0.8967
9	1.32	0.9860
10	1.42	0.3654
11	1.52	0.7530
12	1.32	0.5476
13	1.42	0.8856
14	1.42	0.6490
15	1.52	0.1962
16	1.32	0.0456
17	1.42	0.2542
18	1.52	0.0108
19	1.32	0.5613
20	1.42	0.2543
21	1.42	0.0108
22	1.32	0.0108

TABLE 3: Comparison of mean and accuracy using extended Huckel theory and P_z orbital theory.

Parameter	Group	N	Mean	Std. Deviation	Std. Error Mean

Accuracy	Extended huckel theory	20	0.7817	0.64442	0.14410
	$P_z$orbital theory	20	0.5613	0.55626	0.0.12438

TABLE 4: Independent sample T test in predicting the density of state using Extended huckel theory and P_z orbital theory. There appears to be a statistically significant difference ($p>0.05$) in both methods.

Parameter	**Levene's Test For Equality of Variances**		**t-test for Equality of Means**				**95% Confidence Interval of the Difference**	
	F	**Sig**	**t**	**df**	**Mean Difference**	**Std error difference**	**lower**	**upper**
Equal Variance assumed	0.655	0.423	1.158	38	0.2204	0.19036	-0.1649	0.6059
Equal variance not assumed			1.158	37.206	0.2204	0.19036	-0.1651	0.6059

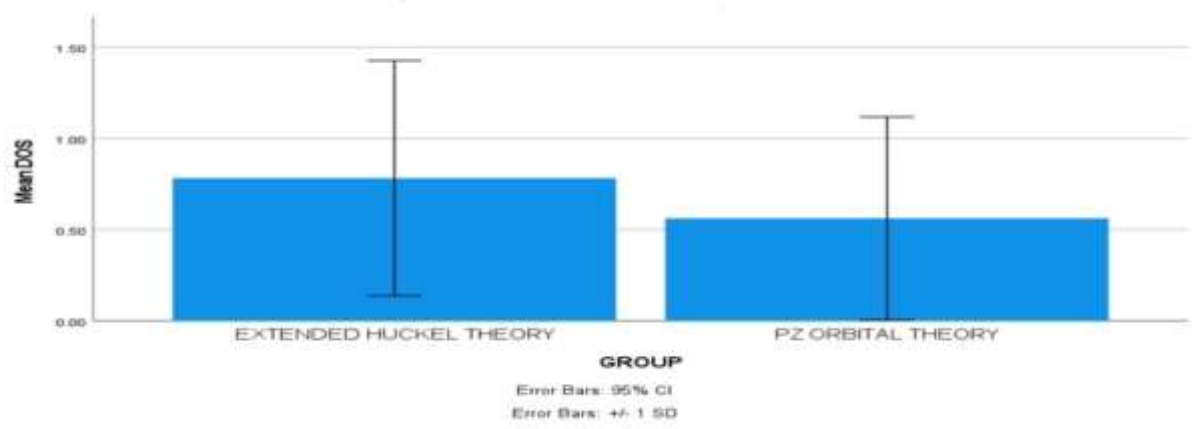
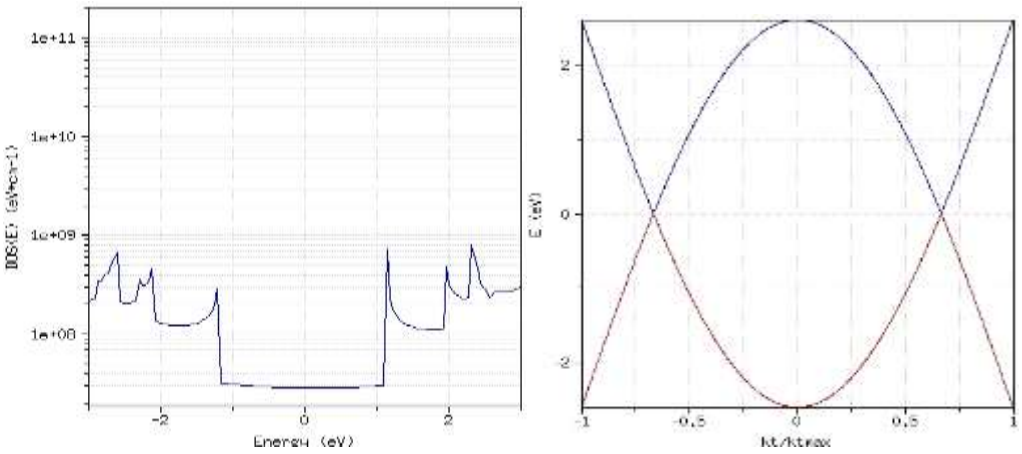


Fig. 1. Bar chart representing the comparison of structure and group of carbon nanotube with Extended huckel theory and P_z orbital theory. Both the comparisons appear to produce the same variable result with accuracy ranging from 0.53% to 0.58% X axis. Extended huckel theory and P_z orbital Y Axis. The standard deviation (SD) was calculated to be +/- 1.



(a) **(b)**

Fig. 2. Graphs represent the outcome of Extended huckel theory and P_z orbital theory of CNT BAND LAB TOOL in nanohub.org. (a) represents the y- axis as density of state and x- axis represents energy. (b) represents the y-axis as energy and x-axis represents energy.