Non Bonded Interactions in cylindrical capacitor of (m, n) @ (m', n') @ (m", n") Three Walled Nano Carbon Nanotubes

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ABSTRACT

In this study we have exhibited that there are regular non-bonded interactions among the layers of Three walled Carbon nanotubes (TWCNTs) and (10, 10), (8, 8) DWCNTs & (6,6) SWBNNTs. It has been observed the energies between three layers are sensitive to chirality dramatically. In other hands the external fields of the inner tubes make strongest fields for the outer tubes. It has been shown the non-bonded quantum mechanics in terms of wave functions and charges densities between three layers. For the systems including charges Q, the densities $(|\psi(x)|^2$ multiplied the atomic charges, yielding toward the charges densities of $|Q(x)|^2$.

Keywords: Non-covalent interaction, Three walled Nano tubes, Cylindrical capacitor.

INTRODUCTION

Three walled nanotubes (TWCNTs) can be considered as a tube twisted from hexagon sheets of graphene or boron nitrides plates which have been synthesized[1] in 1995 firstly. Boron nitrides tubes have structural analogsas carbon nano tubes. SWBNNTs, in contrast of CNTs is metallic or semiconductors depends on its chirality[1], boron nitrides tube are occasionally believed[2] to be a1-dimension insulators regarding of their helicity[3], tube's diameter and the number of tubes wall[4] Since BNNTswere synthesized[1] via arc[5] discharges successfully, the mechanism[6] for its formationsare obscure[7] yet, and the behaviors of the metallic catalyst remain an unknown question[7].

Several experiment results showed which small CNTs are occasionally found inside three-walled tubes[8-12]. Therefore, there are strong motivations for studding in phenomenon of their stabilities in small BNNTs inside the largest one[12-15], which might be helping the experimental[11] synthesis[12-14]. Besides[15], Studding on Three-walled NNTs(TWNTs) has demonstrated[14,15] interesting[16] variations in their electronics properties[17] when they are compared[18] with those of freestanding[17,18] components. Therefore it is also important for seeing the inter-walled coupling[18] behaviors associated with those small BNNTs[19,20].

Internal-layers couplings play a critical[19] function for determining properties[21] of layered three-dimensional[22] material. Truly, the novel studies

have exhibited which mechanical[20] coupling among the outer and inner shells of TWCNT sleads[19,20] for characterizing radials-breathing[20] vibration that corresponds to oscillated modes[21] with concerted[22] inner-and outer-shells motion.

It has been exhibited which TWCNTs are having high oxidativere sistance[21],which were later confirmed[23], by other scientists. Recently, some result sindicate which purified[22] SWBNNTs are resist for oxidase up to 1,100°C[23]. Further more, SWBNNTs are predicted to have piezoelectricity[24] character and are applicable[25] for room-temperatures hydrogen[26] storages.

An elastic[26] property of an individual SWBNNT has been clearly studied through thermal vibration[27]methods.

SWBNNTs were theoretically predicted[28] the uniforms electronics properties[29] which are related to it schirality and also diameters[2,3]. In addition, zigzag schiral are expected[28] for having direct[28] bands gaps. Other word, the arm chairs tubes shall have in directs band[28] gaps. Due to their large band gaps using MWBNNTs as the conduction[29] channel for fields-effects transistors[29] indicated that MWBNNTs allowed transports through the valence[29] bands. Important point sconcerning the bands gap for boron nitrides Nano tube are that those are tunable[12,13] via doping[15] with carbons. The oreticalb and gaps and densities of states calculation in point of view Fermi[17-29] level suggested[27,28] that SWBNNTs can either be *p* - types or *n* –types semi conductor through controlling[24-28] the composition[33] of carbons into SWBNNTs.

The piezoelectricity approaches originated[34] from the deformations effects because of twisting of the h-BNplanes for forming the tubes structures. It is an important behavior in BNNTs[24]. It has been exhibited that BNNTcan be amazing piezoelectric[24] system while the piezoelectric constants for different zigzags BNNT was defined for increasing along[25] with the decreases of the radiuses of BNNTs[25]. One of the most important features of BNNTs is that BNNTs possess large band gaps between 5.0 and 6.0 electron volteirrespective[29] of the number of BNNT's wall, diameter and chirality[2,16-27].

In this study we have exhibited that there are regular[18] non-bonded interactions among the layers of TWCNTs and it has been observed the energies between three layers are sensitive to chirality dramatically[12]. In other hands the external fields of the inner tubes make strongest fields for the outer tubes.

It has been shown the non-bonded quantum mechanics in terms of wave functions and charges densities[16]between three layers[17-19]. For the systems including charges$Q$, the densities ($|\psi(x)|^2$ multiplied the atomic charges, yielding toward the charges densities of $|Q(x)|^2$. Therefore, there are good relationship samong charge and wave functions of those inner tubes rather than outers. Although the wave functionsof each molecule in the systems for $\Phi_n^{Innertube}$ and $\Phi_m^{Innertube}$ under the permutations of electrons coordinate is anti-symmetric, the product of those non-bonded molecule under intermolecular exchanges of the electron couldnot be anti-symmetric.

The unique solution for this purpose is introducing the intermolecular anti-symmetrize operators. However, these would results due two major problem which were shown by Eisenschitz[38], that are, the anti-symmetrized unperturbed stateno longer eigen-function of$H^{(0)}$, which will be followed viathe[A,$H^{(0)}$]≠0, here by the projected excited state, $A^{Inn-out}$ Φ_n^{Inn} Φ_m^{Inn},become linearly dependent[38,39]. and the first-order energies including exchangescould be written as:

$$E_{antisymm}^{(1)} = \frac{\langle \Phi_0^{inn}\Phi_0^{out}|V^{inn-out}\tilde{A}^{inn-out}|\Phi_0^{inn}\Phi_0^{out}\rangle}{\langle \Phi_0^{inn}\Phi_0^{out}|\tilde{A}^{inn-out}|\Phi_0^{inn}\Phi_0^{out}\rangle}$$

Generally, the exchange interactions are commensurate[19] to the differential over laps among other parts. The wave-function as well as the exchange interaction sfades exponentially as functions of distance[38,39]. Therefore, TWCNNs with small diameter and short distance between three layers have been considered based on our previous works[30-49].

Computational details

Calculations were accomplished by Gammas package[50]. In this study, we have calculated for getting the result from DFT method and extended-hackles approaches for the no-bonded interaction samong tubes. The m06-2x,

and m06HF are new method with suitable corresponds in no-bonded interactions and are important for the distance calculations among fragments in thenon-bonded[51] systems, for medium[51] (~3–5Å). We investigated density functional theories with theory of van der Waals densities for modeling exchange-correlation senergies for the nanotubes[3-22]. The double ζ-basis set including polarize orbitals was used for boron and nitrogens atoms while single ζ-basis setincluding polarize orbital was applied for the TWCNTs, respectively[53].

For non-covalent interactions,the BLYP methods are unable for describing van der Waals[51-53] TWCNTs systems by medium-ranges interaction such as interaction between three tubes of TWCNTs. The B3LYP and some other functional are not suitable for illustrating the exchanges and correlations energies indistant medium-range non-bonded system obviously. In addition, some novel studies have exhibited that inaccuracies of the medium-ranges exchanges energies lead to asystematic error to predictof molecular properties[53-58].

Geometry optimization and electronic structures have been accomplished using the semi empirical methods such as CNDO, MINDO, and ZINDO which their approach are based on an semi empirical solution ab-initio and the Kohn-Sham equation[57] also. The density function theories in the plane-waves sets with the projector-augmented wave pseudo-potential are calculated. The Perdew-Burke-Ernzerhof[58] exchange-correlations functional for the generalized gradient approximations or GGA are adopted[58]. The optimization of the lattices constant and the atomics coordinate are made through the minimization of those total energies.

The charge stransferring and electrostatic potentials-derived were also calculated using the Merz-Kollman-Singh[59], chelp[60], or chelpg[61].

The charges calculations method based on molecular electrostatics potentials fitting are not complete-suited for estimating of bigger systems which some of those inner-most atom are located[62] far away from that point at which the MESP[62] is computed[60-62]. In these conditions, variation of the inner-most atomics charge would not leads to a significant change of the MESP[61] outside of the molecules, meaning where the accurate[62] value for the innermost atomics charge are not well-determined by MESP[62] outside[63] of those molecules. The representatives atomics charge for molecule must be computed as averages value over various molecules and conformation. A detailed overview of those effect of those basis sets on the charges distribution might be found in[63,64]. It has been extracted the charges densities prole from the rst-principle calculations through the average process described[65,66].

The interaction energies for capacitors were calculated through equation: $\Delta E_s(eV)= \{E_{TWCNT(1)}(-E_{SWCNT(2)}+E_{SWBCNT(3)})\}+E_{BSSE}$ where the "ΔE_s" are the stabilities energies of non-bonded interactions in TWCNTs.

RESULT AND DISCUSSION

The results are plotted in 6 curves and HOMO LUMO is listed in Table1.

We have estimated the electron densities and gradient norms and Laplacians, values of orbitals wave-functions, electron spin densities, electrostatic potentials from nuclear / atomics charge, electron localization functions or ELF[64-66], localized orbitals locator or LOL[64-66] defined via Becke andTsirelson, total electrostatics potentials, and the exchange-correlations densities, correlations hole and correlations factor, Averages local ionization energiesusing the Multifunctional[66] Wave-functions Analyzer[65,66]

Through density-of-state DOS[66] it has been represented the number of state in the units energies intervals, since energies levelare contiguous, so DOS[66] has drawn as curves map. The systemsare isolated, so the energies levels are discrete[66].

We have investigated the DOS[66] graphs as the tools for analyzing the natures of electron structures in the nanotubes

The original total DOS (TDOS) of our system have calculated based on)$(E)=\Sigma_i\ \delta(E-\varepsilon_i)$ where eigen value set of single-particle Hamilton is, cs Dirac Delta function which after replacing Gaussian, it can be yielded[63].
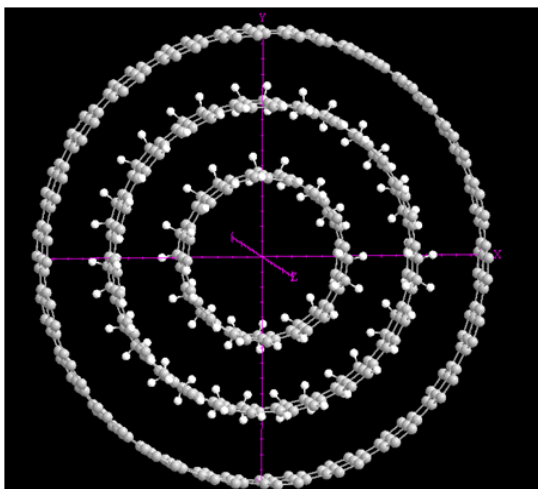
Fig.1. (10,10),(8,8),(6,6) TWCNTs in view point of Cartesian orientation
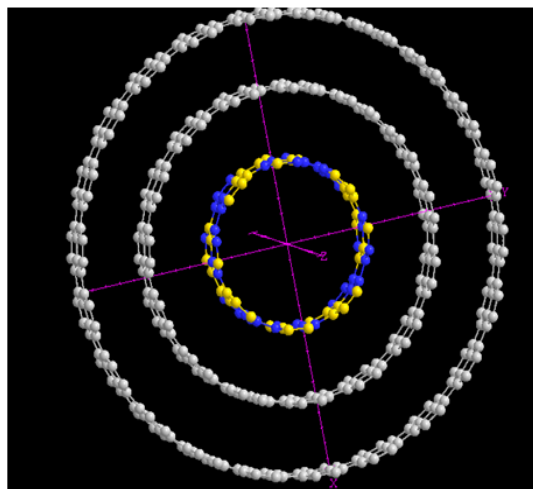

Fig.2. (10,10),(8,8)DWCNTs&(6,6) SWBNNTs in view point of Cartesian orientation
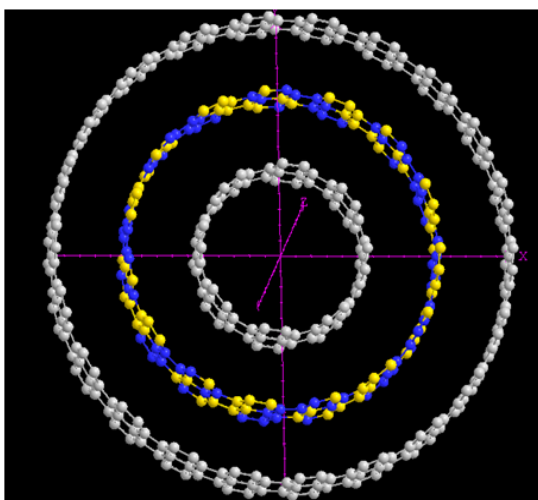

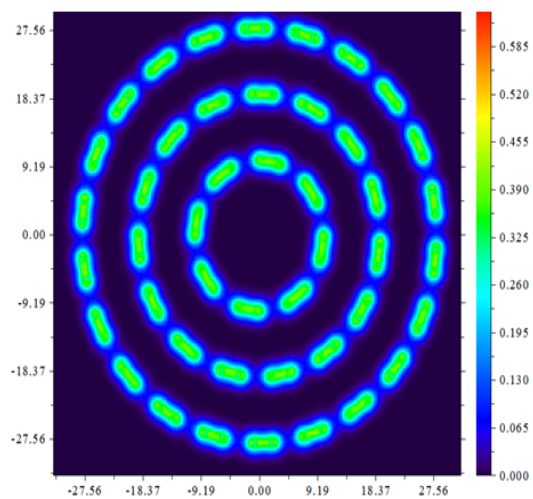**Fig.3. (10, 10), (6, 6) DWCNTs & (8,8) SWBNNTs in view point of Cartesian orientation**

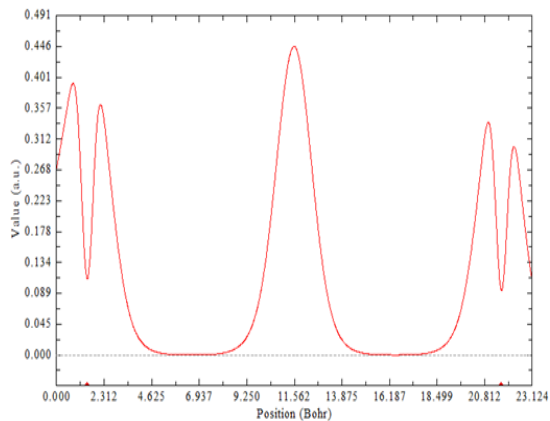**Fig.4. Color-Field map of electron density versus atomic position**

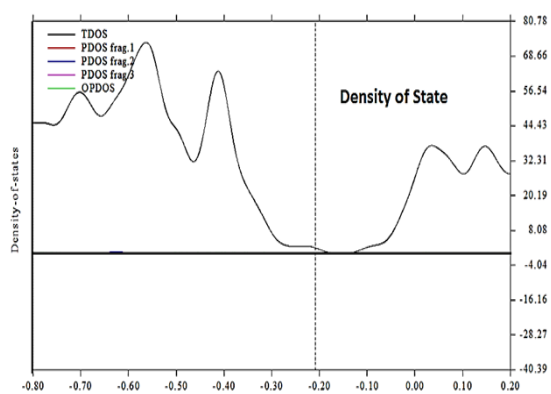**Fig.5. Electron density from atom 1 to atom 588**

Fig.6: TDOS for. (10, 10), (6, 6) DWCNTs & (8,8) SWBNNTs

$G(X) = \frac{1}{c\sqrt{2\pi}} e^{-\frac{x^2}{2c^2}}$ Where $c = \frac{FWHM}{2\sqrt{2ln2}}$ FWHM[63] is acronyms of "full width at half maximum[63], it is an adjustable parameter in multi-wave function, the larger FWHM the TDOS analysis is easier for performing. The normalized Lorentzian function is defined as L$(\chi)=$

$\frac{FWHM}{2\pi}\frac{1}{x^2 + 0.25FWHM^2}$ Pseudo-Voigt function is weighted linear combination for Gaussian function and Lorentzian formula:P(χ)=w$_{gauss}$G(χ)+$(1-$w$_{gauss})$L(χ)

The curve map of broadened partial DOS (PDOS) and overlap DOS (OPDOS) are valuable for visualizing orbital composition analysis, PDOS function of fragment *A* is defined as:

$PDOS_A(E) = \sum_i \Xi_{i,A} F(E - \varepsilon_i)$ where $\Xi_{i,A}$ is the composition of fragment "*A*" in orbital *i*. The OPDOS among fragments *A* and *B* are defined as)$OPDOS_{A,B}(E) = \sum_i X^i_{A,B} F(E - \varepsilon_i)$

where $X^i_{A,B}A,B$ is the composition of total cross term between fragment *A* and *B* in orbital *i*.

Both original and broadened TDOS/PDOS/OPDOS are shown in the graph below. The original DOS graphs are discrete comb-like lines, from which we cannot obtain any additional information other than energies level distributions, it is impossible for distinguishing different types of a line and degenerate energies level sowing for over lapping.

From the height of black curves (TDOS) we can clearly know how dense the energies levels are distributed every where. Besides, the curves corresponding to TDOS, PDOS (red line for fragment 1, blue line for fragment 2) and OPDOS (green line) no longer overlap, we can clearly identifies characters of each orbitals through observing those curves[67].

Table.1: Cartezian and charge density of atoms 550 to 588 and HOMO/LUMO gaps

Orbital	HOMO	LUMO	Gap
969	-0.208359 a.u.	-	-
970	-	-0.101978 a.u.	-
970/980	-	-	0.106381 a.u.
969	-5.669636 eV	-	-
970	-	-2.774965 eV	-
970/980	-	-	2.894771 eV
970/980	-	-	279.302769 KJ/mol

CONCLUSION

In conclusion it has been found that the external fields of the inner tubes make strongest fields for the outer tubes. It has been shown the non-bonded quantum mechanics in terms of wave functions and charges densities between three layers. It is necessary for investigating the density functional theories including theory of van-der-Waals densities for modeling exchange-correlation energies in the nanotubes for any further discussion.

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