Density of State (DOS) for Zig-Zag, Chiral and Armchair SWCNTs and DWBNNTs: In Viewpoint of Electronics and Structure

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ABSTRACT

In this work we have simulated our system based on the various distribution diameters of SWCNTs, SWBNNTs and DWCNTs in three forms of zigzag, armchair and chiral. We have start for answering to some question about the mechanical, electronical and thermochemical properties of the diameter distribution on the various nanotubes, band gape, and potential difference between two layers of a nano cylindrical and finally the radial charge distribution of those systems. It is found that the energy gaps and the energy of those SWBNNTs are strongly dependent on their Chirality and diameters. The energy gap of the formed double-walled (DW-C&BN-NTs)can even be much reduced due to the coupled effect of wall buckling difference and inter-wall π-π* hybridization.

Keyword: SWCNTs, SWBNNTs, Zig-Zag, Chiral and Armchair.

INTRODUCTION

Control and designing of nanotube diameter is needed for developing nanotube growth methods. Nanotubes with a diameter of less than 10 angstrom provide the ideal nano space in one-dimension. Twenty years ago, it was been suggested that the size of the growth catalyst used in metal[1] catalyzed chemical vapor deposition (CVD) can define the diameter of as-grown carbon nanotubes[2]. This idea has been confirmed by the observation that catalytic particles at the ends of CVD-grown nanotubes have sizes proportionate with the nanotubes diameters[3].

Small-diameter carbon nanotubes exhibit many exotic properties such as anisotropic optical absorption spectra[4] and superconductivity originated from a Peierls distortion[5].

These findings have stimulated much interest in study of small nanotubes both experimentally and theoretically.

Boron nitride nanotube (BNNT), which firstly predicted and synthesized by Rubio and Chopra respectively[6,] has a structural analogy to CNT but, contrary to the CNT being metallic (semiconductor) depending on chirality. BNNTs are usually can be an insulator regardless of their helicity, tube diameters and number of tube walls[7].

Besides, the study on double-walled BNNTs (DBNNTs) has demonstrated an interesting variation in their electronic properties when compared with those of freestanding component of BNNTs[8]. So it is also important to see the inter-wall coupling behavior and interaction energies associated with the small BNNTs.

Boron nitride nanotubes possess a large band gap [~(5 — 6) eV)] irrespective of the number of walls, diameters, electronic properties and chirality[9] In addition, they are so stable in viewpoint of chemical and mechanical structures[10]. Therefore, thin single-wall BNNTs (SWBNNs) can widely be used as an ideal nanotube for nano science to produce special materials such as atomic wires, capacitors and semiconductors. In our study the SWBNNs is a suitable material as an insulator to produce nano-cylindrical capacitors.

They used arc-grown SWCNTs (with a diameter distribution of 1.4 ± 0.1 nm) as a template to synthesize thin SWBNNTs. The uniform diameter distribution of SWCNT-templates is essential to realize a diameter selective synthesis of BNNTs (diameter of 0.7 ± 0.1 nm has expected for thin SWBNNTs by them)

In this work we have calculated our systems based on the various distribution diameters of SWBNNTs and SWCNTs .The effects of these doping on the electrostatic properties of the inner and outer tubes can also be calculated for any further comparison and discussion.

Monajjemi and coworkers have simulated a large range of the nanotube carbons and other molecules via a wide range of methods and basis sets[11-127]

Zigzag BNNTs (n, 0) are expected to have direct band gap. On the other hand, armchair BNNTs (m, m) will have indirect band gap[128]. Because of their large band gap of (~5 eV), experiments using BNNTs as the conduction channel for field-effect transistors (FETs) showed that BNNTs allowed transport through only the valence band.

Another important feature about the band gaps of BNNTs is that they are tunable by doping with carbon, radial deformation, or by applying a transverse electric field across the BNNT "so-called giant stark effect"[129].

Theoretical band structure calculations suggested that SWBNNT can either be p-type or n-type semiconductors by controlling the composition of carbon into SWBNNTs. Carbon impurities on the boron sites result in electron carriers while on the nitrogen sites result in hole carriers[130].

On the other hand, the band-gap modification by radial deformation in BNNTs was predicted through first-principles pseudo-potential density-functional calculations.

In zigzag BN nanotubes, radial deformations due to transverse pressures of about 10 GPa decrease the direct band gap of BNNTs from 5 to 2 eV, allowing for optical applications in the visible range[130]. However, the band gaps of armchair BNNTs are found to be insensitive to radial deformations. Finally, theory indicates that the band gap of BNNTs can be reduced and even completely removed by the application of transverse electric field onto BNNTs and simultaneously probing the electronic properties.

In this study we exhibited that the piezoelectricity for BNNTs causes to increase the capacity of BNNTs @ X doped-CNTs capacitor compare to CNTs @ CNTs. This phenomenon theoretically originated from the deformation effect due to the rolling of the planar hexagonal BN networks to form tubular structures[131]. Nakhmanson and coworkers showed that BNNT could be excellent piezoelectric systems[132]. As an example of calculations, piezoelectric constant for different zigzag BNNTs was found to increase along with the decrease of the radius of BNNTs [132] Experimentally, Bai et al. have shown that under in situ elastic bending deformation at room temperature

inside a 300-kV high-resolution transmission electron microscope, a normally electrically insulating MW-BNNT may transform to a semiconductor[133].

One of the main purposes in this study of explaining the capacitor model is concerning the interaction between SWCNTs and SWBNTs is both of electronic transport properties and energy analysis. Although there are many data and a novel method for electronic transport reports for the double-wall carbon nanotubes, for BNNTs @ WCNTs there are not significant works, spatially the subject of this work for BNNTs @ X-doped-WCNTs is completely new.

Based on previous works, we simulated our model in viewpoint of various diameters and chirality by considering the SWCNTs and SWBNNTs.

The electronic structure

The electron density has been defined as

$$\rho(r) = \eta_i \left| \varphi_i(r) \right|^2 = \sum_i \eta_i \left| \sum_l C_{l,i} \chi_i(r) \right|^2$$

...(1)

[134-136]Where ηi is occupation number of orbital (*i*), is orbital wave function, χ is basis function and C is coefficient matrix, the element of i_{th} row j_{th} column corresponds to the expansion coefficient of orbital *j* respect to basis function *i*. Atomic unit for electron density can be explicitly written as $e/Bohr^3$.

$$\nabla\rho(r) = \left[\left(\frac{\partial\rho(r)}{\partial(x)} \right)^2 + \left(\frac{\partial\rho(r)}{\partial(y)} \right)^2 + \left(\frac{\partial\rho(r)}{\partial(z)} \right)^2 \right]^{\frac{1}{2}}$$

...(2)

$$\nabla^2\rho(r) = \frac{\partial^2\rho(r)}{\partial x^2} + \frac{\partial^2\rho(r)}{\partial y^2} + \frac{\partial^2\rho(r)}{\partial z^2}$$

...(3)

[134-136] The kinetic energy density is not uniquely defined, since the expected value of kinetic energy operator

$$< \varphi \left| -\left(\frac{1}{2} \right) \nabla^2 \right| \varphi >$$

...(4)

can be recovered by integrating kinetic energy density from alternative definitions. One of commonly used definition is:

$$k(r) = -\frac{1}{2} \sum_i \eta_i \varphi_i^*(r) \nabla^2 \varphi_i(r)$$

...(5)

Relative to *K*(r), the local kinetic energy definition given below guarantee positivizes everywhere; hence the physical meaning is clearer and is more commonly used.

The Lagrangian kinetic energy density, "G(r)" is also known as positive definite kinetic energy density.

$$G(r) = \frac{1}{2}\Sigma_i \eta_i \left| \nabla(\varphi_i) \right|^2 = \frac{1}{2}\Sigma_i \eta_i \{ [(\frac{\partial\varphi_i(r)}{\partial(x)})^2 + (\frac{\partial\varphi_i(r)}{\partial(y)})^2 + (\frac{\partial\varphi_i(r)}{\partial(z)})^2] \}$$

...(6)

K(r) and *G*(r) are directly related by Laplacian of electron density

$$\frac{1}{4}\nabla^2\rho(r) = G(r) - K(r)$$

...(7)

Becke and Edgecombe noted that spherically averaged likespin conditional pair probability has direct correlation with the Fermi hole and then suggested electron localization function (ELF)[135].

$$ELF(r) = \frac{1}{1+[D(r)/D_{0(r)}]^2}$$

...(8)

where

$$D(r) = \frac{1}{2}\Sigma_i \eta_i \left| \nabla\varphi_i \right|^2 - \frac{1}{8}[\frac{\left| \nabla\rho_\alpha \right|^2}{\rho_\alpha(r)} + \frac{\left| \nabla\rho_\beta \right|^2}{\beta(r)}]$$

...(9)

and

$$D_{0(r)} = \frac{3}{10}(6\pi^2)^{\frac{2}{3}}[\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}}]$$

...(10)

for close-shell system, since

$$\rho_\alpha(r) = \rho_\beta(r) = \frac{1}{2}\rho$$, *D* and *D*0 terms can be simplified as

$$D(r) = \frac{1}{2}\Sigma_i \eta_i \left| \nabla\varphi_i \right|^2 - \frac{1}{8}[\frac{\left| \nabla\rho \right|^2}{\rho(r)}]$$

...(11)

$$D_{0(r)} = \frac{3}{10}(3\pi^2)^{\frac{2}{3}}\rho(r)^{\frac{5}{3}}$$

...(12)

Savin *et al.* have reinterpreted ELF in the view of kinetic energy, which makes ELF also meaningful for Kohn-Sham DFT wave-function or even post-HF wave-function. They indicated that $D(\mathbf{r})$ reveals the excess kinetic energy density caused by Pauli repulsion, while $D0(r)$ can be considered as Thomas-Fermi kinetic energy density. Localized orbital locator (LOL) is another function for locating high localization regions likewise ELF, defined by Schmider and Becke in the paper. We have calculated the Hamiltonian kinetic energy and density Electron localization function of lithium in diffusion model for several of SWBNNTs, SWCNTs and WBNNTs @ SWCNTs

The Total electrostatic potential (ESP) measures the electrostatic interaction between a unit point charges placed at r and the system of interest. A positive (negative) value implies that current position is dominated by nuclear (electronic) charges. Molecular electrostatic potential (ESP) has been widely used for prediction of nucleophilic and electrophilic sites for a long time.

It is also valuable in studying hydrogen bonds, halogen bonds, molecular recognitions and
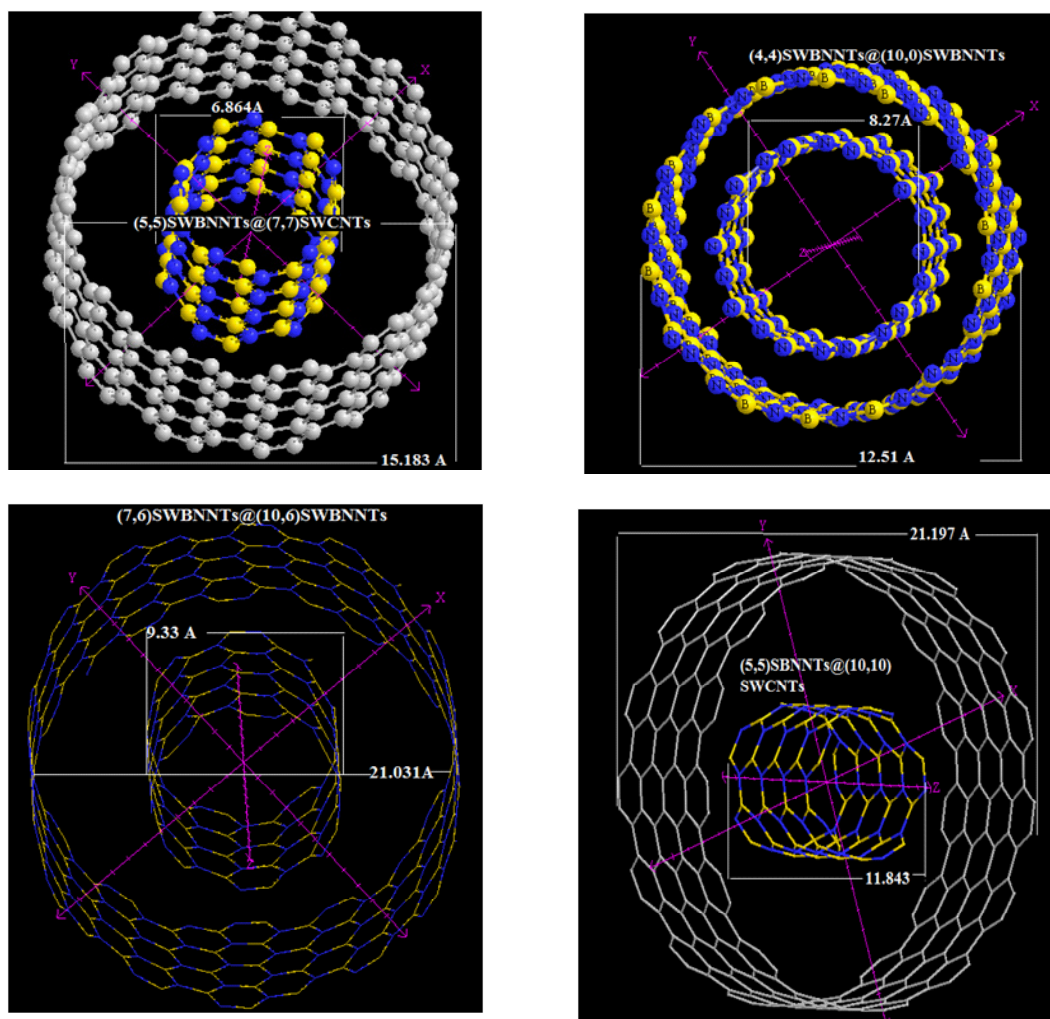

Fig.1: Various SWCNTs and SWBNNTs inside together to produce DWBNNTs &DWCNTs

the intermolecular interaction of aromatics. The ESP evaluated under default value is accurate enough in general cases.

Computational details

     Calculations were performed using Gaussian 09 and GAMESS-US packages[137]. In this study, we have mainly focused on getting the optimized results for each tube from HF and DFT methods including the B3lyp and Blyp. Extendedhuckel calculations using Gaussian program have done for the non-bonded

interaction between BNNTs and X-doped-SWNTs which are monotonous through the comparison between different situations.

     Geometry optimizations and electronic structure calculations for tubes have been carried out using the 6-31g and 6-31g* basis sets.

     A fixed BNNT geometry with B-N bond lengths of 1.445 Å, and B-H and N-H bond lengths of 1.185 Å and 1.05 Å, respectively, are chosen with no further geometry optimization. The outer ring, initially placed at the center of the inner tube, is rigidly axially shifted and rotated around the fixed inner shell.

     The charge transfer and electrostatic potential-derived charge were also calculated using the Merz-Kollman-Singh[138], chelp[139] or chelpG[140] the charge calculation methods based on molecular electrostatic potential (MESP) fitting are not well-suited for treating larger systems whereas some of the innermost atoms are located far away from the points at which the MESP is computed.

     In such a condition, variations of the innermost atomic charges will not lead towards a significant change of the MESP outside of the molecule, meaning that the accurate values for the innermost atomic charges are not well-determined by MESP outside the molecule. This approach (CHELPG) is shown to be considerably less
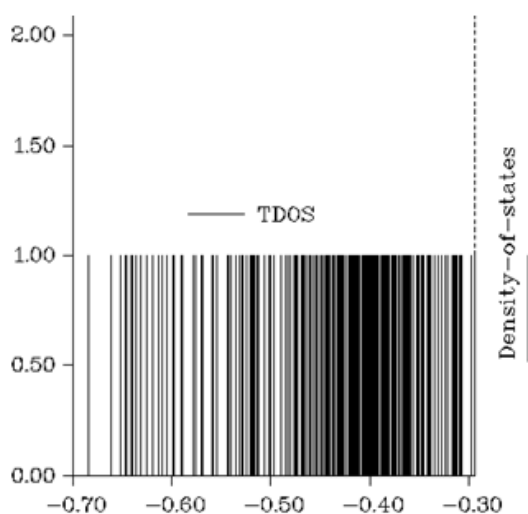

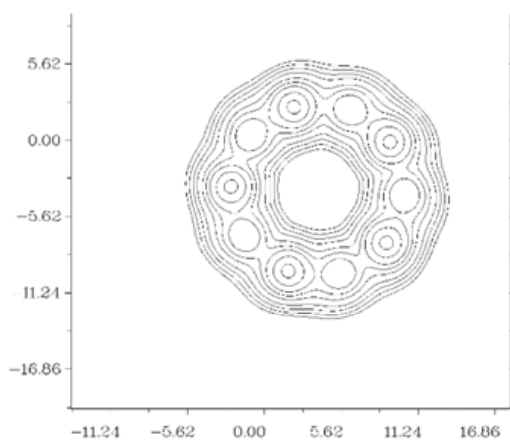**Fig. 2: Density of state for SW (4, 4) BNNTs@ (10, 10) SWBNNTs**

Fig. 3: Counter map of (5,5)SWBNNTs

Fig. 4: Counter map of (5,5)SWBNNTs@(7,7) SWCNNTs

dependent upon molecular orientation than the original CHELP program. The results are compared to those obtained by using CHELP.

In the CHELPG (Charges from Electrostatic Potentials using a Grid based method), atomic charges are fitted to reproduce the molecular electrostatic potential (MESP at a number of points around the molecule. The MESP is calculated at a number of grid points spaced 3.0 pm apart and distributed regularly in a cube. Charges derived in this way don't necessarily reproduce the dipole moment of the molecule. CHELPG charges are frequently considered superior to Mulliken charges as they depend much less on the underlying theoretical

method used to compute the wave function (and thus the MESP)[141-142].

RESULT AND DISCUSSION

The results are shown in Figs 1-7 and tables1. The system has been modeled with Armchair, Zigzag and Chiral as an impurity among the atoms of the outer nanotube layer. The total energy contains three terms including the band structure energy of the inner and outer tubes and the electrostatic energy of the layers charge distribution. In this model, the SWBNNTs compare to SWCNTs tubes have been chosen by various diameters, therefore, as the SWNTCs, the boron atom also
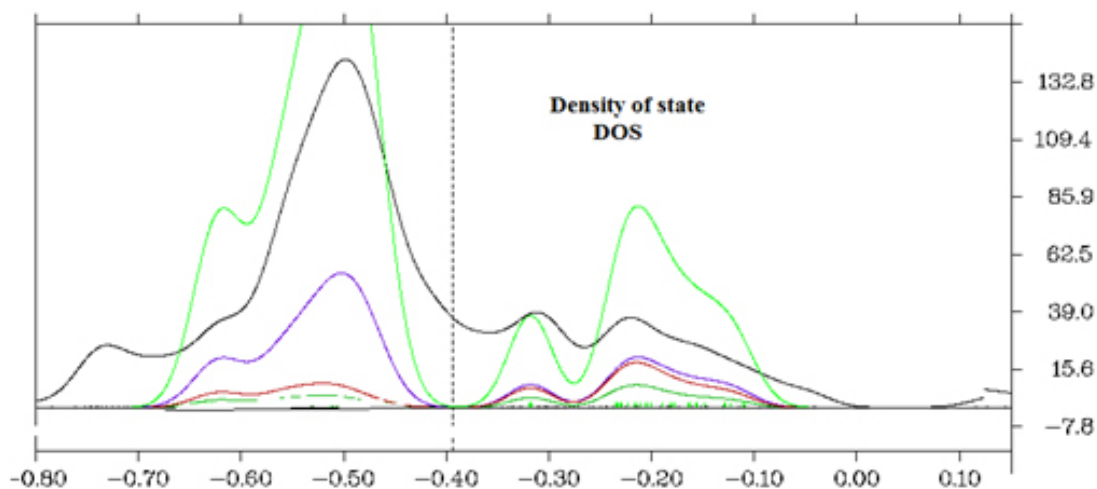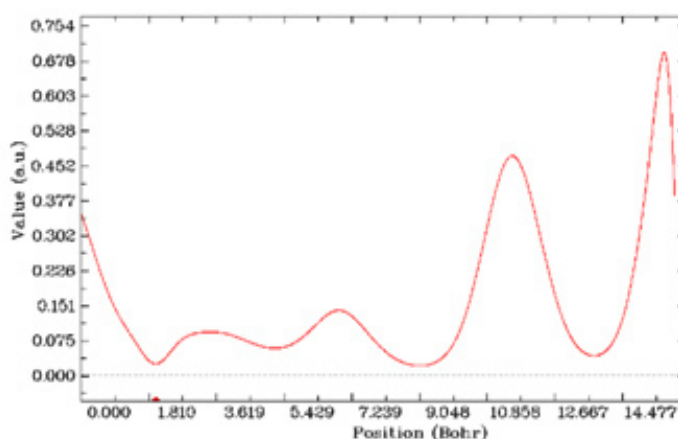

Fig. 5: Density of state

Fig. 6: The electron density between
0.0 to 15.0 (Bohr) position in (10, 10) SWCNTs

Table1: Density, energy, Electron localization function (ELF), Localized orbital locator (LOL) and Local Entropy for C, B and N in various SWBNNTs and SWCNTs

Atom No.	Density of all electron × (10⁻⁴)	Density of α electron (10⁻⁴)	Density of β electron × (10⁻⁴)	Potential energy density (×10⁻³ J)	Hamiltonian kinetic Energy (×10⁻⁴ J)	LOL ×10⁻³	Local Entropy × 10⁻⁶	Local Ellipticity	ELF × 10⁻⁷	Eta index
C(10)	0.28	0.14	0.14	-0.20	-0.10	0.15	0.50	-0.45	0.41	0.15
B(20)	0.20	0.10	0.10	-0.22	-0.14	0.13	0.59	-0.33	0.40	0.13
N(21)	0.24	0.12	0.12	-0.26	-0.12	0.23	0.51	-0.33	0.42	0.14
C(4)	0.26	0.13	0.13	-0.22	-0.14	0.21	0.55	-0.26	0.41	0.15
B(6)	0.32	0.16	0.16	-0.28	-0.15	0.26	0.47	-0.49	0.35	0.11
N(7)	0.36	0.18	0.18	-0.24	-0.17	0.21	0.41	-0.19	0.31	0.12

undergoes the sp² hybridization. Due to the relatively similar size of C and B, no significant distortion in 3-D structure of tube is expected, except for the change in adjoining the bond length. By doping the boron atoms in SWNTCs, the Fermi level shifts significantly below the Dirac point resulting in a p-type doping. This would break the symmetry of tubes into two sub layers due to presence of the B atoms which would eventually lead towards a change of the behavior of tubes from semimetal to conductor.

It is shown that the buckling rapidly increases with decreasing the tube diameter but is nearly independent of the chirality. This result is consistent with the reported trend revealed by tight-binding and ab initio calculations. The wall buckling is driven by different hybridizations related with the B and N atoms.

Two physical effects act in concert to segregate most of the holes onto the outer nanotube. First, the band gaps of the smaller diameter tubes tend to be larger, so they empty last. Second, the cylindrical geometry preferentially raises the electrostatic potential at the inner tube. Only the charge on the inner tube affects the potential difference between the two layers. Figures 1 shows the results of the energy minimization. The stability of small BNNTs encapsulated in a larger x-doped CNT is confirmed by this work. As the total energies of the small BNNTs are higher than those of their uncurled states, examination the behavior of the small BNNTs inside a larger BNNT should be necessary. It is apparent that the small BNNTs become globally stable in their energy favorable outer shells. Encapsulation induced enhancement in stability should be able to extend into other small BNNTs. The electronic properties of SWCNTs and SWBNNTs are listed in table1.

We will call the lowest π* state as singly degenerate state hereafter for all the small BNNTs. In BNNTs, the π* states are mainly distributed on the B atoms from the pz orbitals perpendicularly to the tube wall. So it can be imagined that a shorter B-B distance along the circumference will be more favorable for an overlapping of the singly degenerate state inside the tube, thus enhancing the π* -σ* hybridization. With increasing chiral angle of the BNNT, there are two primary variations that could

significantly affect such overlapping: (i) Increasing nearest B-B distance along the circumference.

Besides, we also note that the repulsion between the NFE and π* bands becomes increasingly significant from the (2, 2) to (4, 0) BNNTs, indicating that the NFE-π* hybridization becomes stronger with decreasing chiral angle as well. This phenomenon gives us a hint that the amplitude of NFE-π hybridization is proportional to that of π* -σ* hybridization. On the other hand, it is found that the nearest B-B distance along the circumference can also be reduced by decreasing the tube diameter, which is decreased to 2.16 Å in the (3, 0) BNNT. That is why the energy gap displays apparent diameter dependence in the small zigzag BNNTs.

The data of Density of all electron, Density of electron, Density of β electron, Potential energy density, Hamiltonian, kinetic energy, Hamiltonian kinetic Energy, LOL, local Entropy, ellipticity, ELF, eta index of several atoms in nanotube have listed in table1. For calculation the electron spin density from the difference between alpha and beta density, we have used $\rho^s(r) = \rho^\alpha(r) - \rho^\beta(r)$ then the spin polarization parameter function will be returned instead of spin density $\xi(r) = \frac{\rho^\alpha(r) - \rho^\beta(r)}{\rho^\alpha(r) + \rho^\beta(r)}$. The kinetic energy density, Lagrangian kinetic energy density, and the electrostatic potential from nuclear / atomic charges can be calculated as the 1-5 eqs.

The larger the electron localization is in a region, the more likely the electron motion is confined within it. If electrons are completely localized, then they can be distinguished from the ones outside. Bader found that the regions which have large electron localization must have large magnitudes of Fermi hole integration. However, the Fermi hole is a six-dimension function and thus difficult to be studied visually.

Since $D0(\mathbf{r})$ from eqs. 5-10 is introduced into ELF as reference, what the ELF reveals is actually a relative localization. ELF is within the range of [0, 1]. A large ELF value means that electrons are greatly localized, indicating that there is a covalent bond, a lone pair or inner shells of the atom involved. ELF has been widely used for a wide variety of systems, such as organic and inorganic small molecules, atomic crystals, coordination compounds, clusters, and for different problems, such as the revealing atomic shell structure, classification of chemical bonding, verification of charge-shift bond, studying aromaticity.

LOL has similar expression compared to ELF. Actually, the chemically significant regions that highlighted by LOL and ELF are generally qualitative comparable, while Jacobsen pointed out that LOL conveys more decisive and clearer picture than ELF, Obviously LOL can be interpreted in kinetic energy way as for ELF; however LOL can also be interpreted in view of localized orbital. Small (large) LOL value usually appears in boundary (inner) region of localized orbitals because the gradient of orbital wave-function is large (small) in this area. The value range of LOL is identical to ELF, namely [0, 1].

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