



## Calculating the Electronic Transport Properties of Different Carbon Nanotube Based Intramolecular Junctions

<sup>1</sup>Rashid Nizam, S. Mahdi <sup>2</sup>A. Rizvi and <sup>1</sup>Ameer Azam

<sup>1</sup>Department of Applied Physics, Aligarh Muslim University, Aligarh, India

<sup>2</sup>Department of Mechanical Engineering, Aligarh Muslim University, Aligarh, India

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**Abstract:** The electronic structure and the conductance of carbon nanotube based metal/semiconductor/metal intramolecular junctions are investigated numerically. The nature of electronic states at the interfaces and in the semiconductor section is analysed with the help of tight-binding method. The quantum conductance of the system is calculated in the logical regime and its variations with energy have been observed. These quantum conductances have been compared among the different carbon nanotubes and that have been correlated with the pentagon and heptagon that formed in the intramolecular junction.

**Key words:** Transport properties, Electronic structure, Semiconductor, Intramolecular junction, Carbon nanotube

### INTRODUCTION

The study of transport through molecular junctions is an important topic in nanotechnology [1]. Single-wall carbon nanotubes are interesting in this context, thanks to several of their remarkable properties: they are stable; they can be manipulated; they can be contacted to external leads; they can be both metallic and semiconducting depending on the diameter and helicity of their atomic structure. Last but not least, semiconducting nanotubes can be doped by application of an electric field [2], as in conventional MOS field-effect transistors. The possibility of realizing seamless connections between single-walled nanotubes with different helicities has stimulated a great interest, because metal/semiconductor junctions with simple interfaces can be obtained in this way. Rectifying current properties were predicted for these systems [3], as in a diode and were further verified experimentally [4]. A simple end to end connection between two different nanotubes, called an intramolecular junction, can be realized by the incorporation of an equal number of pentagons and heptagons, just a single pair in the simplest case [5, 6]. More complex structures can be formed, still by incorporating pentagons and heptagons in the otherwise perfect honeycomb arrangement of the carbon atoms.

It is believed that intramolecular junctions can also be produced, perhaps in a controlled way, by electron irradiation of individual single-wall nanotubes [7]. If a two-terminal device like a metal/semiconductor intramolecular junction offers little interest for logical circuits compared to all-transistor devices, it presents the advantage of being a simple object to deal with. On the theoretical side, intramolecular junctions are ideal systems to consider for the study of the electronic structure of metal/semiconductor [8-11], metal/metal [12] and semiconductor/ semiconductor [13] interfaces, to investigate the Schottky barrier formation in such junctions [14, 15] and to calculate their transport properties [6, 16-18].

### Model and numerical method

**Individual Carbon Nanotube Electronic Properties:** CNT can be perceived as a wrapped graphene, which is a 2-dimensional carbon atom lattice. Therefore, all of the atoms in the CNT have  $sp^2$  hybridization. The way how to wrap the graphene to become a carbon nanotube is the most important concept to comprehend structure and properties of CNT. The way how to wrap the graphene is so called as the chiral vector [19]. This chiral vector is one of the parameters that define the symmetry of CNT,

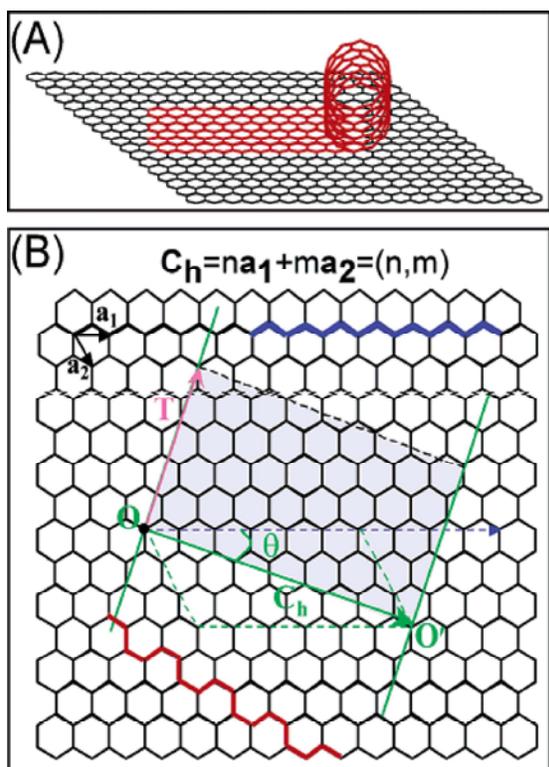


Fig. 1: Wrapped graphene

which is a non-bravais lattice. One unit cell of CNT is bound by two vectors, which are the chiral vector and its perpendicular pair, the translational vector.

On the 2-dimensions graphene sheet unit vector reference, the chiral vector is defined as

$$\vec{C} = n\vec{a}_1 + m\vec{a}_2 \quad (1)$$

Where  $n$  and  $m$  are integers, which satisfies  $0 = |m| = n$  as shown in fig. 1 ; meanwhile,  $\vec{a}_1$  and  $\vec{a}_2$  are the real space unit vectors of the hexagonal lattice, which are expressed as

$$\begin{aligned} \vec{a}_1 &= a \left( \frac{\sqrt{3}}{2} \hat{i} + \frac{1}{2} \hat{j} \right) \\ \vec{a}_2 &= a \left( \frac{\sqrt{3}}{2} \hat{i} - \frac{1}{2} \hat{j} \right) \end{aligned} \quad (2)$$

Where  $\hat{i}$  and  $\hat{j}$  are the unit vectors in cartesian coordinate,  $a = |\vec{a}_1| = |\vec{a}_2| = 1.423 \text{ \AA}$  is the lattice constant of two dimensional graphite. On the other hand, the translational vector, which derived from the perpendicular condition, is expressed by

$$T = t_1 a_1 + t_2 a_2 \equiv (t_1, t_2) \quad (3)$$

Where  $t_1$  and  $t_2$  are expressed as

$$\begin{aligned} t_1 &= (2m + n)/d_R \\ t_2 &= -(2n + m)/d_R \end{aligned} \quad (4)$$

Here  $d_R$  is the greatest common divisor of  $(2m + n)$  and  $(2n + m)$ . From those two geometrical features of CNT, it could be derived some other CNT parameters which would be useful for the CNT electronic properties identification. By using the Laue conditions, it could be obtained two reciprocal lattices of CNT, which are

$$\begin{aligned} \vec{K}_1 &= \frac{1}{N_{hex}} (-t_2 \vec{b}_1 + t_1 \vec{b}_2) \\ \vec{K}_2 &= \frac{1}{N_{hex}} (-m \vec{b}_1 - n \vec{b}_2) \end{aligned} \quad (5)$$

The reciprocal lattices of 2-dimensional graphene sheet are  $\vec{b}_1$  and  $\vec{b}_2$ ; meanwhile, the number of hexagonal in one CNT's unit cell is  $N_{hex}$ .

**Model:** To build models of the intramolecular junctions (IMJs), the SWNT  $(n,m)$  indices that correspond to a specific combination of  $d$  and  $\theta$  [20] were determined by using an iterative projection matching method [21]. For the semiconducting and metallic portions, various indices are used such as  $(5, 5)$  and  $(7, 4)$ , respectively. Here each nanotube  $20 \text{ \AA}$ , almost the same radii is used with total length  $40 \text{ \AA}$ . The energy grid of different nanotube is used  $=12\text{eV}$  and  $\pm 2\text{eV}$  at the lower and upper bound of nanotube respectively. SWNT segments with these indices can be joined faultlessly along a common axis using different configurations of 5-7 defects.

Various low-energy structural models are shown (Fig. 2-8), which have been optimized using molecular mechanics energy minimization. It is possible to evaluate the possibility of these atomic models by calculating the local electronic density of states (DOS) and comparing these with experiment [22]. But very few experiments have done to join the different various carbon nanotubes. The simulation of each intramolecular junction is done, that contain 1000 energy points including on the both grids. The system is described by a simple tight-binding Hamiltonian with constant nearest neighbour. In this study, the same parameter is used for the bonds of the pentagon-heptagon pairs. For a more accurate model, parameters fitted from tight-binding

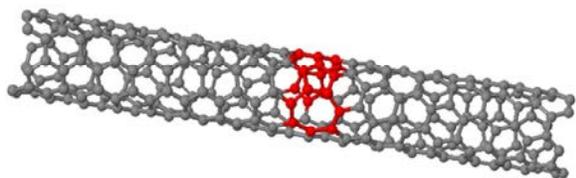


Fig. 2: Intramolecular junctions of first carbon nanotube

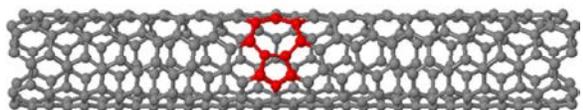


Fig. 3: Intramolecular junctions of second carbon nanotube

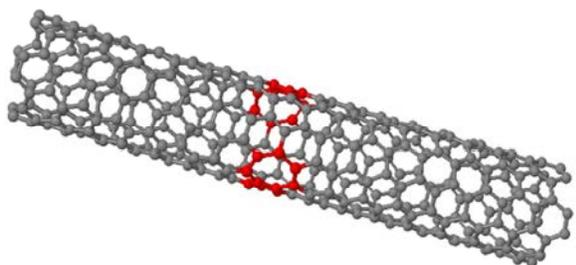


Fig. 4: Intramolecular junctions of third carbon nanotube

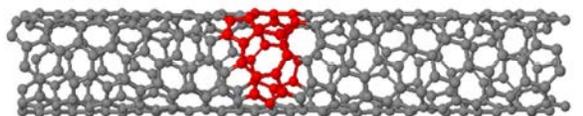


Fig. 5: Intramolecular junctions of fourth carbon nanotube

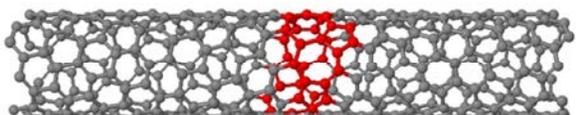


Fig. 6: Intramolecular junctions of fifth carbon nanotube

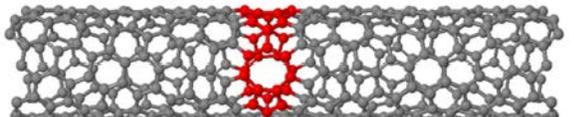


Fig. 7: Intramolecular junctions of sixth carbon nanotube

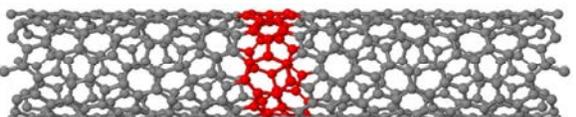


Fig. 8: Intramolecular junctions of seventh carbon nanotube

calculations should be used. The Hamiltonian is divided in two blocks corresponding to two semiconductors nanotube or semiconductor-metallic nanotubes or two metallic nanotubes as shown in different figures.

The quantities of interest in this study are the local density of states (DOS) and the multi-channel Landauer-Buttiker conductance in the coherent regime [23]. The DOSs is computed using the standard recursion technique [24]. The Landauer-Buttiker conductance at energy  $E$  is expressed with the trace formula [25, 26].

$$\zeta(E) = \frac{2e^2}{h} Tr[\Gamma_1 G^r \Gamma_2 G^a] \quad (6)$$

The conductance is proportional to the conductance quantum  $\zeta_0 = 2e^2/h$  and to the sum of the transmission coefficients of conducting channels at energy  $E$ .  $G^{r,a}$  are the retarded and advanced Green functions inside the system  $S$ , taking into account the coupling with the electrodes via the self-energies  $\sum_1^{r,a}$  and  $\sum_2^{r,a}$  [26].

$$G^{r,a}(E) = [E - H_s - \sum_1^{r,a}(E) - \sum_2^{r,a}(E)]^{-1} \quad (7)$$

The operators  $\Gamma_{1,2}$  are also related to the self-energies

$$\Gamma_i(E) = i \left( \sum_i^r(E) - \sum_i^a(E) \right) \quad (8)$$

The self-energies and the Green functions are calculated by the decimation technique [26-28]. The system is divided along the tube axis into main layers, each one being only coupled to its two nearby layers. In the present paper we have connected fourteen chiral carbon nanotubes into seven carbon nanotubes with almost same radius respectively but the simplification chiral is used again and again as follows.

- Semiconductor (5, 3)-semiconductor (5, 3) radii, 2.74 Å and 266 number of atoms respectively. As shown in fig 2
- Semiconductor (5, 4)-semiconductor (5, 4) radii, 3.06 Å and 294 number of atoms respectively. As shown in fig 3
- Semiconductor (6, 4)-semiconductor (6, 4) radii, 3.11 Å and 332 number of atoms respectively. As shown in fig 4
- Semiconductor (6, 4)-metallic (6, 3) radii, 3.11 Å, 3.41 Å respectively and 314 number of atoms. As shown in fig 5
- Semiconductor (7, 3)-metallic (7, 4) radii, 3.48 Å, 3.77 Å respectively and 353 number of atoms. As shown in fig 6
- Metallic (7, 4)-metallic (7, 4) radii, 3.77 Å, 3.77 Å respectively and 364 number of atoms. As shown in fig 7
- Semiconductor (8, 4)-semiconductor (8, 4) radii, 4.14 Å and 406 number of atoms respectively. As shown in fig 8

## RESULTS AND DISCUSSION

The nanometer dimensions of the carbon nanotubes together with the unique electronic structure of a two dimensional graphene sheet make the electronic properties of these one-dimensional carbon nanotube structures highly unusual. The aim of the present section is to relation between the atomic structure and the electronic conductance properties of SWNTs. The rich interplay between the structural and electronic properties of carbon nanotubes gives rise to new physical phenomena and the possibility of novel nanoscale device applications.

As shown in the previous section, a SWNT is geometrically just a graphene strip. Its structure can be specified or indexed by its circumferential periodicity and its chiral vector ( $C_h$ ) in terms of a pair of integers ( $n,m$ ). Early theoretical calculations [29, 30 and 19] have shown that the electronic properties of the carbon nanotubes are very sensitive to their geometric structure. Although graphene is a zero-gap semiconductor, theory has predicted that carbon nanotubes can be either metals or semiconductors with different size energy gaps, depending very sensitively on the diameter and helicity of the tubes, i.e., on the indices ( $n,m$ ). We observe that the density of state in every nanotube change due to the present of pentagon and heptagon. The greater the number of pentagon and heptagon greater will the deviation in the carbon nanotube density of state. Although the same carbon nanotubes are used in the formation of intramolecular junction still it shows the variation in the density of state. It becomes extensive large when the different carbon nanotubes are joined to form intramolecular junction. It is represented in the other two carbon nanotube.

In each case, the red colour line in the density of state diagram represents the previous density of state before joining of the carbon nanotube and the blue colour line represents the density of state after joining of the carbon nanotubes with intramolecular junction. But when different carbon nanotubes i.e. one semiconductor and the other is metallic are used, greater deviation occur and it is seen in 4) and 5) above mention cases. In these cases the green colour line and the red colour line represent the density of state of metallic and semiconductor carbon nanotube before joining of intramolecular junction. The final resultant density of state is represented by blue colour line in the same respective diagram. It appears that the resultant density become metallic type due to the formation of pentagon and heptagon at the intramolecular

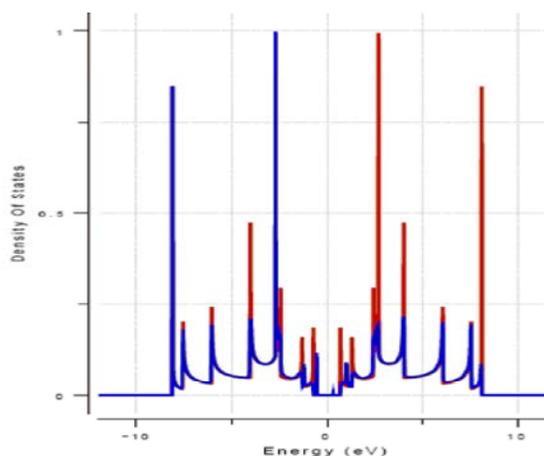


Fig. 9: Density of states for the case 1)

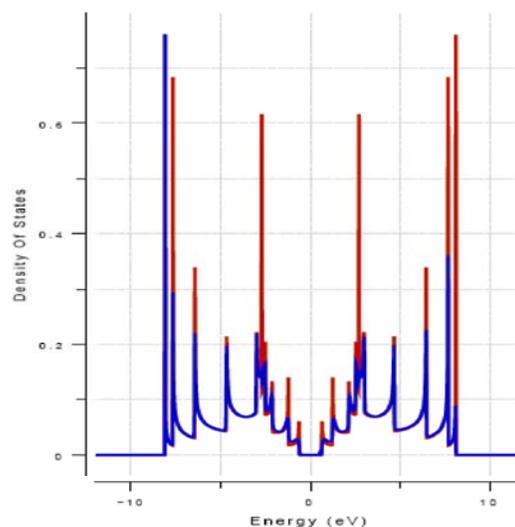


Fig. 10: Density of states for the case 2)

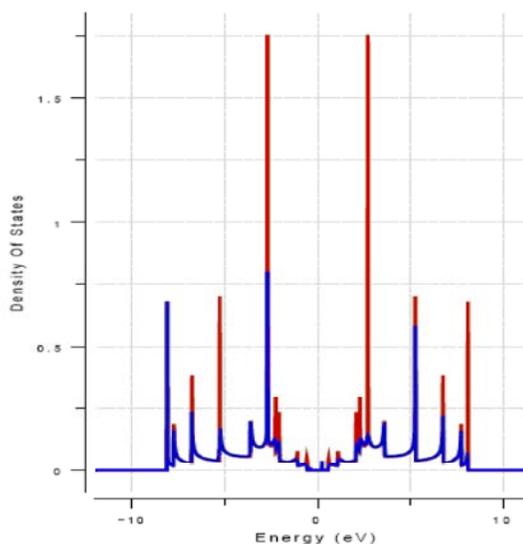


Fig. 11: Density of states for the case 3)

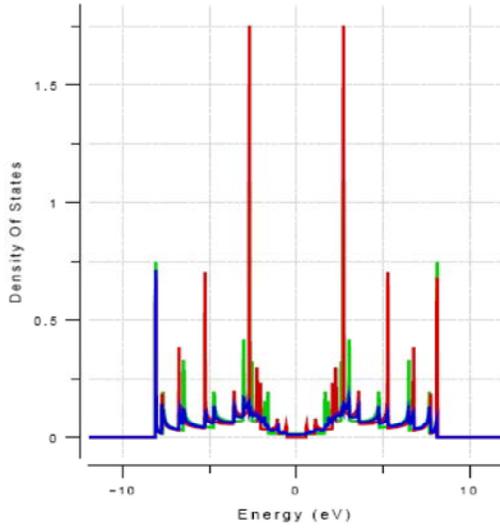


Fig. 12: Density of states for the case 4)

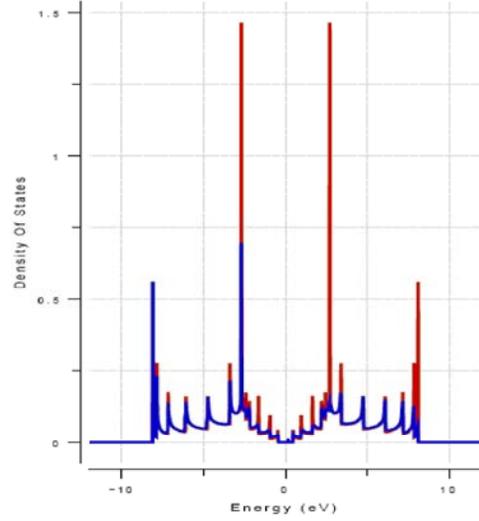


Fig. 15: Density of states for the case 7)

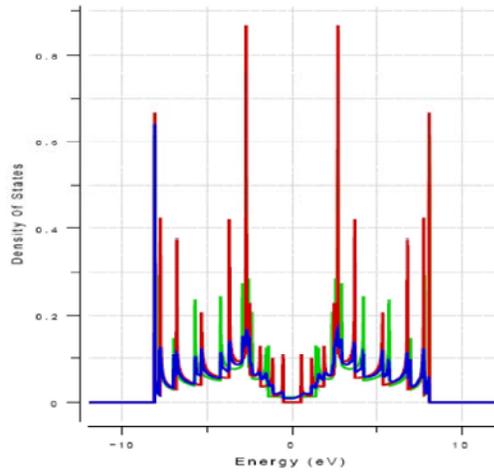


Fig. 13: Density of states for the case 5)

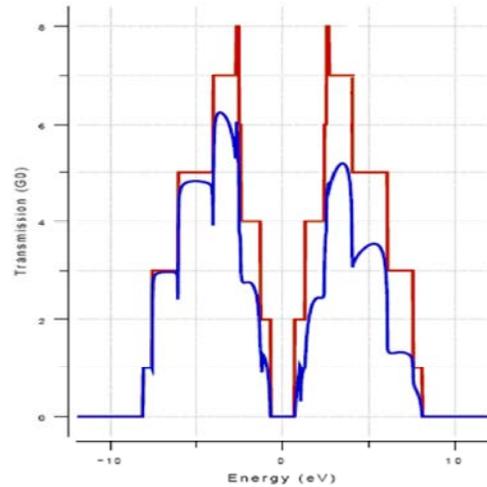


Fig. 16: Transmission function for the case 1)

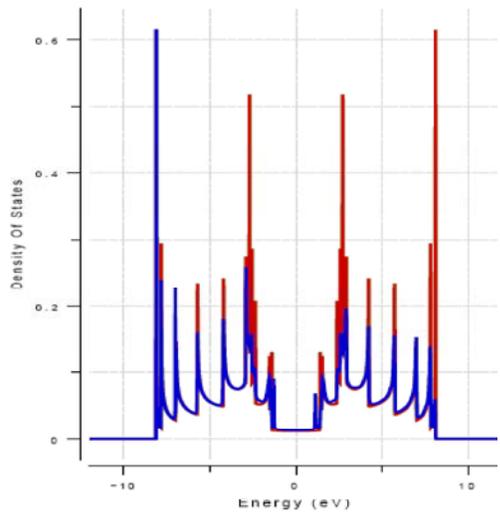


Fig. 14: Density of states for the case 6)

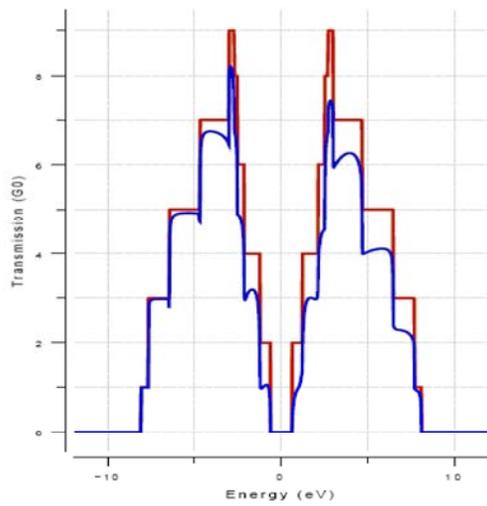


Fig. 17: Transmission function for the case 2)

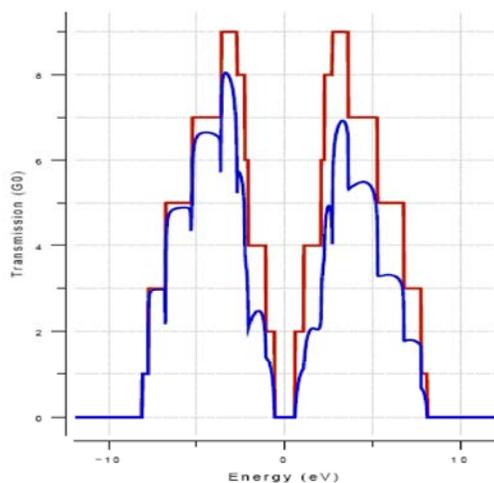


Fig. 18: Transmission function for the case 3)

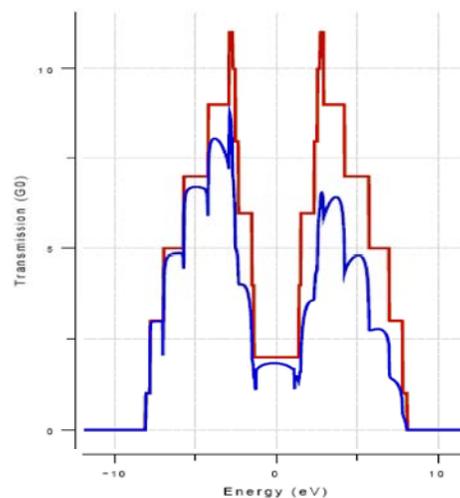


Fig. 21: Transmission function for the case 6)

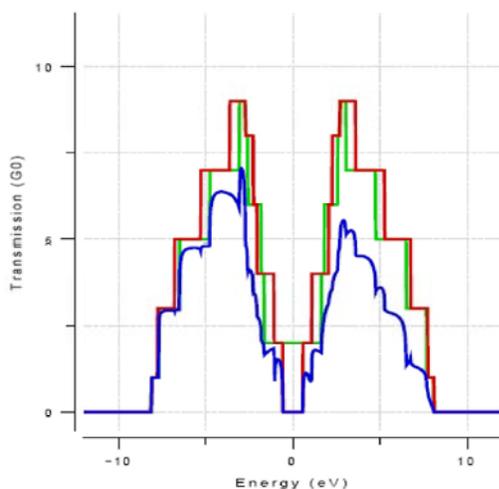


Fig. 19: Transmission function for the case 4)

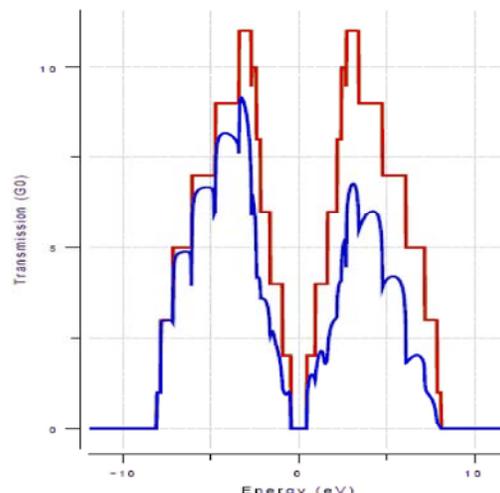


Fig. 22: Transmission function for the case 7)

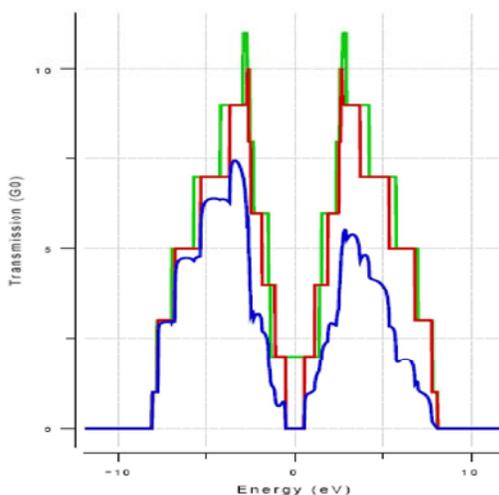


Fig. 20: Transmission function for the case 5)

junction and thus modified the properties of semiconductor carbon nanotube to metallic. It is seen that when two the semiconductor are joint the resultant carbon nanotube becomes semiconductor and the density of states predicted the same thing but when the semiconductor and the metallic carbon nanotube are joint then the resultant carbon nanotube become metallic at the room temperature as shown in the respective diagram where the different carbon nanotube are joint.

Similarly the red colour line in the transmission function diagram represents the previous transmission function before joining of the carbon nanotube and the blue colour line represents the transmission function after joining of the carbon nanotubes with intramolecular junction.

In 4) and 5) cases when different carbon nanotubes i.e. one semiconductor and the other is metallic are used, greater deviation occur in transmission function. In these cases the green colour and the red colour represent the metallic and semiconductor respectively. The final resultant transmission is given by the blue colour line in the respective diagram. The resultant transmission modified so much from the initial transmission because of the formation of pentagon and heptagon at the intramolecular junction. It is seen that the curvature is formed instead of sharp edges at the particular voltage in the transmission function when the same type carbon nanotube are used. The transmissions decrease when it passes through the intramolecular junction. This is because the passage of the electron decrease at intramolecular junction in the carbon nanotube due to the formation of pentagon and heptagon as the transmission is directly proportional to chirality in the carbon nanotube. The variation of transmissions are maximum in the cases when different carbon nanotubes are used to intramolecular junction; it is seen that the transmission mostly depends on the passage of the electron at the intramolecular junction than the later joining carbon nanotube.

### CONCLUSION

Carbon nanotubes often exhibit defects such as pentagons, heptagons, vacancies, or dopants that drastically modify their electronic properties. The electronic properties of defective nanotube-based structures are, of course, more complex than those for infinitely long, perfect nanotubes. The introduction of defects into the carbon network is thus an interesting way to tailor its intrinsic properties to create new potential nanodevices and to propose new potential applications for nanotubes in nano-electronics.

Because carbon nanotubes are metals or semiconductors, depending sensitively on their geometrical structures, they can be used to form metal-semiconductor, semiconductor-semiconductor, or metal-metal junctions. These junctions have great potential for applications because they are of nanoscale dimensions and are made entirely of a single chemical element. In constructing this kind of on tube junction, the key is to join two half-tubes of different helicities seamlessly with each other, without too much cost in energy or disruption in structure. The introduction of pentagon-heptagon pair defects into the hexagonal

network of a single carbon nanotube can change the helicity of the carbon nanotube and fundamentally alter its electronic structure.

The defects, however, must make zero net curvature to prevent the tube from flaring or closing. The smallest topological defect with zero net curvature is a pentagon-heptagon pair, which can be treated as a single local defect because it creates only topological changes (but no net disclination). Such a 5/7 pair will create only a small local deformation in the width of the nanotube and may also generates a small change in the helicity, depending on its orientation in the hexagonal network. Joining a semiconducting nanotube to a metallic one, using a pentagon-heptagon 5/7 pair incorporated in the hexagonal network can be the basis of a nanodiode (or molecular diode) for nano-electronics. Nanotube junctions thus can behave as nanoscale metal-metal junctions, metal-semiconductor Schottky barrier junctions, or semiconductor intramolecular junctions with novel properties and these different types of junctions can serve as building blocks for nanoscale electronic devices.

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