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Electron Transport Properties of Peapods

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Abstract: We have investigated the electronic transport properties of molecular junctions constructed by open and closed peapods molecules. In addition have investigation behavior NDR in the open and closed peapods. Our results indicate that the absence of Coulomb interaction decreases current and shifts the NDR behavior to higher voltage.

Key words: Negative differential resistance · Peapods · Model SSH

INTRODUCTION

In recent years structural and properties of fullerenes and also peapod has attracted attention of many scientists in physics and chemistry to research electronic, optical, mechanical properties and other properties [1-3]. Due to the unique structure of fullerenes, has been used this material in various sciences such as the construction of optical parts manufacturing, electronic equipment, medical and pharmaceutical, etc. [4].

Electronic transport through single molecules strongly depends on the nature and quality of the contacts with electrodes. Among many types of molecules, the fullerene C_{60} is suitable for molecular bridge because its LUMO is situated at relatively lower energies in comparison with the other organic molecules.

Using a tight-binding model was indicated that the strength of the metal/ molecule interaction and the geometry of the contact between the tip and the molecule play an important role in the drastic increase in the conductance.The study of negative differential resistance (NDR) effect in molecular electronics is a very useful property due to its utility in molecular electronic devices such as molecular switch, logic cell and memory. By applying nonequilibrium Green's functions (NEGF) in combination with the density-functional theory, Chen et al. observed NDR in molecular junctions constructed by the porphyrin molecule with donor or acceptor side groups [26]. Zhao *et al*. indicated NDR behavior can be observed in the N-terminated carbon nanotube junction [27]. Taylor *et al*. found that the side groups play a crucial role NDR [5].

Theoretical Methods: In the way without Coulomb interaction SSH, approximate Hamiltonian model SSH (Su - Schrieffer - Heeger), a model based on the interaction of electrons-phonon with strong techniques in the formulation Hamiltonian C_{60} molecule lack presence of magnetic field can be written as [6]:

$$H_{ssh} = \sum_{\langle i,j\rangle}[-t_0 - \alpha y_{i,j}](C_i^{\dagger} + H.C) + \frac{1}{2}K(y_{ij})^2 \qquad (1)$$

Here t_0 mutation rate (hopping integral) in the channel region of the C- C bond between the two carbons. α fixed coupling of electron - phonon (electron-phonon coupling constant), K factor, spring constant, $C_{i,s}$ and $C^{\dagger}_{i,s}$ operators of creation and annihilation operator electrons π at ith carbon atoms with spin s and length Change y_{ij} bond between carbon atoms i and j are location and is close to the <i,j> summation on neighbors. Finally phrase, the elastic energy of the phonon system with spring constant k is a constant factor. Hamiltonian eq. (1) can be approximated by the standard method without adiabatic, the Schrödinger equation may be solved for π electrons [7-9]:

$$\varepsilon_k Z_{ks}(i) = \Sigma_{\langle i,j\rangle})(-t_0 - \alpha y_{ij}) Z_{ks}(i=j) \qquad (2)$$

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In particular ϵ_k values of kth mode Z_{ks} electron wave function is related to it. The total energy C_{60} molecule as a function of y_{ij} obtained from the following equation:

$$E_T(y_{ij}) = 2\sum\nolimits_k^{'} \varepsilon_k + \sum_{\langle i,j\rangle} \frac{k}{2} y_{ij}^2 \quad (3)$$

Primed sign indicates that summation is only over the occupied levels. Using the equation Schrödinger For the total energy we have:

$$E_T(y_{ij}) = 2\sum\nolimits_{k,s}^{'} \sum_{\langle i,j\rangle} (-t - \alpha y_{ij}) Z_{ks}^*(i) + \sum_{\langle i,j\rangle} \frac{k}{2} y_{ij}^2 \quad (4)$$

The minimization of the total energy E_T of all y_{ij} and Lagrange undetermined coefficients $\psi = \Sigma_{\langle i,j\rangle}\, y_{ij}$ that the constraint is satisfied, the Lagrange equations can be written as follows:

$$\frac{\partial E_T}{\partial y_{ij}} + \lambda \frac{\partial \psi}{\partial y_{ij}} = 0 \quad (5)$$

Then:

$$2\sum\nolimits_{k,s}^{'} \sum_{\langle i,j\rangle} -\alpha Z_{ks}(j) Z_{ks}^*(i) + \sum_{\langle i,j\rangle} k y_{ij} + \lambda \sum_{\langle i,j\rangle} 1 = 0 \quad (6)$$

Considering $\Sigma_{\langle i,j\rangle}$, where N is the total number of nearest neighbor bonds. Defined as:

$$\lambda = \frac{1}{N} \sum\nolimits_{k,s}^{'} \sum_{\langle i,j\rangle} -\alpha Z_{ks}(j) Z_{ks}^*(i) \quad (7)$$

Put the equation in (3-6)

There by:

$$\sum_{\langle i,j\rangle} [2\sum\nolimits_{k,s}^{'} -\alpha Z_{ks}(j) Z_{ks}^*(i) + \sum_{\langle i,j\rangle} K y_{ij} + \lambda \frac{1}{N} \sum\nolimits_{k,s}^{'} \sum_{\langle i,j\rangle} -\alpha Z_{ks}(j) Z_{ks}^*(i)] = 0 \quad (8)$$

In view of the above equation to reach a series of self- equations for y_{ij} follows:

$$y_{ij} = \frac{2\alpha}{K} \sum\nolimits_{k,s}^{'} Z_{ks}(j) Z_{ks}^*(i) - \Delta y \quad (9)$$

That:

$$\Delta y = \frac{1}{N} \sum_{\langle i,j\rangle} \frac{2\alpha}{K} \sum\nolimits_{k,s}^{'} Z_{ks}(j) Z_{ks}^*(i) \quad (10)$$

Here N =220 total number of bonds π is in the open peapod molecule and N =360 total number of bonds π in the close peapod molecule. Coupled equations (2) and (9) and (10) can be solved to replicate. These values, have in good agreement with other methods like methodology LDA and strong correlation method[10].

RESULT AND DISCUSSION

Study and was discussed a molecular junction made by open and closed peapods molecules using the non-equilibrium Green's functions (NEGF) in combination with density functional theory[11].

One of the physical phenomena that occur in the calculation of current molecule finds a negative differential resistance behavior (NDR). Negative differential resistance behavior in V <0.2v and V> 0.6v order to for open and close peapods is observed (without Coulomb effects).

In this study, was seen the behavior the stepped current- voltage and also the difference in open and closed peapod [12].

Peapod have nanotubes and fullerenes with C_{60} or C_{60} @ *SWCNT* two sides open are and 330 molecules of carbon, it is known that the open peapods, close peapods are like open peapods but is closed on both sides with carbon molecules to the number of carbon atoms in its molecules to reach 540. As recently by researchers in the field of nanotechnology is mentioned a lot of attention peapod capsule form [13].

Fig. (1) and (2) overview of both -See open and closed peapods closed to be placed later. Purposes of single contact is the metal electrode, only one carbon atom attached to the molecule is forms.

A of the properties of electron transport in molecular systems, is negative differential resistance (NDR). In fact, it occurs when the current through the molecule is reduced with increasing bias voltage. NDR behavior first by LG. Azaky in tunnel diodes was discovered and then in quantum dots and bonds metal-molecule-metal was observed.

Importance of applications due to its technological in many cases, such as switching, amplifiers, digital devices and instruments fluctuating flow electric [14]. Several reasons explain the NDR behavior in electron transport through bonds molecular offered. In cases such as tunnel diodes, reduce the displacement of the Fermi level of the into the conduction band or band gap semiconductor capacity occurs.

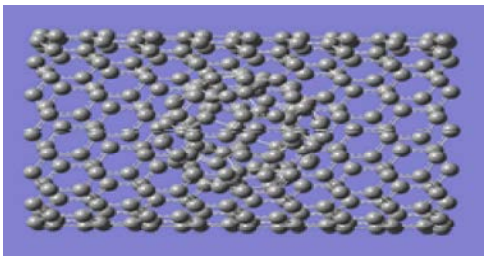

Fig. 1: Open peapod

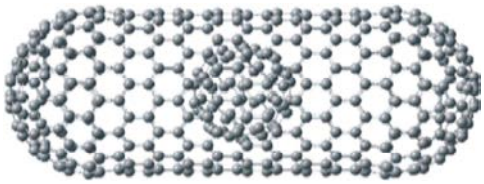

Fig. 2: Close peapod

Metal bonds in molecules, the NDR can be caused by queuing and consequently the Fermi level of electrodes alignment with the orbital that the effect of increasing the bias voltage molecular happen[15].

NDR peaks can also arise inductive effect or interaction of electrons with orbital Coulomb barrier is vibrating molecule. However, the research shows that NDR characteristic in curve the current - voltage, usually matching or not matching the energy levels of molecules with energy levels of the electrodes.

The NDR is a well-known concept in many physical systems, such as one-dimensional systems, supper networking and double quantum wells have been discovered [16]. Resonator and resonator electronic tunneling mechanism can explain satisfactorily the NDR behavior. We compared NDR behavior in our study for open and closed peapods.

As is clear from the opening peapods limited to the voltage (0-0.2v) and voltage (0.6-0.8v), with voltage increasing, done the current decreases, namely as the negative differential resistance. But these changes have not been observed in close peapods this can be very important and useful for bonds be open. Results show that without the Coulomb interaction, the behavior of the negative differential resistance (NDR) the voltage above changes, also with increasing atomic number of contact points, NDR behavior is shift over voltage [17].

Was shown in the Figure (3), the peapod molecule through is a single atomic contact, current is a function of bias voltage. In the case of one point contact, a threshold voltage is needed to the system to produce current and voltage -current curve shows a stepped behavior.

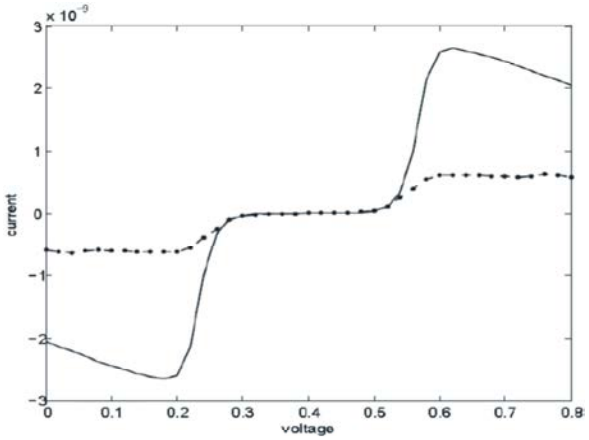

Fig. 3: Current-voltage chart show for open peapods (_) and closes peapds (._._)

Calculations showed that in current-voltage characteristics (I-V), a Ohmic behavior at low applied voltage for a single contact. The reason for problem is that the hybrid electrodes is stronger and here more pathways for electrons there, to increase the number of points of contact between the electrodes and the molecule, the molecule passes toward the metal. The difference between the currents in single and multiple contact state and changes is due to interference effects and the peaks transfer coefficient rate (TC). Measurement all quantities such as current and transfer function, etc., depends to Hamiltonian of the molecule and the electrodes and also contact. Constants that in the variety Hamiltonian of electrodes and molecules and their binding was introduced in the numerical calculation are as follows: (t_0) value jumps between nearest neighbor carbon atoms C-C bonds the molecule put equal 2.5 ev. Size of the binding constant of electron – phonon is considered $\alpha_0 = 3.31\frac{ev}{A^0}.(V_0)$ the quantity of Coulomb force intensity between nearest neighbors and the positions i and j equal t_0 and value Coulomb repulsion force in any situation (U_0) doubled t_0 choose form $U_0 = 2V_0 = 2t_0$. The amount of heat that is selected in the Fermi function comes T = 300k. The connection between nearest the atomic positions of the electrodes t_0 and between the molecule and the electrodes t consider [18-20].

If the mutation coefficient between the electrode and the carbon atoms molecule proportion the mutation coefficient between electrode atoms or between molecules atoms is much weaker, then we can be placed $t' = 0.5t_0$. Well assume that the energy per atom in the molecule is constant. The Figures (4) transfer coefficients (TC)

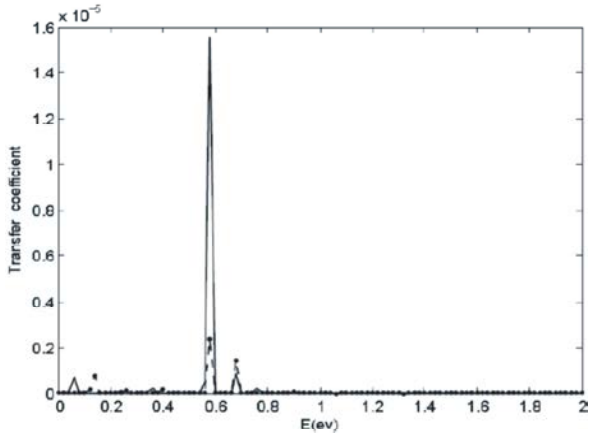

Fig. 4: Transfer coeffcient per the energy (ev) is plotted for open (___) close (¯ ¯ . ¯ ¯) peapods

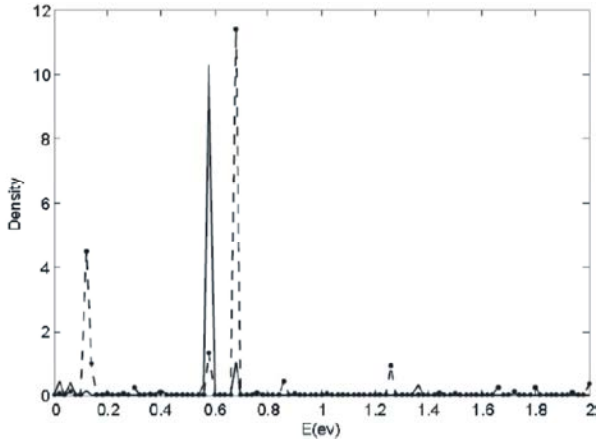

Fig. 5: Density of state open (___) and close (_._) peapods molecules unitage a function of energy with out coulomb interaction

are displayed like a function of electron energy. These figures, is shown in both state and for open and close peapods and without Coulomb interaction and with V = 0.5 *v*.

As can be seen in figure the peak in the transfer coefficient viewing 0.5ev for open and close peapod that peak open peapod transfer coefficient is larger than the peak transfer coefficient closed peapod [21-23].

It should also be noted that the intensity of the transfer spectrums, which depends on the electronic energy. So large amounts of transfer function (peaks) near the molecular level in are open and closed peapods. All the above conditions with is caused by Coherent electron emission. Coherent transmission assumption the electron wave function is spread uniformly throughout the system [24].

When the electron emission is coherent with the phase dispersion process that alters the state is not broke. If some electrons transfer energy to the grid, began to vibrate, which causes the network to in case of failure of one phase of the process and thus fails to account for the Hamiltonian system comes. Thus, the electron energy almost matches the molecular level, there is a large transfer Comes resonant electrons in a molecule can move on. Calculations is shown the behavior of different transmission coefficients (TC) system, in the states of contact one open and close peapods [25-27].

In coherent quantum transport, width resonant transfer depends on power of contact the electrode - molecule. The one-dimensional electrodes, only one atom in the last position, is Pair of carbon atoms. When molecule via a carbon atom attached to the electrode, transport through molecules depends the effects of tunneling resonance. By increasing the number of contact points, interference effects around these parts, contact it is important, some of which may disappear entirely resonance transfer curves shift said.

Physical meaning of interference effect is the molecular electron wave different have been from the contact points, possible to have a phase shift [28]. Thus, a constructive or destructive interference of the diffusion of electrons, it can happen through the molecule. Effect of contacts described by the matrix self- energy. With these explanations, Green's function and the density of the molecules state pair and transmission range, are changed by changing the number of points of contact [29-31]. In Figure (5) density of state open and closed peapods molecules are shown unit age a function of energy and without coulomb interaction and considering the $V = 0.5\,v$.

In Figure (5), density of state open and closed peapods molecules are shown unit age function of energy and without coulomb interaction and considering the $V = 0.5\,v$.

In Fig. (5) density of states toward energy in confine 0.1v until 0.5v viewing, that is for close peapod in under 0.5v and whatever energy more, transmission pike for open and close peapod move toward forward.

CONCLUSION

Non-equilibrium Green's function technique and theory of education and contact for Landauer without Coulomb interactions on the electronic transport properties of a molecule, applied.

The results showed that the number of contact points between the device electrodes and molecules, a very important factor is in electron transfer. Also, the absence of Coulomb interaction, the peak transfer coefficients (TC) the lower energy changes.

Addition of negative differential resistance (NDR), can in curves (I-V) open and close peapods molecule with the touch of a single seeing, but this behavior peak in open peapods is much larger than peapods of closed.

The results suggest that the open peapod molecules chosen are interesting and exciting to work with such systems, is current on the nanoscale.

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REFERENCES

1. Kroto, H.W., J.R. Heath, S.C. O'Brien, R.F. Curl and R.E. Smalley, 1985. Nature, 318: 162.
2. Krätchmer, W., L.D. Lambd, K. Fostiropoulos and D.R. Huffman, 1990. Nature, 347: 354.
3., Schön, J.H., C.H. Kloc, T. Siegrist, M. Steigerwald, Svensson and B. Batlogg, 2001. Nature, 413: 831.
4. Kalhor, D., R. Zahiri, S.A. Ketabi and A. Ebrahimzad, 2010. Indian J. Phys., 84(5): 483-484.
5. Smith, B.W., M. Monthioux and D.E. Luzzi, 1998. Nature (London,) 396: 323.
6. Harigaya, K. and S. Abe, 1995. Phys.: Condens. Matter, 7, B 49, 4061.
7. Liu, J., S. Iwata and B. Gu, 1994. J. Phys. Condens. Matter, 6, L2, 53.
8. Harigaya, K., 1992. Phys. Rev., B 45, 13676.
9. Cuo, T., G.K. Odom and G.E. Scuseria, 1994. J. Phys. Chem., 98: 7745.
10. Wang, Y., G.F. Bertsch and D.Z. Tomanek, 1993. J. Phys. D., 25: 181.
11. Kurita, N., K. Kobayashi and H. Kumahora, 1993. Phys. Rev. B, 48: 4850.
12. Dong, J., J. Jiang, Z.D. Wang and D.Y. Xing, 1995. Phys. Rev. B, 51: 1977.
13. Dong, J., J. Jiang, J. Yu, Z.D. Wang and D.Y. Xing, 1995. Phys. Rev. B, 52: 9066.
14. **Missing**
15. Yaghobi, M. and M.Yuonesi, 2011. Molecular Phys., 109: 14.
16. Zheng, X., W. Lu, T.A. Abtew, V. Meunier and J. Bernholc, 2005. J. Phys. Chem. B, 109: 3334.
17. Yaghobi, M. and H.R. Vanai, 2011. Phys. Lett. A, 375: 1249.
18. Shuai, Z., B.S. Qing Wan, Zou and Yan Zhang, 2009. Appl. Phys. Lett., 94: 073503.
19. Esaki, L., 1958. Phys. Rev., 109: 603.
20. Esaki, L. and P.J. Stiles, 1966. Phys. Rev. Lett., 16: 1108.
21. Esaki, L., 1974. Mod. Phys. Rev., 46: 237.
22. Meisam Valizadeh Kiamahalleh, Ghasem Najafpour, Suhairi Abd Sata, Surani Buniran and Sharif Hussein Sharif Zein, 2010. World Applied Sciences Journal, 9: 10.
23. Gaudioso, C.J., L.J. Lauhon and W. Ho, 2000. Phys. Rev. Lett., 85: 1918.
24. Chang, L.L., E.E. Mendez and C. Tejedor, 1991. Resonant Tunneling in Semiconductors, New York, Plenum.
25. Zhao, P., P.J. Wang, Z. Zhang and D.S. Liu, 2010. Phys. Lett. A, 374: 1167.
26. Zheng, X., W. Lu, T.A. Abtew, V. Meunier and J. Bernholc, 2005. J. Phys. Chem. B, 109: 3334.
27. Yaghobi, M. and H.R. Vanai, 2011. Phys. Lett. A, 375: 1249.
28. Esaki, L., 1958. Phys. Rev., 109: 603.
29. Esaki, L. and P.J. Stiles, 1966. Phys. Rev. Lett., 16: 1108.
30. Esaki, L., 1974. Mod. Phys. Rev., 46: 237.
31. Bedrossian, P., D.M. Chen, K. Mortensen and J.A. Golovchenko, 1989. Nature, 342: 258.