Investigation the C-C Bonds with
Morse Potential in the CNT

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Abstract: This work is concerned with molecular devices based carbon nano tubes (CNT), i.e., devices based on the use of one or several electrically - contacted molecules. Clearly, the experimental difficulty in contacting one or a small number of molecules is formidable, largely because of the scale reduction by a factor of $10^3$ to $10^6$ between the size of the molecule (of nano metric order) and the macroscopic world. We consider the C - C bonds with Morse potential to the review the chemical and physical ideas underlying the novel families of components, born from the current and future requirements of nano science.

Key words: Thin film • Nano science • Carbon nano tubes and Morse potential

INTRODUCTION

Some workers during the centuries have tried to formulate the details of atomistic structure of materials. We have now entered the nano science and nano technology which pop up new branch when chemistry and physics dedicated to understanding phenomenon on the smallest scales. However, there are some issues from both fundamental and applications standpoint, which cause the realization of devices comprising one or several molecules, extending the ideas slightly one or several objects of size comparable to a small molecule, i.e., typically about 5 nm [1-7]. These nano objects may the organic molecules, metal or semiconductor nano particles, CNTs nano wires or biomolecules [8-10].

In this works, we focus on new transport regime of SWCNT (Single - Walled - Carbon - Nano - Tubes) by considering Morse potential for C - C bonds and connecting nano objects directly to conducting electrodes. The obtained results help us to understand and control the relationship between molecular structures and transport properties in such a way it will one day the possible to exploit it.

Theory: There are two regimes, strong coupling regime and weak coupling regimes, which limit the carrier transport through the SWCNT due to variation between C - C bond length and angle. In the weak coupling limit, the passage of an electron from one electrode of CNTFET to the other occurs sequentially in which, it passes through a charged state of the carbon, viz., $\text{C}^0 \rightarrow \text{C}^+$

We use Morse potential for describing the electronic properties of an isolated carbon atom orbitals (CO) [11]. In general, the highest occupied molecular orbital is referred to as HOMO and the lowest unoccupied molecular orbital as the LUMO. We shall assume here that the atoms and or molecules retain their identity during the changes in C - C length and angles, which can cause energy levels of their CO are broadened due to hybridization by the interaction between carbon atoms with the CNTFET gate and electrodes under the effects of fractional charge transfer. This degree of broadening of the levels allows us to distinguish between weak and strong coupling. Indeed, the broadening with the energy $U$ (Morse energy) shows how electrons transfer from a carbon atom to the electrodes. Alignment the position of the Fermi level with respect to the HOMO and LUMO of the molecule determines the I (v) characteristic of a molecular conductor. Furthermore, the potential profile, here, Morse potential, across the molecular conductor leads a method of I (v) characteristic.

As stated above, we use an approximation which the molecular levels can shift in a rigid manner by a change in the average potential $< V(r) >$ in the molecule in the presence of an applied bias $V$. The Morse potential is given by

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\[ V(\mathbf{r}) = V_{\text{bond}} + V_{\text{angle}} \]
\[ V_{\text{bond}} = 6.03 \times 10^{-10} \text{ nm} \left[ \left( 1 - \frac{e^{\theta}}{\theta} \right) \right] \]
\[ V_{\text{angle}} = \frac{1}{2} K \Delta \theta \left( 1 + \Delta \theta \right) \]

Where \( V_{\text{bond}} \) indicates the bond energy associated with bond stretch and \( V_{\text{angle}} \) is bond energy due to angle bending, \( \mathbf{r} \) is the length of the C - C bond and \( \theta \) is the angle between the adjacent bonds [5].

Therefore,
\[ <V(\mathbf{r})> = \alpha e \nu \]

The factor \( \alpha \) multiplying the voltage is a number between 0 and 1. By fixing the HOMO energy as reference, the electrochemical potentials are then obtained as follows:
\[ \mu_1 = E_F - <V(\mathbf{r})> = E_F - \alpha e \nu \]
\[ \mu_2 = E_F + (1-\alpha)e\nu \]

The number of electrons on electrode 1 and 2 denoted \( N_1 \) and \( N_2 \), respectively. They are determined under the equilibrium conditions.

\[ N_1 = \frac{2}{1 + e^{\frac{\varepsilon - \mu_1}{k_B T}}} \]

and

\[ N_2 = \frac{2}{1 + e^{\frac{\varepsilon - \mu_2}{k_B T}}} \]

The number of electrons \( N \) out of equilibrium will lie between \( N_1 \) and \( N_2 \), so that the net current through electrodes is found as follows:

\[ I_1 = \frac{e}{h} \gamma_1 (N_1 - N) \]

and

\[ I_2 = \frac{e}{h} \gamma_2 (N - N_2) \]

Where \( \gamma_{12} \) are the broadening energy levels and electrodes 1 and 2. In the stationary state, \( I_1 = I_2 \), and hence

\[ I = I_1 = I_2 = \frac{2 e}{h} \gamma_1 \gamma_2 \left( \frac{1}{1 + e^{\frac{\varepsilon - \mu_1}{k_B T}}} + \frac{1}{1 + e^{\frac{\varepsilon - \mu_2}{k_B T}}} \right) \]

By doing some calculations and introducing a potential similar to the one used in Morse potential and or in the Hubbard model [11], viz.,

\[ U \approx V(\mathbf{r}) \]

Due to the change in the number of electrons from the equilibrium value of \[ \frac{2}{1 + e^{\frac{\varepsilon - \mu_1}{k_B T}}} \], the energy level, \( \varepsilon \), will be floated in where,

\[ U = U_0 \left[ N - \frac{2}{1 + e^{\frac{\varepsilon - \mu_1}{k_B T}}} \right] \]

and

\[ \varepsilon = \varepsilon_0 + U \]

It yields to the facts that the asymmetry in the C - C bonds in the graphene case, causes the overlap of carbon atoms wave functions and perturbations in the carrier transport through the SWCNT as a channel of the CNTFET transistor.

CONCLUSIONS

The Morse potential rather than the Coulomb attractive potential indicates that the carrier transports are strong temperature dependence and exponential gate dependence, which indicated that the tunneling mechanism is responsible for this phenomenon. This simple model illustrates the main principles of transport in the weak coupling case and can be used for modeling the next CNTFET devices.

REFERENCES


