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The Resonance Tunneling Process in the Scanning Tunneling Microscope with Carbon Nanotube as a Tip

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Abstract

In our work we present an integrated calculation model to investigate the possibility of using carbon nanotubes as a tip for the scanning tunneling microscope. Our model takes into consideration the electronic properties of the substrate and tip that fabricated by using carbon nanomaterials . since we calculated the hybridization function and the quantum shift(as well as the assistant function) due to coupling between the molecule and the tip and the substrate . This calculation are utilized to calculate the local density of states on the molecule . We firstly studied the effect of all the properties of the carbon nanotube tip , since different carbon nanotubes chiral and achiral , metallic and semiconductor with different diameters are considered . Also , we calculated the transport properties for the used system (substrate - molecule – carbon nanotube tip) , these calculations can be considered as an additional step to enhance our results . We conclude that the carbon nanotube tip is not suitable for investigation in the most cases ,since that depends on the molecule effective energy level position with respect to the Van Hove (V.H) singularities in the electronic density of states of the carbon nanotube . And as the normal distance between the tip and the molecule is one of the most important experimental parameters that enhance the process of investigation , the effect of the tip distance on the process of investigation is studied for the carbon nanotube (12,0) . According to our calculations , its concluded that it is possible to get the exact density of states by controlling the distance which is a function of the molecule effective energy level position .

Key words: carbon nanotube , Dyson equation , Green function ,density of states , transport properties .

Introduction

Since its invention in 1982 , the scanning tunneling microscopy (STM) opened an experimental frontier for determining the electronic structure and material surface morphology at the atomic resolution [1,19] . It has been widely used in physical phenomenon observation ,

manipulation of crystal growth [2] , single – molecule probing [3] and surface modification [4] . The probe tip is considered as the critical component of the STM which making the atomic resolution possible . The resolution of STM depends on the physical and chemical properties of the probe tip materials[5-7] . The tip is usually composed of tungsten (W) or

platinum/ iridium (Pt-Ir) [8,9] . The W tip is the earliest STM tip due to its simple preparation , mechanically stable and low cost [10] .But the radius of curvature is hard to reach 5nm , which would limit the scanning resolution , as well as a thick oxidation layer may exist on the surface of W tip which minimizes the electric conductivity. For the Pt-Ir tip [11,12] it is usually prepared using the mechanical cutting . In this tip , the oxidation layer cannot be exist on its surface ,but the multiple tips are usually produced. This will affect the quality of the scanning images , and the atomic resolution . Recently , single walled carbon nanotubes (SWCNTs) are used as a tip for the STM . SWCNTs are chemically inert and mechanically robust , they have small specific weight , record high elastic modulus , have a large aspect ratio , good electric conductivity and the tip end is well defined [13] . In this paper , model calculation is presented to study and investigate the ability of using the single walled carbon nanotube as a tip for the STM.

The Model Calculation

A model calculation for the electron tunneling during probing process of single molecule placed on substrate with Scanning Tunneling Microscope whose tip is Single Walled carbon nanotubes (see figure (1)) is presented . Carbon nanotube has very special energy bands structure which including several sub bands where the quantum confinement is in two directions . Figure (1) shows the schematic representation for the system used (substrate – molecule – probe) in our study .

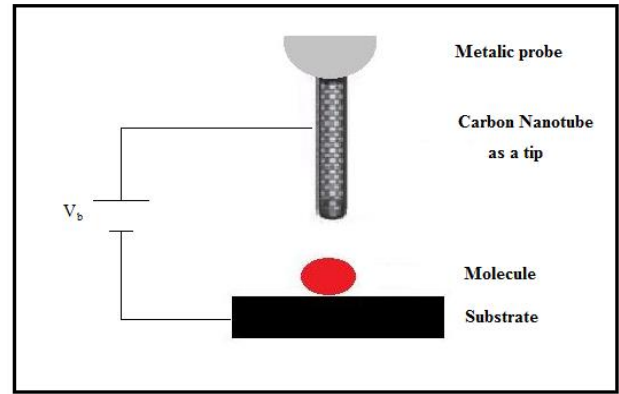


Fig.(1): SWCNT as a tip for scanning tunneling microscope .

The Hamiltonian ,that describes the system , includes four main terms[18] :

$$H = H_p + H_s + H_m + H_t \quad (1)$$

Where the symbols (s and p) refer to the substrate and probe . The first term presents the Hamiltonian for the probe which is given by :

$$H_p = \sum_{k_p, \sigma} E_{k_p}^{\sigma} C_{k_p}^{\sigma\dagger} C_{k_p}^{\sigma} \quad (2)$$

while for the substrate it is given by :

$$H_s = \sum_{k_s, \sigma} E_{k_s}^{\sigma} C_{k_s}^{\sigma\dagger} C_{k_s}^{\sigma} \quad (3)$$

$C_{k_i}^{\sigma\dagger}$ (i=s ,p) is the creation operator and $C_{k_i}^{\sigma}$ is the annihilation operator for the electrons in the probe or in the substrate . $E_{k_i}^{\sigma}$ represent the spin – dependent energy levels in the substrate and probe energy bands .

The special SWCNT density of states includes the Van Hove singularities (see fig

(2)) . It is clear from the scheme that there are two or three Van Hove singularities in the SWCNT density of states which are lying within the energy range $-2 \text{ eV} < E < 2\text{eV}$.

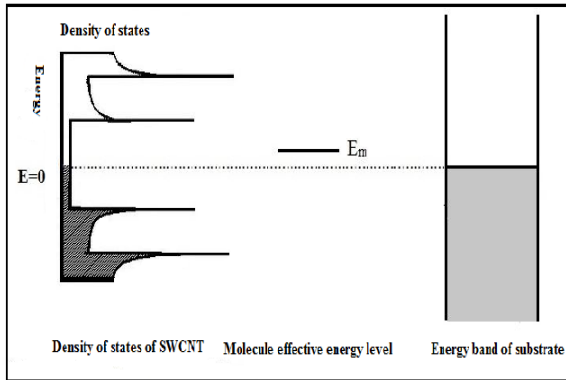


Fig.(2) :The energy diagram for (SWCNT-molecule-substrate) system .

The Hamiltonian of the considered molecule is given by :

$$H_m = \sum_{\sigma} E_m^{\sigma} d^{\sigma\dagger} d^{\sigma} \quad (4)$$

d^{σ} and $d^{\sigma\dagger}$ are the creation and annihilation operators for the electrons on the energy level of spin σ in the molecule . For simplicity ,the Coulomb interaction energy in our work is neglected and the molecule is presented by a single effective energy level E_m .

The Hamiltonian H_t is concerned to the coupling interaction between the three parts (substrate – molecule – probe tip) ,

$$H_t = \sum_{k_s, \sigma} (V_{k_s}^{\sigma} C_{k_s}^{\sigma\dagger} d^{\sigma} + H.C. + \sum_{k_p, \sigma} (V_{k_p}^{\sigma} C_{k_p}^{\sigma\dagger} d^{\sigma} + H.C.) \quad (5)$$

$V_{k_s}^{\sigma}$ ($V_{k_p}^{\sigma}$) is the spin – dependence coupling interaction between the substrate (probe) and molecule .The coupling interaction may be considered as a constant (i.e. energy independent) or it depends on the normal distance between the subsystems.

The model calculation is based on the nonequilibrium Green function method to represent the theoretical model of the electron resonance tunneling in one dimension . The molecule Green function was solved based on solving the Dyson equation [14,17]:

$$G_{m\sigma}^r(E) = g_{m\sigma}^r(E) + g_{m\sigma}^r(E) \sum_{\sigma}^r(E) G_{m\sigma}^r(E) \quad (6)$$

Where $G_{m\sigma}^r(E)$ is the Fourier Transform for the following function :

$$G_{m\sigma}^r(t) = -i \theta(t) \langle [d_{\sigma}(t), d_{\sigma}^{\dagger}(0)] \rangle \quad (7)$$

The $g_{m\sigma}^r(E)$ function is the molecule Green function in absence of the coupling between the substrate and molecule and between the probe and molecule i.e $V_{k_s}^{\sigma} = V_{k_p}^{\sigma} = 0$. The $g_{m\sigma}^r(E)$ given by the following relation[14] :

$$g_{m\sigma}^r(E) = \frac{1}{E - E_m + i\eta} \quad (8)$$

η is very small positive number .

The retarded self – energy $\sum_{\sigma}^r(E)$ is written in the following form :

$$\sum_{\sigma}^r(E) = \sum_{\sigma p}^r(E) + \sum_{\sigma s}^r(E) \quad (9)$$

The first and second terms on the right eq (9) represent the retarded self –energies of the probe and the molecule respectively .

Where,

$$\sum_{\sigma p}^r(E) = \sum_{k_p} V_{k_p}^{\sigma} g_{k_p\sigma}^r(E) \quad (10)$$

$$\sum_{\sigma s}^r(E) = \sum_{k_s} V_{k_s}^{\sigma} g_{k_s\sigma}^r(E)$$

and ,

$$g_{k_p\sigma}^r(E) = \frac{1}{E - E_{k_p}^{\sigma} + i\eta} \quad (11)$$

$$g_{k_s\sigma}^r(E) = \frac{1}{E - E_{k_s}^{\sigma} + i\eta}$$

To get the total retarded self – energy we must find the correct forms of the functions $\sum_{\sigma p}^r(E)$ and $\sum_{\sigma s}^r(E)$ which will be denoted as $\sum_p^r(E)$ and $\sum_s^r(E)$, respectively .

The retarded self – energy is written as following [16]:

$$\sum_{\sigma p}^r(E) = \sum_{k_p} \frac{|V_{k_p}^{\sigma}|^2}{E - E_{k_p}^{\sigma} + i\eta} \quad (12)$$

Then we rewrite the retarded self – energy by using simple mathematical steps as :

$$\begin{aligned} \sum_{\sigma p}^r(E) &= \sum_{k_p} \int dE' \frac{|V_{k_p}^{\sigma}|^2 \delta(E' - E_{k_p}^{\sigma})}{E - E'} - \\ &i \sum_{k_p} \int dE' |V_{k_p}^{\sigma}|^2 \delta(E' - E_{k_p}^{\sigma}) \frac{\eta}{(E - E')^2 + \eta^2} \end{aligned} \quad (13)$$

by taking the principal value for the first term of eq. (13), the quantum shift in the molecule energy level due to the coupling with the probe energy levels is given as follow :

$$\Lambda_p^{\sigma}(E) = P \int \frac{dE'}{\pi} \frac{\Delta_p^{\sigma}(E')}{(E - E')} \quad (14)$$

Where $\Delta_p^{\sigma}(E)$ represents the broadening function in the molecule effective energy level due to the coupling with the probe energy band levels ,

$$\Delta_p^{\sigma}(E) = \sum_{k_p} |V_{k_p}^{\sigma}|^2 \delta(E - E_{k_p}^{\sigma}) \quad (15)$$

The second term of equation (13) can be written as :

$$\int dE \Delta_p^r(E') \delta(E - E') = \Delta_p^{\sigma}(E) \quad (16)$$

By using the following definition[17] :

$$V_{k_p}^\sigma = v_{k_p} V_p^\sigma \quad (17)$$

eq.(16) will be written as follows ;

$$\Delta_p^\sigma(E) = \pi |V_p^\sigma|^2 \rho_p^\sigma(E) \quad (18)$$

where $\rho_p^\sigma(E)$ is the density of states of the probe :

$$\rho_p^\sigma(E) = \sum_{k_p} |v_{k_p}|^2 \delta(E - E_{k_p}^\sigma) \quad (19)$$

and eq. (14) becomes ,

$$\Lambda_p^\sigma(E) = |V_p^\sigma|^2 P \int dE' \frac{\rho_p^\sigma(E')}{(E - E')} \quad (20)$$

Similarly the retarded self – energy due to substrate can be written as :

$$\Lambda_s^\sigma(E) = |V_s^\sigma|^2 P \int dE' \frac{\rho_s^\sigma(E')}{(E - E')} \quad (21)$$

and also ,

$$\Delta_s^\sigma(E) = \pi |V_s^\sigma|^2 \rho_s^\sigma(E) \quad (22)$$

The total quantum shift in the effective energy level of molecule is written as following :

$$\Lambda^\sigma(E) = \Lambda_p^\sigma(E) + \Lambda_s^\sigma(E) \quad (23)$$

and the total quantum broadening :

$$\Delta^\sigma(E) = \Delta_p^\sigma(E) + \Delta_s^\sigma(E) \quad (24)$$

Now we can write the local density of states on the molecule in the following form :

$$\rho_m^\sigma(E) = \frac{1}{\pi} \frac{\Delta^\sigma(E)}{(E - E_m^\sigma - \Lambda^\sigma(E))^2 + (\Delta^\sigma(E))^2} \quad (25)$$

Then the current that passes between the probe tip and substrate through the molecule can be written in the following form [15] :

$$I = \frac{2e}{\hbar} \int dE \frac{\Delta_p^\sigma(E) \Delta_s^\sigma(E) [f_p(E) - f_s(E)]}{[E - E_m - \Lambda^\sigma(E)]^2 + (\Delta^\sigma(E))^2} \quad (26)$$

$f_p(E)$ and $f_s(E)$ are the Fermi distribution functions for the probe and substrate ,

$$f_\alpha(E, \mu_\alpha, T) = \frac{1}{1 + \exp\left(\frac{E - \mu_\alpha}{K_B T}\right)} \quad (27)$$

μ_α represents the chemical potential for the α ($\equiv p, s$) lead , T is the lead's temperature and K_B is Boltzmann constant .The differential conductance is calculated by finite differences.

The Calculations and the Results

To calculate the transport properties , it is necessary to display the energy diagram scheme when applying a certain bias voltage equals to eV_b (see fig . 3) where $\mu_p = eV_b$, $\mu_s = -eV_b$.

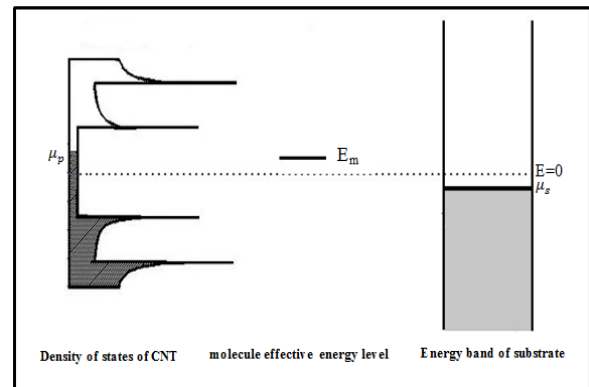


Fig.(3):energy diagram for (SWCNT- molecule - substrate) system when the bias voltage is applied .

It is worth mentioning that our calculations take the following into consideration ,

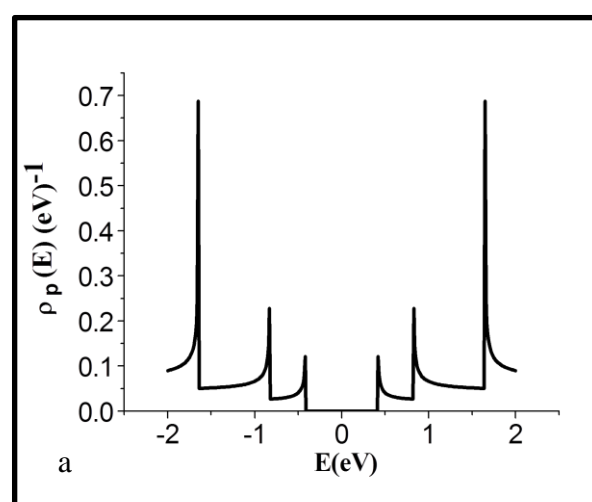
1- The noninteraction case where the spin is neglected .

2- The wide band approximation when calculating the self – energy due to the coupling between the molecule and substrate .

The parameters which used in our calculations are $V_s= 0.1$ eV and $V_p=1$ eV while the temperature is equal to 300 K , i.e. the system in a thermal equilibrium . The electronic density of states of the single walled carbon nanotube and the hyperdization function and function and the quantum shift is calculated according to equations (18) and (20) to state the role of the special density of states of carbon nanotube in determining the behavior of the hyperdization function and quantum shift as a function of energy system when $V_p= 1$ eV.

According to fig .(4), it is obvious that the

behavior of hyperdization function and quantum shift have also Vane Hove Singularities. Therefore , in this case , neither the hyperdization function nor quantum shift can be neglected . It is worth mentioning that the hyperdization function and quantum shift play a role in determining the behavior of the local density of states on the molecule . If the coupling interaction of molecule with substrate is equals to 0.1 eV ,the quantum shift due to substrate will become zero according to the wide band approximation where $\rho_s = \frac{1}{4\beta}$, and 4β ($\beta =2$ eV) represents the width of the substrate energy band



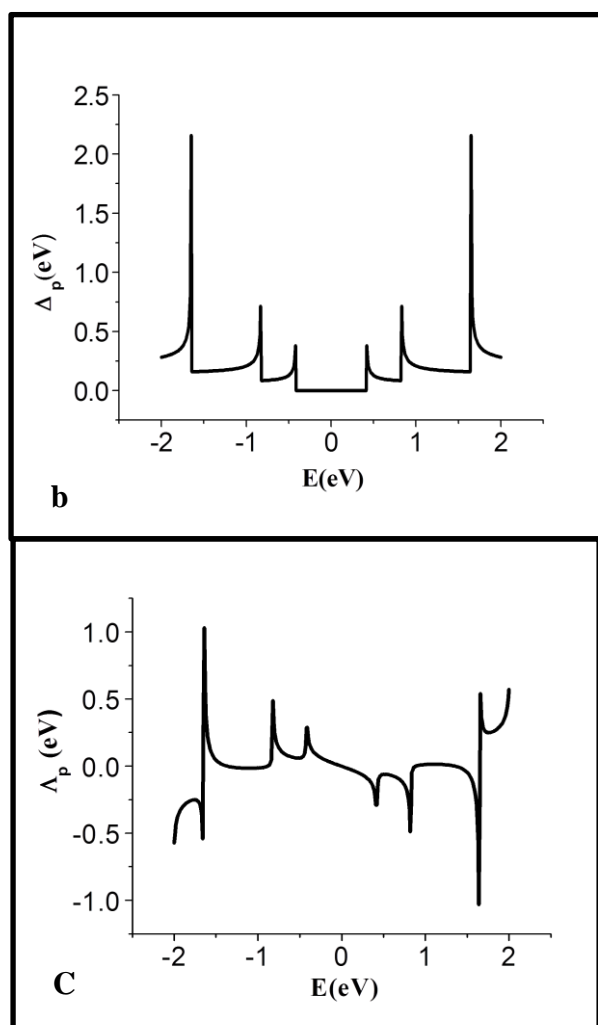
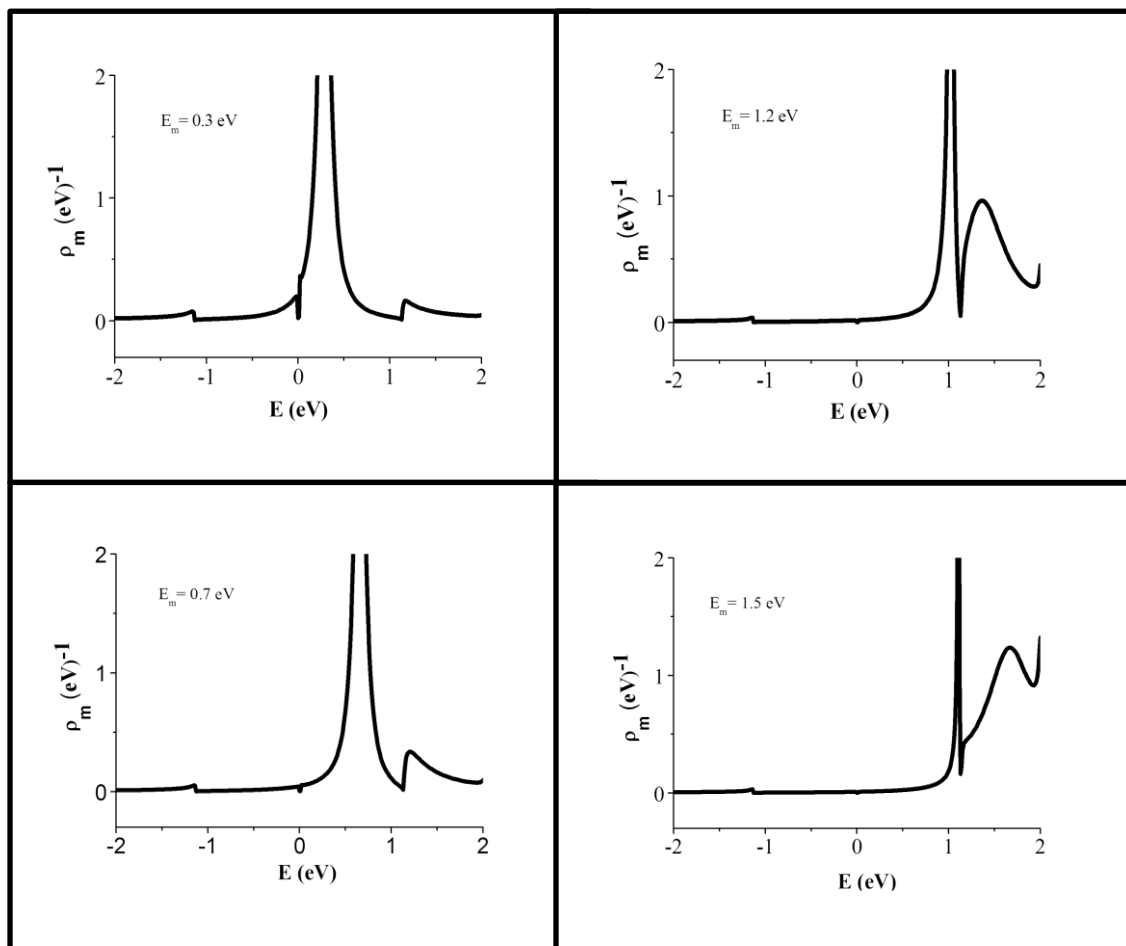


Fig.(4) :(a) the density of states for SWCNT (12,0) , (b) the hyperdization function and (c) the quantum shift for probe as a function of energy when $V_p=1$ eV .

The molecule local density of states is calculated according to equation (25) . The highest value of the local density of states on the molecule is $(1/\pi \Delta)$, since the term $(E-E_m-\Lambda(E))$ equals to zero (see fig.(5)) . Therefore , the assistant function $(E-E_m-\Lambda(E))$ is an important function , it can be employed useful for determining the new position of E_m which is equals to $E_m+\Lambda(E)$. The change of the position of E_m is due to the coupling with the substrate and the tip .

In order to check all the parameters that affect the measurement process , the local density of states on the molecule and also the corresponding assistant function are calculated for the values $E_m= 0.3 ,0.7 ,1.2 ,1.5$ eV . We note that the SWCNT(12,0) show a resonance peak when E_m equal to 0.7 eV and another separated peak to the side of the resonance peak .



Fig(5) : the local density of states on molecule for different values of E_m , since the investigation is done by using SWCNT (12,0) .

In order to get the transport properties of the (SWCNT- molecule – substrate) system , the current and the differential conductance must be calculated . Since the conductance gives an important property about any system or nanostructure . The

current and the differential conductance are calculated as a function of the bias voltage when the coupling interaction between the probe tip SWCNT (12,0) and molecule is equal to $V_p = 1$ eV for different values of E_m , see figures (6-9) .

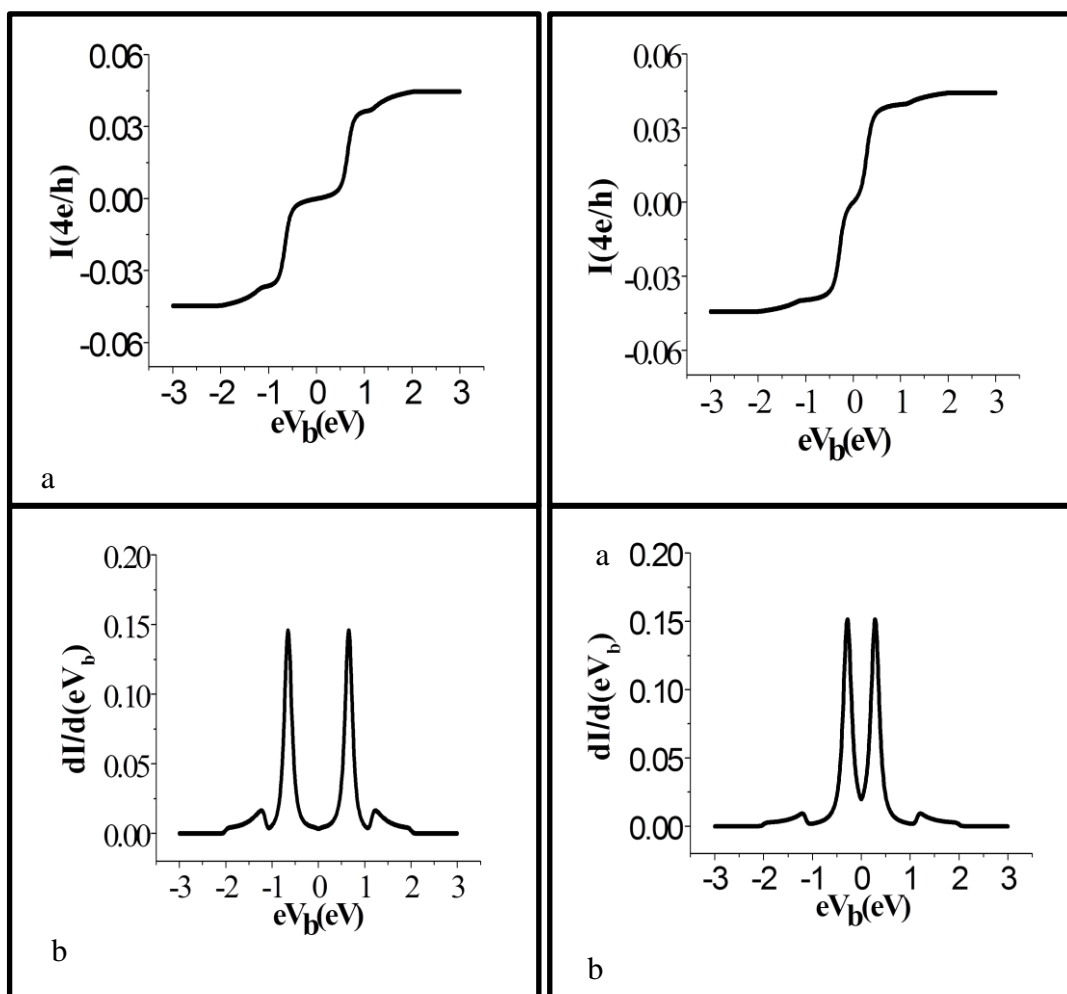


Fig.(6) : (a) the current and (b) the differential conductance as a function of the bias voltage when $E_m=0.3$ eV by using SWCNT (12,0)as a tip .

Fig.(7) : (a) the current and (b) the differential conductance as a function of the bias voltage when $E_m=0.7$ eV by using SWCNT (12,0)as a tip .

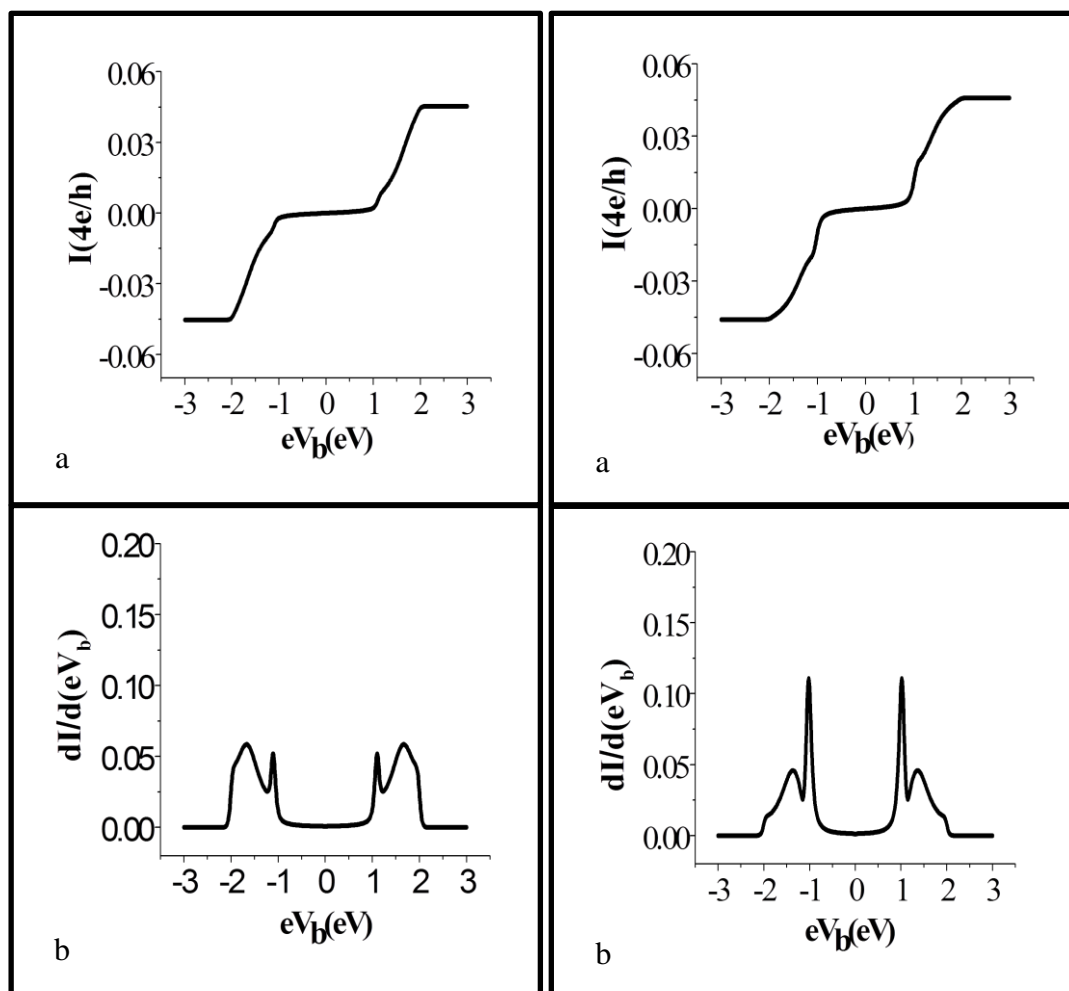


Fig.(8) :the (a) current and (b) the differential conductance as a function of the bias voltage when $E_m=1.2$ eV by using SWCNT (12,0)as a tip .

Fig.(9) : (a) the current and (b) the differential conductance as a function of the bias voltage when $E_m=1.5$ eV by using SWCNT (12,0) as a tip .

According to these figures one can report the following notes :

1- It is well known that the differential conductance calculation is an important step which gives important informations about the local density of states on the molecule . The differential conductance spectrum displays resonance peak with suppressed side peaks when $E_m = 0.3$ and 0.7 eV . Accordingly , we can conclude that when the values of E_m are close to the low bias voltages , the CNT (12,0) can be used as a probe tip and vice versa .

2- The $I-eV_b$ characteristics show that the current becomes zero at a certain region , this region may called the bias voltage gap . We conclude that when the bias voltage gap is relatively small , the CNT tip can be used to investigate the nanoparticle .

These results can be also exploited to write important notes about the carbon nanotube that can be used as a normal electrode in molecular devices in which the molecule operates as a switch .

The Effect of the Normal Distance between the CNT Tip and Molecule

Experimentally , the probe tip can be brought close to the samples . until the normal distance becomes finite and

suitable for the manipulation procedure to be allowed . At this position , applying a bias voltage between the tip and sample will makes the electrons to tunnel between them . Thus one can get a measurable current crosses between the tip and sample .When the current starts , the position of the probe tip and its bias can be tuned during the experiment and so one can get information from the changes that happen in the conductance spectrum .

In the following we investigate the variation of the coupling strength with the normal distance (Z) between the tip and molecule . This coupling strength can be described as follows :

$$V_p = V_{p0} e^{-\frac{Z}{Z_0}} \quad (28)$$

Where V_{p0} is the coupling strength at $Z=0$, Z_0 is the decay factor of the waves functions of the tip and molecule in the vacuum between them . Experimentally , the normal distance between the molecule and the tip is considered as the most important factor that related to the measurement process .

In order to investigate the normal distance effect on the measurement process and manipulation , we use SWCNT (12,0) to calculate the local density of states on the molecule as well as the current and differential conductance for different values

of Z such as $Z= 0.5 , 1.0$ nm at $T= 300$ K .
These results are shown in the figures (10-17) . according to these results , one can conclude that when the distance Z is relatively large , the broadening and quantum shift will be as low as possible and the maximum peak is located at E_m .
In the figure (14) where $E_m = 1.2$ eV and $Z =0.5$ nm , the peak in the conductance spectrum has a splitting , while in the fig. (15) the peak is resonant and clear .

In order to enhance the investigation process , the control on the distance between the tip and molecule must be investigated . These calculations must be done for every value of E_m in order to guess the corresponding normal distance .

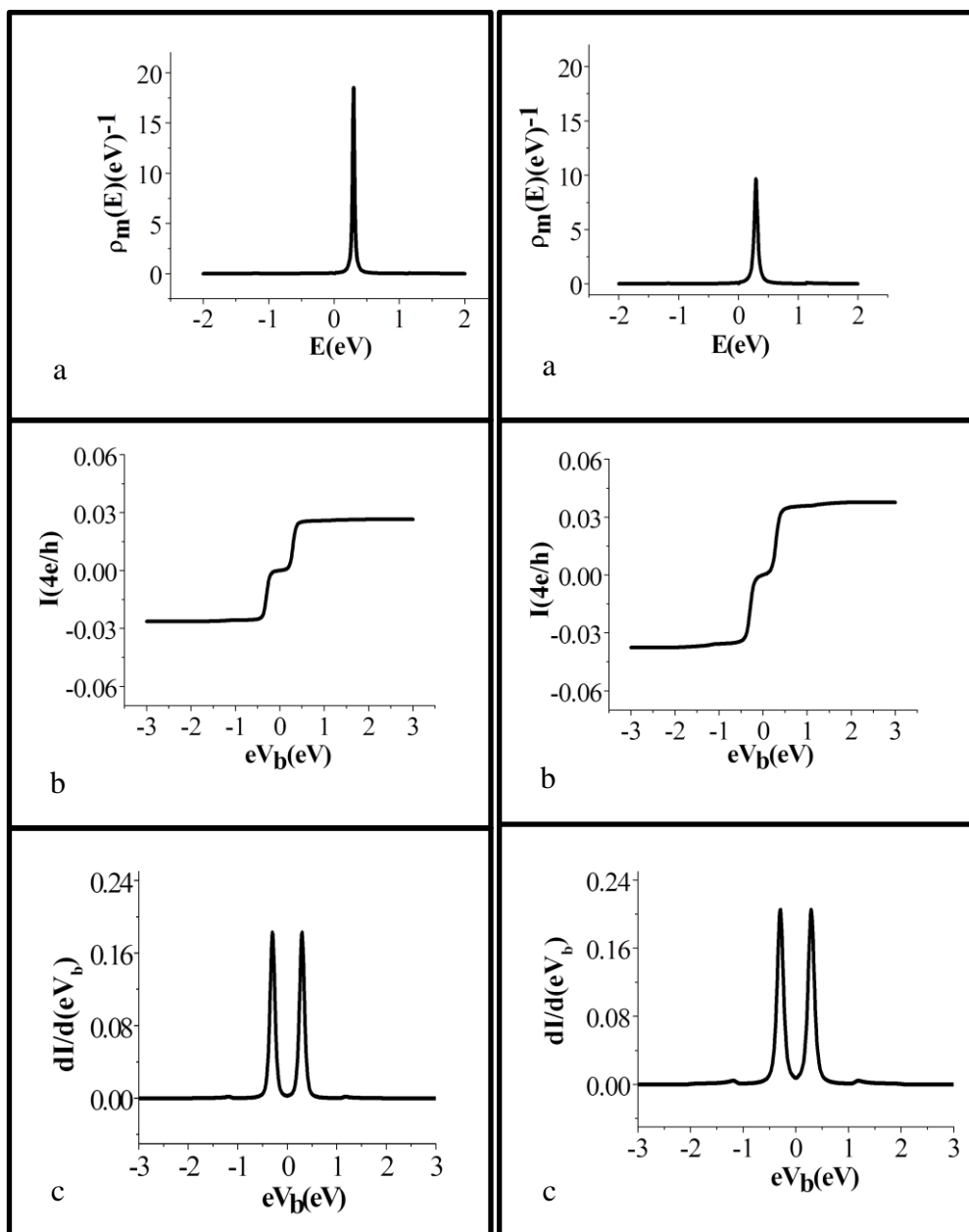


Fig.(11) : (a) local density o states on molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=0.3$ eV and $Z=0.5$ nm.

Fig.(10) : (a) local density of states on molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=0.3$ eV and $Z=1.0$ nm.

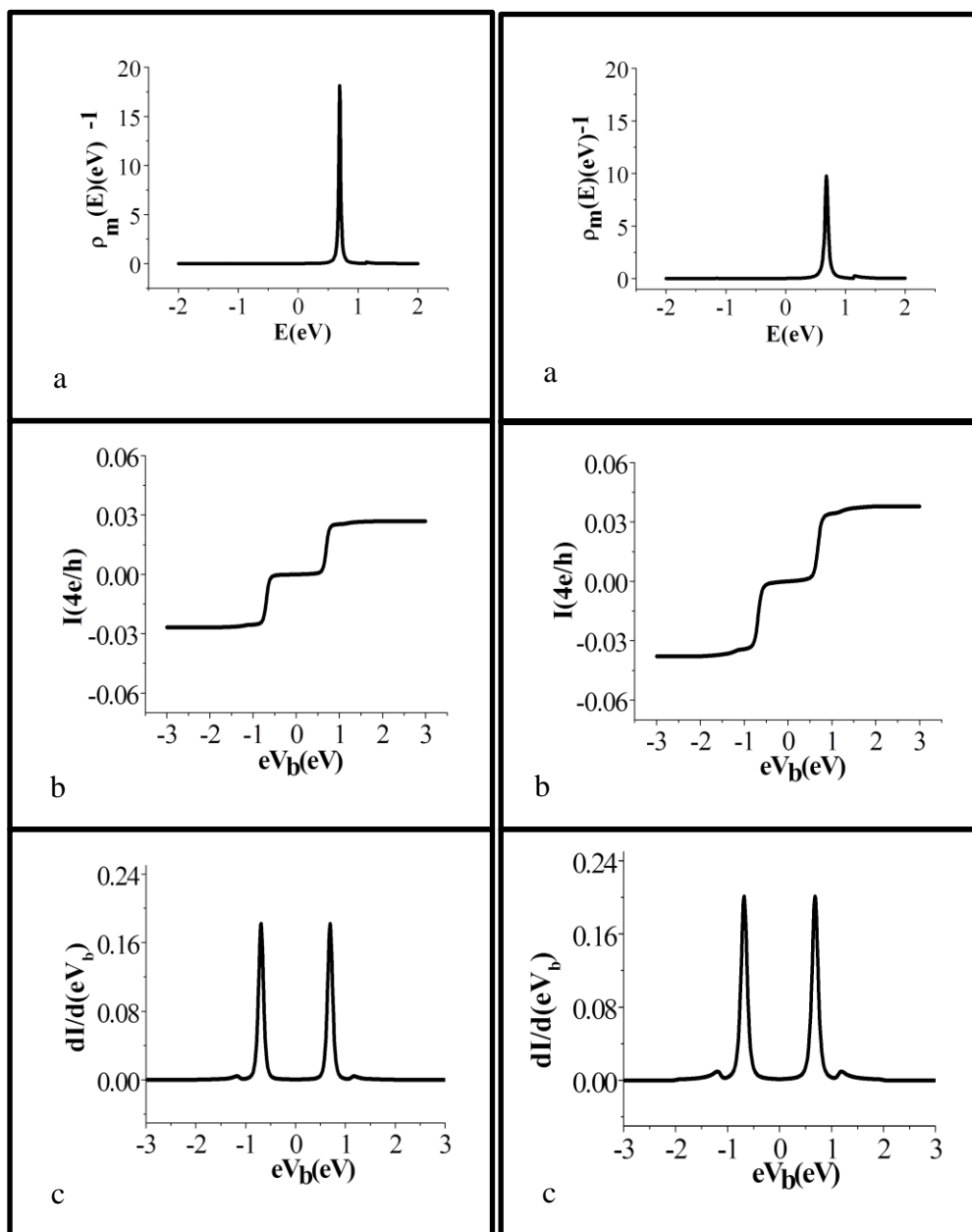


Fig. (12): (a) local density of states on molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=0.7$ eV and $Z=1.0$ nm.

Fig.(13) : (a) local density of states on molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=0.7$ eV and $Z=0.5$ nm.

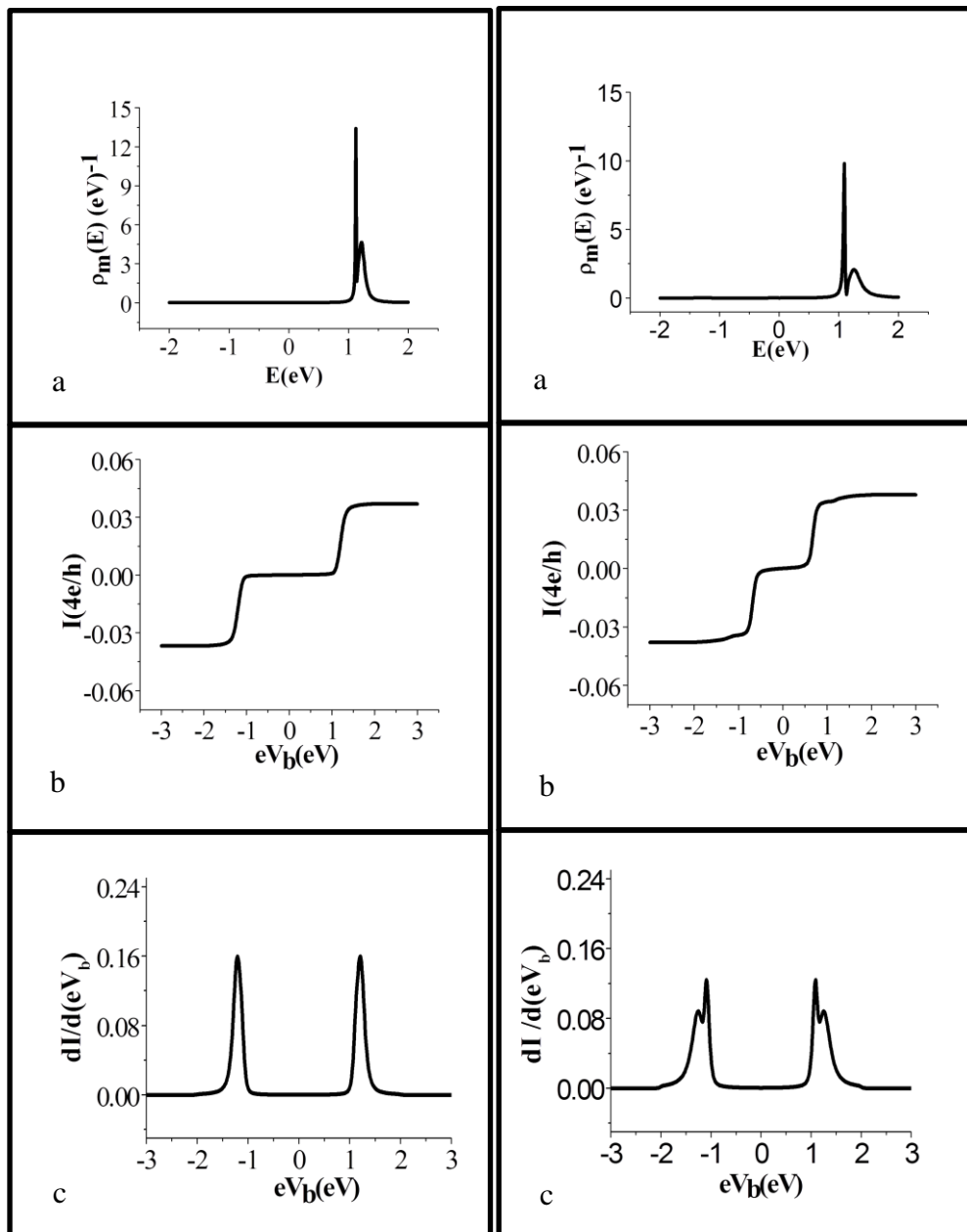


Fig.(14) : (a) local density of states of molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=1.2$ eV and $Z=1.0$ nm.

Fig.(15): (a) local density of states on molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=1.2$ eV and $Z=0.5$ nm.

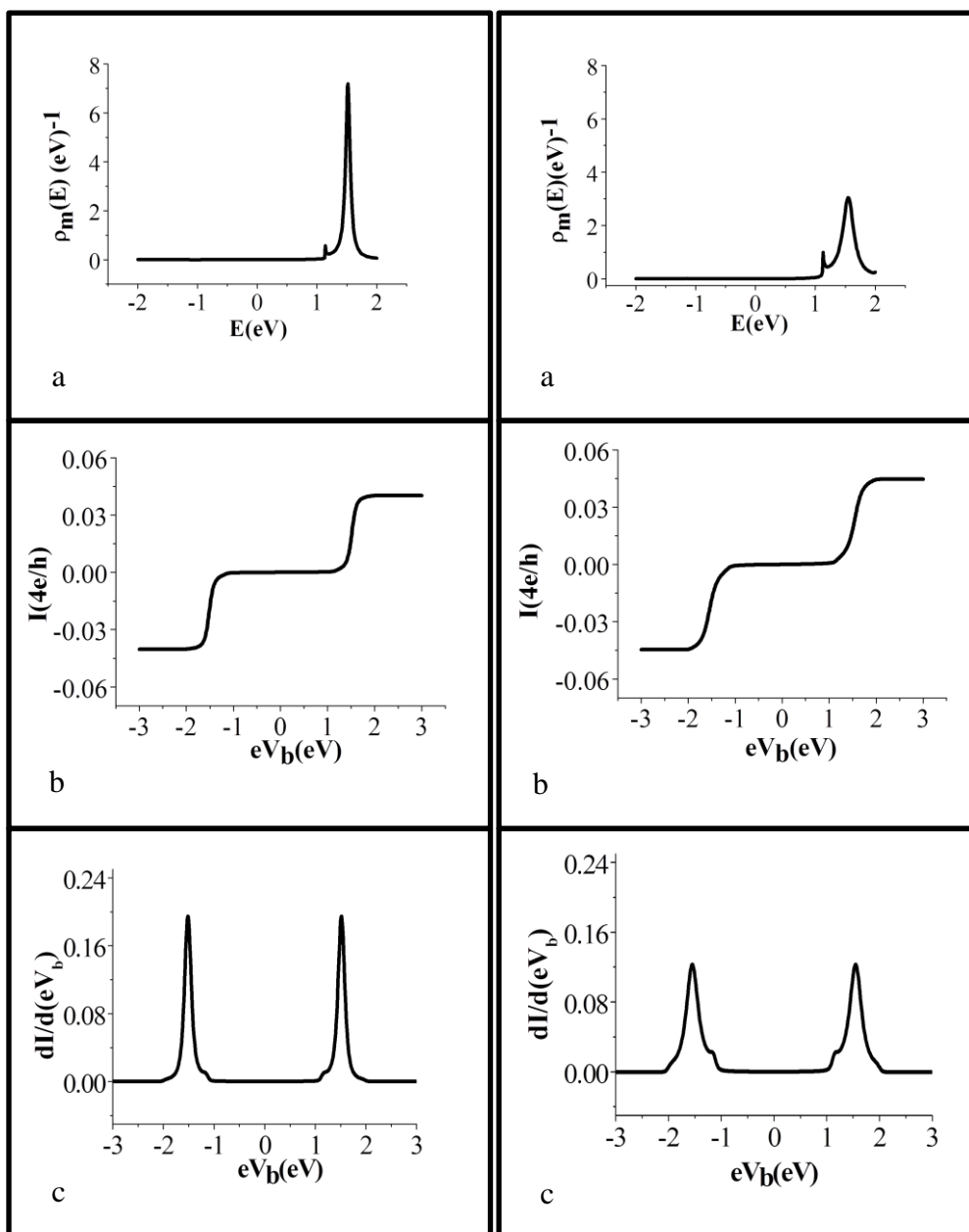


Fig.(16) : (a) local density of states of molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=1.5\text{eV}$ and $Z=1.0\text{ nm}$.

Fig.(17) : (a) local density of states of molecule , (b) the current and (c) differential conductance as a function of the bias voltage when $E_m=1.5\text{ eV}$ and $Z=0.5\text{ nm}$.

Conclusions

1- The theoretical method that includes the calculation of the hybridization function, between the tip (which made from carbon nanomaterials) and the molecule that one aims to examine its electronic properties, is the promising method to determine the properties early. Since the assistant function is considered as an important function for determining the position of molecule effective energy level. This important calculations determine the local density of states on the molecule.

2- The transport properties calculation of the system (SWCNT-molecule-substrate) is necessary step for two reasons: the first is to enhance the obtained physical properties that related to experiments. While the second reason is that the study of the device (CNT – molecule – substrate) can be developed to study the accuracy of using CNT as a normal electrode in the structures, systems and nano devices.

3- It is well known that every carbon nanomaterial can be investigated by using normal metal tip. This make it easy to knowing the properties of the carbon nanomaterial before use it as a tip for the STM.

4-According to our calculations, There is no rule for determining which one of the carbon nanotubes (chiral or achiral, metallic or

semiconductor with different diameters) can be used as a tip for STM. But according to our calculations we can say that the best SWCNT for investigation, is the tube where the number of the Vane Hove Singularities in the density of states is few and the energy spacing between the Vane Hove Singularities is relatively large. Experimentally, this can be achieved easily by investigation the density of states of SWCNT using normal metal tip.

5- We have confirmed that the position of molecule effective energy level, with respect to the position of singularities energies in the density of states of CNT tip, has a role in determining which one of the SWCNTs can be used successfully to investigate the molecule. Depending on our calculations it has been confirmed that for finite distance and as the hybridization function and the absolute value of quantum shift are as low as possible, the value of the energy which corresponds to the assistant function that equals zero represents the effect energy level of molecule.

6- The strength of coupling, between the tip and the particle to be examined, can be experimentally tuned by many ways. one of them is the distance between the tip and the molecule which can be easily controlled. Finally, the extended model calculation that we have presented and our motivated results can be exploited to investigate the ability of using more carbon nanomaterials

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عملية النفق الرنيني في المجهر النفقي الماسح مع أنبوب كاربون نانوي كراس مجس

علاء خالد بندر وجنان مجيد المخ

قسم الفيزياء / كلية التربية للعلوم الصرفة / جامعة البصرة / البصرة / العراق

الخلاصة

في عملنا هذا , قدمنا أنموذجاً حسابياً متكاملًا لفحص إمكانية استخدام أنابيب الكربون النانوية كراس مجس للمجهر النفقي الماسح. يهتم أنموذجنا بالخصائص الإلكترونية للقاعدة ورأس المجس المصنوع من مواد الكربون النانوية , حيث تم حساب دالة التهجين والإزاحة الكمية (بالإضافة إلى الدالة المساعدة) بسبب الإقتران بين الجزيئة مع رأس المجس والقاعدة . هذه الحسابات تم توظيفها لحساب كثافة الحالات الموضعية على الجزيئة . ثم درسنا تأثير كل خصائص أنبوب الكربون النانوي كراس مجس , إذ تم أخذ أنابيب كاربون نانوية مختلفة كيرالية chiral وغير كيرالية achiral , معدنية وشبه موصلة وبأقطار مختلفة . كذلك تم حساب خصائص النقل للنظام قاعدة - جزيئة - رأس مجس , هذه الحسابات تعد خطوة إضافية لتعزيز نتائجنا . لقد إستنتجنا إن رأس المجس أنبوب الكربون النانوي لا يكون مناسباً للفحص في معظم الحالات إذ يعتمد ذلك على موقع مستوى طاقة الجزيئة المؤثر بالنسبة إلى مواقع الطاقات المعتلة ل فان هوف في كثافة الحالات الإلكترونية لرأس مجس أنبوب الكربون النانوي . ولما كانت المسافة العمودية بين رأس المجس والجزيئة من العوامل العملية المهمة التي تُعزز عملية الفحص , تم دراسة تأثير هذه المسافة على عملية الفحص وذلك بإستخدام أنبوب الكربون النانوي (12,0) . لقد إتضح من حساباتنا أنه بالإمكان الحصول على كثافة الحالات المضبوطة عن طريق التحكم بالمسافة التي تكون دالة لموقع مستوى الطاقة الفعال للجزيئة .