

## Conductance-Voltage Characteristics of Single Molecule Junction: in Resonant Tunneling Regime

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**Fouad Nimr Ajeel**

College of Science, Thi Qar University/Thi Qar.

Email: fouad\_noor@hotmail.com

**Dr. Jenan Majeed AL-Mukh**

Education for Pure Sciences College /Basarh.

**Dr. Lafy Faraj Al-Badry**

College of Science, Thi Qar University/Thi Qar.

### Abstract

Electronic transport characteristics through a single molecule junction are investigated by using the Keldysh non equilibrium Green function (NEGF) model. The model consists of a molecular bridge (represented by a molecular orbital) attached with two free electron reservoirs (represents two metallic leads) and it is coupled with a vibrational degree of freedom (represents a molecular vibrational mode). The behavior of the electronic transfer through the molecular junction becomes more clearly visible by studying of the conductance-voltage characteristics. The numerical calculations are done based on this model to study the changes in conductance behavior through a single molecule junction in the resonant tunneling regime. According to our results, the conductance-voltage characteristics are influenced by (I) the electron-vibration interaction, (II) the molecular bridge-leads coupling strength, (III) the junction temperature, and (IV) the molecular vibrational mode energy. We conclude that the previous parameters have a significant role in determination of the electron conduction through the single-molecule junctions. Especially, the conductance is very sensitive to the molecular bridge-leads coupling strength and the junction temperature. These features provide important information about the study of the electronic transport phenomena in molecular junctions.

**Keywords:** Molecular junction; nonequilibrium Green function theory; electronic transport; conductance; electron-vibration coupling.

### خصائص التوصيلية-الفولتية لوصلة احادية الجزيئة : في نهج الرنين النفقي

#### الخلاصة

تم فحص خصائص النقل الإلكتروني عبر وصلة احادية-الجزيئة باستخدام نموذج دالة كرين غير المتزنة (NEGF). حيث يتألف هذا النموذج من الجسر الجزيئي (تم تمثيله بالمدار الجزيئي) المرتبط بخزاني الإلكترون الحر (تمثلان قطبين معدنيين) والمرتبط كذلك بدرجة الحرية الاهتزازية (والذي تم تمثيله بالنمط الاهتزازي الجزيئي). ان سلوك النقل الإلكتروني من خلال الوصلة الجزيئية يصبح أكثر وضوحاً بدراسة خصائص التوصيلية-الفولتية. انجزت الحسابات العددية استناداً على هذا النموذج

لدراسة التغيرات في سلوك التوصيلية عبر الوصلة احادية-الجزئية في نهج النفق الرنيني. ووفقاً لنتائجنا، فإن خصائص التوصيلية-الفولتية تتأثر بـ: (I) تفاعل الكترولن-اهتزاز، (II) قوة اقتران المدار الجزيئي-الاقطاب، (III) درجة حرارة الوصلة، و (IV) طاقة النمط الاهتزازي الجزيئي. واستنتجنا بان المعاملات السابقة لها دور هام في تحديد توصيل الإلكترولن عبر وصلة احادية-الجزئية. وبالخصوص تكون التوصيلية حساسة جداً لقوة اقتران المدار الجزيئي-الاقطاب ودرجة حرارة الوصلة. هذه السمات توفر معلومات هامة حول دراسة ظواهر النقل الإلكترولني في الوصلات الجزيئية.

**الكلمات المرشدة:** الوصلة الجزيئية، نظرية دالة كرين غير المترنة، الانتقال الإلكترولني، التوصيلية، اقتران الكترولن-اهتزاز.

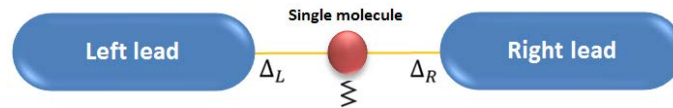
## INTRODUCTION

Electronic transport through molecular junctions is of immense scientific and technological interest because it may form fundamental nano and molecular electronics devices. In addition to their potential industrial application, these devices provide an ideal test ground for the study of basic physics including the nano size [1-3]. Single molecule junctions are among the smallest electric circuits, and they are structures in which a single molecule forms a stable electrically conducting bridge between two metal and/or semiconductor leads. The flow of currents through these junctions can be studied and controlled [2-4]. These systems have been studied intensively experimentally [5, 6] and theoretically [7, 8]. The electronic transfer behavior through these junctions becomes more clearly visible by studying of the conductance-voltage characteristics [6, 9]. Many early studies of molecular junctions were interested to measurement of the conductance-voltage characteristics of such junctions and their dependence on some of junction parameters [10-14]. Scientists and researchers recently studied and investigated how current is flowing through a single molecule and if the molecular synthesis may be used to control currents on a molecular scale [4, 6]. Two important aspects have to be considered on the molecular scale: the wave nature of the electron and the electron-vibration interaction of the molecular bridge [15-19]. These aspects are important in electronic transport through single molecule junctions due to their small size and mass, especially electron-vibration coupling and the respective current-induced vibrational excitation influences the electronic transport characteristics for these systems profoundly [20].

The complete knowledge of the conduction mechanism in this scale is not well understood even today. Therefore, we try in this article to investigate the effect of the electron-vibration interaction (via the electron-vibration coupling strength), the molecular bridge-leads distance (via the molecular bridge-leads coupling strengths) and the junction temperature on the electronic transport (the electrical conductance) through single molecule junction using Keldysh non equilibrium Green function model in the resonant tunneling regime.

**Theoretical Model**

The total system consists of subsystems, a single molecule connected to the two metallic leads. The electrons in the molecule are also coupled to a single phonon mode. The energies (annihilation operators) of a left and right lead, a molecular orbital and a vibrational mode are denoted by  $E_L (C_L), E_R (C_R), E_M (C_M)$ , and  $\omega, (b)$  respectively. For simplicity, often use a molecular bridge model that corresponds to one molecular orbital of energy  $E_M$  (we consider the lowest unoccupied molecular orbital, LUMO) to represent the molecular electronic system. The model system under consideration is illustrated in Fig. 1. By applying a potential bias at the leads, electrons flow from one lead to the other through the molecular bridge. This state can be controlled by the polarity and the magnitude of the potential bias [21].



**Figure 1 (Color online) Schematic representation of a single molecule junction, where a single molecule attached to two (left and right) metal leads through the couplings  $\Delta_L$  and  $\Delta_R$ . The molecule's electrons are also interacting with a single phonon mode.**

The Hamiltonian of this system is given by [20, 22-26]

$$H = \sum_L E_L C_L^\dagger C_L + \sum_R E_R C_R^\dagger C_R + E_M C_M^\dagger C_M + \omega \left( b^\dagger b + \frac{1}{2} \right) + \sum_L (V_{LM} C_L^\dagger C_M + h.c.) + \sum_R (V_{RM} C_R^\dagger C_M + h.c.) + \lambda C_M^\dagger C_M (b^\dagger + b).$$

Electronic tunneling matrix elements  $V_{LM}$  (left lead-molecule) and  $V_{RM}$  (right lead-molecule) give rise to a stationary current between the left and the right lead through the molecular bridge. The electron-vibration coupling constant is denoted by  $\lambda$ . The junction is assumed to be in thermal equilibrium, and have independent chemical potentials of left and right leads  $\mu_L$  and  $\mu_R$ , respectively. At zero bias,  $V_{bias} = 0$ , the chemical potentials in the left lead  $\mu_L$  and the right lead  $\mu_R$  are at the same level as the Fermi energy (the chemical potential in the equilibrium case) of the system  $E_F = 0$ , while at  $V_{bias} \neq 0$  they are different. The difference that corresponds to the bias voltage  $V_{bias}$  where is added to the system according to [20, 27, 28],

$$eV_{bias} = \mu_L - \mu_R \quad \text{with} \quad \mu_L = E_F + V_{bias}/2 \quad \text{and} \quad \mu_R = E_F - V_{bias}/2 \quad (2)$$

The finite bias voltage is necessary to achieve transport in molecular junctions. In the absence of the applied voltage, the stationary electrons distribution functions of the two leads are given by the Fermi distribution functions,

$$f_{L/R}(E) = \left[ \exp\left(\frac{E - \mu_{L/R}}{k_B T}\right) + 1 \right]^{-1} \quad \dots(3)$$

Where

$E$  is the energy of the tunneling electron and  $k_B$  the Boltzmann constant, while the stationary phonons distribution function is given by the Bose-Einstein distribution function,

$$f(\omega) = \left[ \exp\left(\frac{\omega}{k_B T}\right) - 1 \right]^{-1} \quad \dots(4)$$

Where

$\omega$  is the energy of the vibrational system. The electron-vibration coupling  $\lambda$  is not only responsible for the vibrational excitation and deexcitation upon temporal occupation of tunneling electrons in the molecule, but also for the vibrational relaxation due to electron-hole pair excitations in the leads [20, 24, 25, 28].

The electrical conductance  $dI/dV_{bias}$  curve can be obtained by numerical differentiation of the tunneling current ( $I$ ). In what follows we give a detailed description for the calculation of the net current formula through a single molecule junction [20, 25, 29, 30],

$$I = \frac{2e}{h} \frac{\Delta_L \Delta_R}{\Delta} \int dE \rho_M(E) [f_L(E) - f_R(E)]. \quad \dots(5)$$

The coupling of the molecular bridge to the leads is characterized by the level-width functions [20, 25],

$$\Delta_{L/R}(E) = 2\pi \sum_{K \in L/R} |V_{KM}|^2 \delta(E - E_K) \quad \text{and} \quad \Delta = \Delta_L + \Delta_R \quad \dots(6)$$

Where

$\Delta$  is the total level-width function to describe the broadening of the energy level on the molecule due to the hybridization between the molecule and the leads by

interaction matrix elements  $V_{KM}$ . For simplicity, these functions are assumed to be energy independent in the wideband approximation. The molecular bridge and the leads are exchanging energy. In our description, such energy exchange is the result of

electron-vibration coupling and mediated by inelastic electron tunneling processes. The influence of the electron-vibration interaction enters into Eq. (5) through the full molecule density of states [20, 24]

$$= -\frac{1}{\pi} \text{Im } G_M^r(E), \tag{7}$$

Where:

The molecule retarded Green's function  $G_M^r(E)$  is given by

$$= \frac{1}{E - E_M - i\Delta - \Sigma_M^r(E)} \tag{8}$$

The imaginary part of the self-energy  $\Sigma_M^r(E)$  in Eq. (8) is calculated to the second-order of  $\lambda$  as [25, 31]

$$\text{Im}\Sigma_M^r(E) = \pi\lambda^2 \int \rho_{ph}(\omega) \times \{f_{ph}(\omega) [\rho_{ei}(E - \omega) + \rho_{ei}(E + \omega)] + [1 - f_{ei}(E - \omega)] \times \rho_{ei}(E - \omega) + f_{ei}(E + \omega) \rho_{ei}(E + \omega)\} d\omega, \tag{9}$$

In the absence of electron-phonon coupling (the unperturbed case) the densities of states are given by [25, 27],

$$\rho_{ei}(\omega) = \frac{\Delta}{\pi} [(E - E_M)^2 + \Delta^2]^{-1}, \tag{10}$$

$$\rho_{ph}(\omega) = \frac{\Gamma_{ph}(\omega)}{\pi} [(\omega - \omega_0)^2 + \Gamma_{ph}^2(\omega)]^{-1}, \tag{11}$$

The vibrational damping rate  $\Gamma_{ph}(\omega)$  due to electron-hole excitation is given by [20, 25, 32]

$$\Gamma_{ph}(\omega) = \pi\lambda^2 \int \rho_{ei}(E) \rho_{ei}(E + \omega) \times [f_{ei}(E) - f_{ei}(E + \omega)] dE, \tag{12}$$

Where  $f_{ei}(\omega)$  and  $f_{ph}(E)$  are the electrons and phonons occupation functions in the junction, respectively,

$$f_{el}(E) = \frac{\Delta_L f_L(E) + \Delta_R f_R(E)}{\Delta}, \quad \dots(13)$$

$$f_{ph}(\omega) = \left[ \exp\left(\frac{\omega_c}{k_B T}\right) - 1 \right]^{-1} + \frac{\pi \lambda^2}{\Gamma_{ph}(\omega)} \frac{\Delta_L \Delta_R}{\Delta} \int \rho_{el}(E) \rho_{el}(E + \omega) \times [f_L(E) - f_R(E)][f_L(E + \omega) - f_R(E + \omega)] dE. \quad \dots(14)$$

Eq. (14) includes the vibrational heating (in the second term) by inelastic tunneling electrons [24, 25, 27].

### Results and Discussion

In this section, we present our results that obtained by numerical calculations to study the conductance-voltage characteristics for a single molecule junction in the resonant tunneling regime based on NEGF model. Numerical Results of the conductance-voltage characteristics are shown in figures 2(a-c) and 3(a-c). In our numerical calculations, the following notes are taken into consideration: (1) the electron tunneling process with resonant limit  $\Delta \gg |E - E_M|$  is studied. (2) Using the atomic units system ( $\hbar = e = 1$ ) for the conductance quantum  $2e^2/h$ , with  $e$  is the electron charge and  $\hbar = 2\pi\hbar$  is Planck constant. (3) A set of energy parameters used are appropriate to energies in small molecules. (4) For simplicity, the molecular bridge-leads coupling interactions are symmetry ( $\Delta_L = \Delta_R$ ) and the leads have broad and flat density of states (i.e., the wideband approximation) are considered. This symmetry can be rationalized by noting that tunneling distances between the molecule and the left and right leads are equal, resulting in same tunneling probabilities towards these leads for an electron that lost energy to molecular vibrations. (5) The parameters values used to describe the system in this work are representing typical values for molecular junctions as they are found for example in experiments [33-35] or employing ab-initio calculations [15, 36, 37]. (6) The voltage division parameter  $\eta (= \Delta_R/\Delta)$  is used, this parameter determines the voltage induced shifts in the leads electrochemical potentials  $\mu_L$  and  $\mu_R$  relative to  $E_F$  using the formula  $\mu_L = E_F + \eta eV_{bias}$  and  $\mu_R = E_F - (\eta - 1) eV_{bias}$ . The effect of this parameter on the numerical results translates into the relative positioning of electronic energies of the system by the applied bias voltage [27].

In our calculations, we use as a representative set of molecular junction parameters  $E_M = 0 \text{ meV}$  (that is in principle controllable by applied gate voltage),  $\lambda = 50 \text{ meV}$ ,  $\Delta_L (= \Delta_R) = 5 \text{ meV}$  and  $T = 10 \text{ K}$ , since we interest in the change of the parameter value used to investigate the conductance dependence.

Figures 2 and 3 show the dependence of the conductance on the bias voltage. Physically meaningful values of the tunneling current correspond to the inelastic threshold voltage  $eV_{bias} = \omega_0$ , as a result of the electron energy associated with the

Applied bias is just enough to excite the vibrational mode. Thus, at the threshold the inelastic transmission channels open up and appear a peak in the conductance.

In Fig. 2(a) the effect of electron-vibration coupling on the conductance is investigated. The conductance shows resonant peak associated with the energy eigen value of the corresponding molecule. Thus, it can be emphasized that the conductance spectrum manifests itself as the energy eigen value of the molecule. The size of the conductance drop can be scaled with  $\lambda$ . This is due to the fact that a larger electron-vibration coupling gives a larger change (decreasing) in the conductance at the inelastic threshold voltage  $eV_{bias} = \omega_0$ , where the conductance exhibits an additional broadening due to energy dissipation to the vibrational mode. It is important to observe the conductance exhibits a peak at  $eV_{bias} = \omega_0$  and dip prominent at  $eV_{bias} \approx \Delta$  for increasing electron-vibration coupling strength, this dip mean occurrence of the backscattering processes of electrons near the leads. Change point can be seen in the behavior of the conductance for increasing this interaction at  $eV_{bias} \approx 24$  meV due to current-induced heating of the vibrational mode. Conductance curves are vanishes at  $eV_{bias} = 2\omega_0$  as a result another vibrational excitation.

Figure 2(b) shows the change in the conductance with changing the coupling strength to the leads. In the molecular bridge-leads weak coupling limit the conductance shows very sharp resonant peaks at the position of the resonance level of the molecule. While, with increasing the molecular bridge-leads coupling strength, the widths of these resonances get enhanced substantially. This is due to the substantial broadening of the quantized energy levels of the molecule. The contribution for such broadening of the energy levels comes from the imaginary parts of the two self-energies (for left and right lead). Thus, for the strong coupling limit, the electron conducts through the molecule for a wide range of energies, while, a fine tuning in the energy scale is necessary to get the electron conduction through the molecule in the limit of weak coupling. Therefore, it can be predicted that the molecular bridge-leads coupling strength has a significant role in the determination of the electron conduction through a molecular junction. The Electronic resonance of the molecule overlaps with Fermi level of the leads, the onset of the vibrational excitation leads to an overall decrease in the conductance due to the suppression of elastic tunneling. For a molecule resonance near the Fermi level, the conductance decreases

at  $eV_{\text{bias}} = \omega_e$  due to the additional broadening associated with energy dissipation to the vibrational excitation. This gives rise to plateaus, separated by thermally broadened steps. Due to the symmetric application of the bias, the steps occur at voltages of twice the corresponding excitation energy. The plateau heights depend on the coupling parameters  $\Delta_L$  and  $\Delta_R$  only, i.e. they are independent of  $\lambda$  and  $T$ .

Inelastic tunneling processes become active at slightly different bias voltages or energies, because the vibrational frequencies  $\omega$  are renormalized due to the coupling of the molecule to the leads.

The effect of temperature is demonstrated in Fig. 2(c) where the results of the conductance for low temperatures and up to room temperature are presented. The resonant peak of the conductance becomes wider and lower with increasing the temperature. At the same time the peaks at the inelastic threshold voltage disappear, and the difference in the resonance peak heights becomes more pronounced. As can be observed in Fig. 2(c), the conductance exhibits small steps which can be associated with the onset of inelastic emission of phonons. This width is in turn controlled by the mechanical coupling of the molecule with the leads, thus providing an intrinsic width of the steps in the conductance. In this work, we performed all the previous calculations in Figures 2(a) and 2(b) at low temperature  $T = 10 \text{ K}$ , the reason for such an assumption is that the broadening of the energy levels of the molecule due to its coupling to the leads is much larger than that of the thermal broadening.

The set of parameters in Fig. 3 are the same parameters used in Fig. 2, with  $\omega_e = 100 \text{ meV}$ . We observe one resonance at the resonance level for all values of electron-vibration coupling in Fig. 3(a), while all dips and peaks disappear, which are appearing in  $\omega_e = 50 \text{ meV}$  in Fig. 2(a). Therefore, the electron-vibration coupling strength insignificantly influence on the conductance spectra, because enhancement the inelastic threshold voltage lead to suppression the backscattering processes of electrons near the leads. In Fig. 3(b), the plateaus disappear from the conductance spectra for all values of the molecular bridge-leads coupling, except at the molecular bridge-leads weak coupling limit. The temperature dependence of the conductance calculated at  $\omega_e = 100 \text{ meV}$ , is shown in Fig. 3(c). By comparing Fig. 3(c) with Fig. 2(c), we observe none difference in the spectra so we conclude that the conductance is not enhanced by increasing  $\omega_e$ .

## Conclusions

In the conclusion, we have studied the effects of the electron-vibration interaction strength, the molecular bridge-leads coupling strength and the junction



temperature on the conductance-voltage characteristics through single molecule junctions using the Keldysh nonequilibrium Green function model in the resonant tunneling regime. That junction comprises a one level bridge (it is chosen as the molecular LUMO) between two metallic leads, the level is coupled with a vibrational degree of freedom that represents a molecular vibration. It is found that these parameters are important parameters to determine the nature and the mechanisms of the conductance-voltage characteristics in a single molecule junctions. According to our calculations, important features are reported in the following notes: (a) The

Conductance-voltage characteristic shows very sharp resonant peaks at the position of the resonance level of the molecule. (b) With increasing of the electron-vibration interaction strength, the conductance-voltage characteristic exhibits a peak at the inelastic threshold voltage. This change in the conductance due to the additional broadening associated with energy dissipation to the vibrational excitation. (c) When the molecular bridge-leads coupling strength increases, the width of these resonances gets more enhancement substantially, where the plateau heights depend on the molecular bridge-leads coupling parameters. (d) The resonant peak of the conductance-voltage characteristic becomes wider and lower with increasing the junction temperature. (e) None difference in the spectra of the conductance with increasing of the vibrational mode energy. Finally, it is observed that the molecular bridge-leads coupling strengths and the junction temperature have a significant role in the determination of electronic transport characteristics (the electron conduction) through a single molecule junction in the presence of electron-vibration coupling.

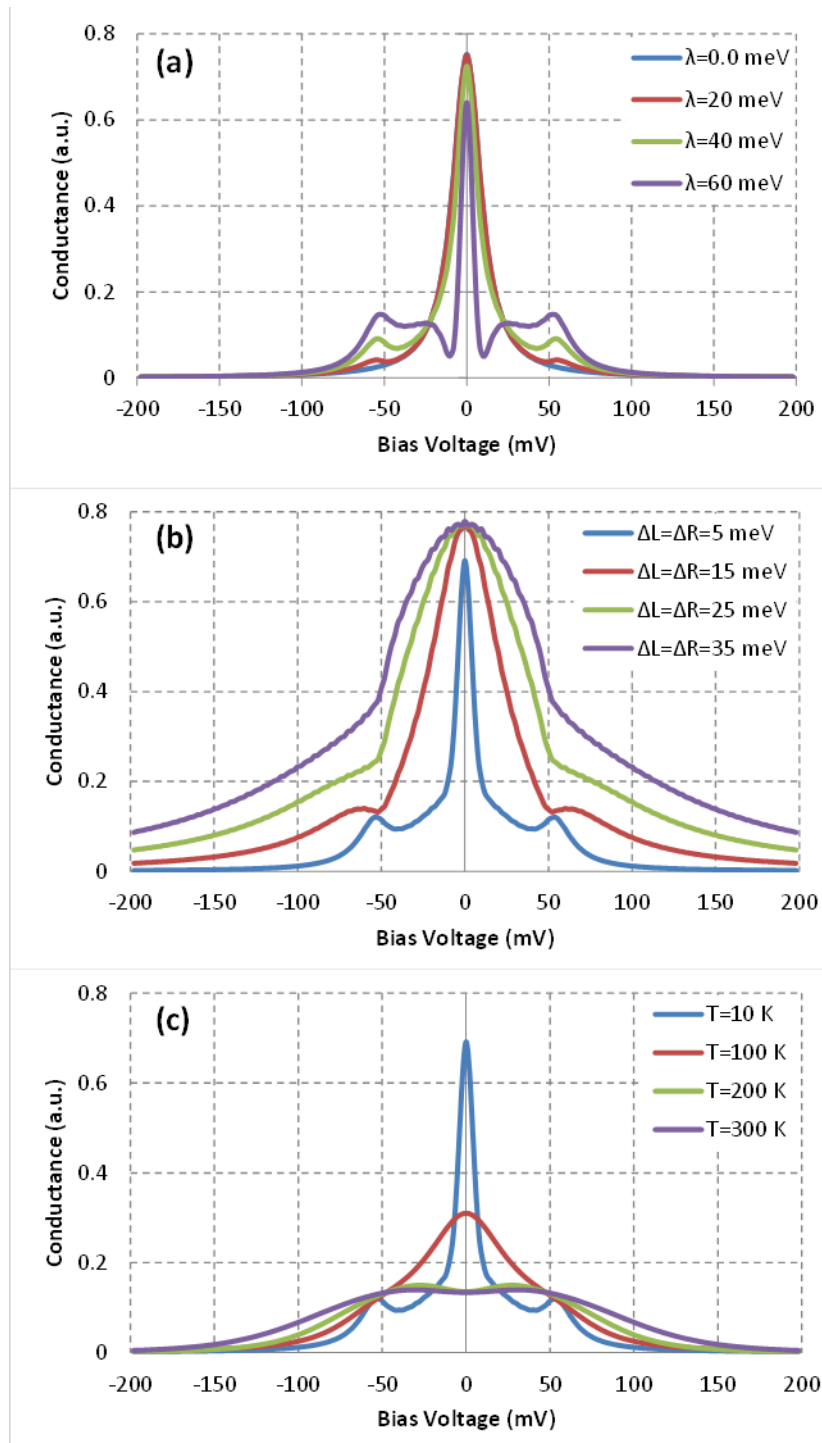


Figure (2) (Color online) Conductance-voltage characteristics of a single molecule junction in the resonant tunneling regime, See the text for the rest of parameters used here in  $\omega_0 = 50$  meV.

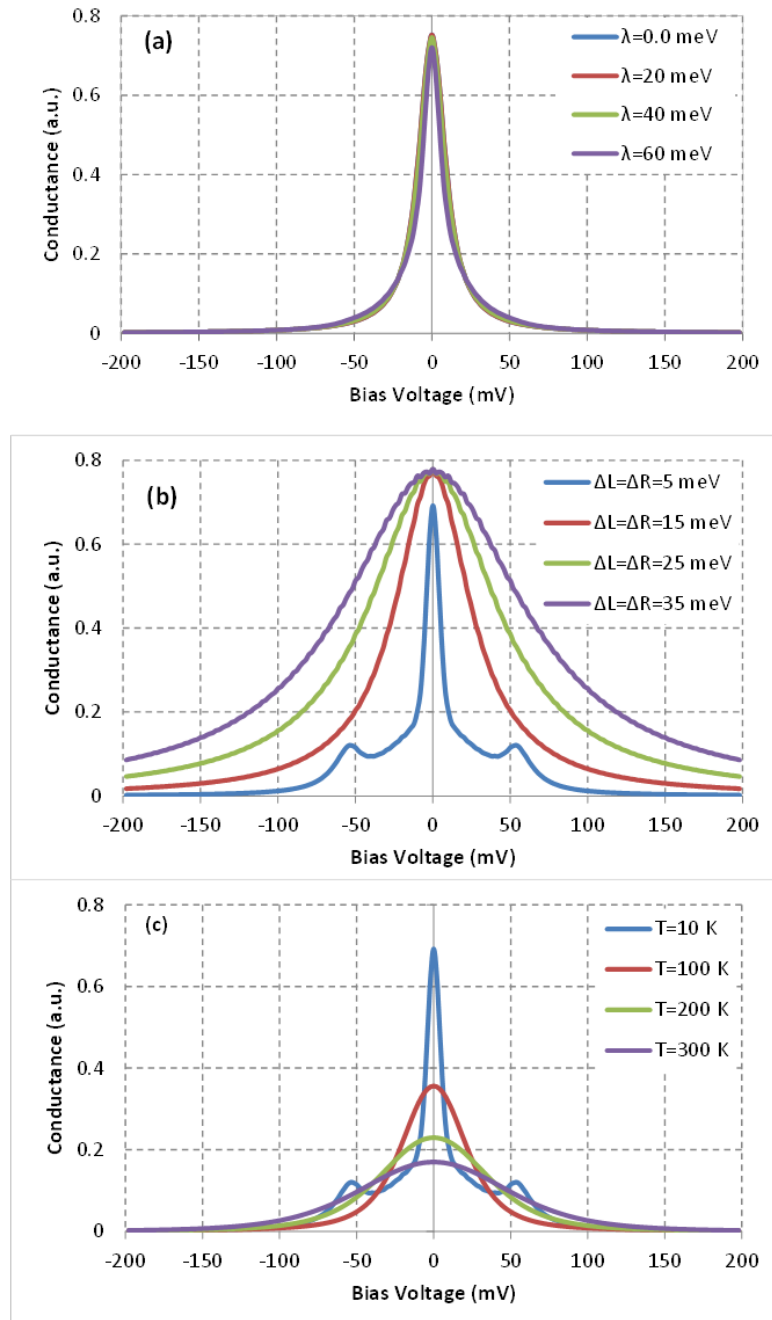


Figure 3) (Color online) Conductance-voltage characteristics of a single molecule junction in the resonant tunneling regime, see the text for the rest of parameters used here in  $\omega_s = 100 \text{ meV}$ .

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