

A Theoretical Study of Charge Transport y at Au/ ZnSe and Au/ZnS Interfaces Devices

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Abstract

A quantum mechanical description of the dynamics of non-adiabatic electron transfer in metal/semiconductor interfaces can be achieved using simplified models of the system. For this system we can suppose two localized quantum states donor state $|D\rangle$ and acceptor state $|A\rangle$ respectively. Expression of rate constant of electron transfer for metal/semiconductor system derived upon quantum mechanical model and perturbation theory for transition between $|D\rangle$ and $|A\rangle$ state when the coupling matrix element coefficient is smaller than 0.025eV . The rate of electron transfer for Au/ ZnSe and Au/ZnS interface systems is evaluated with orientation free energy using a Matlap program. The results of the electron transfer rate constant are calculated for our modeas well as with experimental results .

Key Word :Charge Transport Theory, Metal/ Semiconductor Interfaces

Introduction

Electron transfer is an integral part of many biophysics[1], physical chemistry[2] processes and technology[3], which occurs in a large variety of molecules ranging from small ion pairs up to large system [4].The theory of electron transfer reaction is the subject of persistent interest in physics [5] , over the past several decades, researchers have investigated the transfer of electron through molecule and solid state structure [6] , molecule metal interfaces [7], and metal semiconductors interfaces [8].Metal semiconductor contact from interfaces that give basic features of many metal /semiconductor devices .To construct the diagram of an metal/ semiconductor contact ,we consider the energy band diagram of metal /semiconductor , and align .These ET systems seen important from technological and biological ? where a metal is placed in intimate contact with a semiconductor , the electrons from the conduction band in one material ,which have higher energy ,flow into the other material until the Fermi level on the two sides are brought into coincidence [9].

The energy level in the two material are rearranged relatively to the new common Fermi level. However, the Fermi energy of the metal and semiconductor do not change right away [10].. Fundamental studies, as performed in this paper are expected to provide guidelines for design of such practically useful ET system In this paper, Our main theoretical model to study of electron transfer is at metal/semiconductor interface system .There orientation energy and the rate of electron transfer constant are calculated according to this model.

Theoretical Model

The fundamental starting point is the derived formula for the transition probability given by first order perturbation theory for a transition from a discrete state to continuum state the state a quantum system which is described by a wave function [11].

$$\Psi(r, t) = \sum_n A_n e^{-\frac{iE_n t}{\hbar}} \Psi_n(r) \dots \dots \dots (1)$$

Where $\Psi(r, t)$ is the time dependent state vector in Hilbert space at quantum system state, A_n is the coefficient of wave founction , E_n is the energy ,and t is time .Model Hamiltonians operator used to describe the electron transfer in donor /acceptor system can be written as [12].

$$H = H_{op} + V \dots \dots \dots (2)$$

Where H_{op} is the Hamiltonian before perturbation ,and V refers to the potential where the electron is either on the donor $|D\rangle$ or acceptor $|A\rangle$, respectively ,it is given [13].

$$H_{op} = |D\rangle H_D \langle D| + |A\rangle H_A \langle A| \dots \dots \dots (3)$$

The Hamiltonian operator obeys the Schrödinger equation $H\Psi(r, t) = E_n\Psi(r, t)$.Substituting Eq.(3) and Eq. (2) into Eq.(1)the results

$$(H_{op} + V) \sum_n A_n(t) |\phi(t)\rangle = i\hbar \frac{d}{dt} \sum_n A_n(t) |\phi(t)\rangle \dots \dots \dots (4)$$

The first term on each side in Eq.(4) is cancelled that because $|\phi(t)\rangle$ is a solution to time dependent schrodinger equation with H_{op} Eq. (3) becomes .

$$i\hbar \sum_n \frac{d}{dt} A_n(t) |\phi(t)\rangle = \sum_n A_n(t) V |\phi_n(t)\rangle e^{-\frac{iE_n t}{\hbar}} \dots \dots (5)$$

Multiply both sides of the Eq.(5) by $\langle \Phi_m(t) |$ for the final state and integral over space, we get :-

$$i\hbar \sum_n \frac{d}{dt} A_n(t) \langle \Phi_m(t) | \Phi_n(t) \rangle e^{-\frac{iE_n t}{\hbar}} = \sum_n A_n(t) \langle \Phi_m(t) | V | \Phi_n(t) \rangle \dots (6)$$

By normalizing the left hand side of Eq. (6) all terms vanish except $n=m$ then.

$$\frac{d}{dt} A_n(t) = \frac{1}{i\hbar} \sum_n A_n(t) V_{DA} e^{\frac{i(E_m - E_n)t}{\hbar}} \dots \dots \dots (7)$$

Here V_{DA} is the coupling coefficient of donor and acceptor state, and $E_m - E_n$ is the difference in the energy between the state m and n respectively with direct integration for Eq. (7), and mathematical treatment, results.

$$A_n(t) = -iV_{DA} e^{\frac{i(E_m - E_n)t}{2\hbar}} \frac{\sin\left(\frac{(E_m - E_n)t}{2\hbar}\right)}{\left(\frac{(E_m - E_n)t}{2\hbar}\right)} \frac{t}{\hbar} \dots \dots \dots (8)$$

The total probability of finding the particles at time (t) in the final state $|m\rangle$ is given by.

$$P_n(t) = |V_{DA}|^2 \frac{t^2}{\hbar^2} \frac{\sin^2\left(\frac{(E_m - E_n)t}{2\hbar}\right)}{\left(\frac{(E_m - E_n)t}{2\hbar}\right)} \dots \dots \dots (9)$$

The term $\frac{\sin^2\left(\frac{(E_m - E_n)t}{2\hbar}\right)}{\left(\frac{(E_m - E_n)t}{2\hbar}\right)} = \pi \delta\left(\frac{(E_m - E_n)t}{2\hbar}\right)$ [14].

Where δ is delta function $\delta(ax) = \frac{1}{|a|} \delta(x) a \neq 0$ [14]

$$\delta\left(\frac{(E_m - E_n)t}{2\hbar}\right) = \delta\left(\frac{t}{2\hbar}(E_m - E_n)\right) = \frac{2\hbar}{t} \delta(E_m - E_n) \dots \dots \dots (10)$$

So that Eq. (9) becomes :

$$P_n(t) = \left|\frac{2\pi t}{\hbar}\right| |V_{DA}|^2 \delta(E_m - E_n) \dots \dots \dots (11)$$

The rate of the probability transition per unit time is the rate constant K_{et} of electron transfer that means [15].

$$K_{et} = \frac{d}{dt} P_n(t) = \frac{2\pi}{\hbar} |V_{DA}|^2 \rho(E) \dots \dots \dots (12)$$

Such that [16].

$$\int_{-\infty}^{\infty} \rho(E) \delta(E) dE = \rho(E) \dots \dots \dots (13)$$

In place of the wave function, one introduces the density operator [17].

$$\rho = \sum_n \rho_n |\Psi_{\psi_n}\rangle \langle \Psi_{\psi_n}| \quad , \sum_n |\rho_n|^2 = 1 \dots \dots (14)$$

According to Eq.(14) and mathematically the corresponding density operator becomes.

$$\rho = N \sum_n e^{-\frac{(E_d - E_a)}{k\beta T}} |\Phi_n\rangle \langle \Phi_n| \Psi \rangle \dots \dots \dots (15)$$

Eq.(15) indicates that the probability is proportional to the Boltzmann's factor $e^{\frac{-(E_d-E_a)}{k_B T}}$. In non-adiabatic metal/semiconductor interface system the energy difference $\Delta E = E_d - E_a$ and equals the activation free energy ΔG^+ , and can be written Eq.(15) in expression.

$$\rho(\Delta G) = N \exp\left(\frac{-\Delta G}{k_B T}\right) = N \exp\left(\frac{-\Delta G^{++}}{k_B T}\right) \dots\dots\dots(16)$$

The activation energy according Marcus theory is given by [18].

$$\Delta G^{++} = \frac{(\lambda + \Delta G^0)^2}{4\lambda} \dots\dots\dots(17)$$

Inserting Eq.(17) in Eq.(16) results.

$$\rho(\Delta G) = N \exp\left(\frac{-(\lambda + \Delta G^0)^2}{4\lambda k_B T}\right) \dots\dots\dots(18)$$

To Find N we note that using definition of Gamma integral [19].

$$\int_0^\infty e^{-\alpha(\lambda + \Delta G^0)^2} d\Delta G^0 = \left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}} \dots\dots\dots(19)$$

And for complete set $|\Phi_n\rangle$ we found $\sum \Phi_n^* \Phi_m = \sum |\Phi_n|^2 = 1$

$$N = \left(\frac{1}{4\pi\lambda k_B T}\right)^{\frac{1}{2}} \dots\dots\dots(20)$$

Inserting value of N in Eq.(18) we can get the influence of temperature on the electron transfer rate with Boltzmann distribution to give the common classical expression for the Franck-Condon factor.

$$FC = (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{-(\lambda + \Delta G^0)^2}{4\lambda k_B T}\right) \dots\dots\dots(21)$$

Inserting Eq(21) in Eq.(12) we get the Landau-Zener formula to describe the rate of a non-adiabatic electron tunneling from one electronic state to another [20].

$$K_{ET} = \frac{2\pi}{\hbar} |V_{DA}(E)|^2 FC \dots\dots\dots(22)$$

where $V_{DA}(E)$ is the electronic coupling matrix element of the donor and acceptor. The total electron transfer rate from semiconductor (donor state) to the metal (acceptor state) can be expressed as the sum of electron transfer rates to all possible accepting states in the metal that are given by [21].

$$K_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^\infty f(E, E_F) |V_E|^2 (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{-(\lambda + \Delta G)^2}{4\pi k_B T}\right) \dots\dots(23)$$

Where $f(E, E_F)$ is the Fermi-Dirac function can be related to electron by [22].

$$f(E, E_F) = \frac{1}{1 + \exp\left(\frac{E_{CB} - E_F}{k_B T}\right)} \dots\dots\dots(24)$$

Here E_{CB} is the conduction band energy and E_F is the Fermi level energy. Inserting Eq.(24) in the Eq.(23) we get

$$K_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^\infty \frac{1}{1 + \exp\left(\frac{E_{CB} - E_F}{k_B T}\right)} |V_{(k,r)}|^2 (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{-(\lambda + \Delta G)^2}{4\pi k_B T}\right) dE \dots\dots(25)$$

The free energy ΔG is related to occupy energy E by [23].

$$\Delta G = \Delta G^\circ - E \dots \dots \dots (26)$$

Where ΔG° is the standard free energy of reaction. Substituting Eq.(26) in Eq.(25) results.

$$K_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \frac{1}{1 + \exp\left(\frac{E_{CB} - E_F}{k_B T}\right)} |V_{(k,r)}|^2 (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{-(\lambda + \Delta G^\circ - E)^2}{4\pi k_B T}\right) dE \dots \dots \dots (27)$$

The exponent $\exp\left(\frac{(\lambda + \Delta G^\circ - E)^2}{4\pi k_B T}\right) = \exp\left[\frac{(\lambda + \Delta G^\circ)^2}{4\lambda k_B T} - \frac{(\lambda + \Delta G^\circ)E}{2\lambda k_B T} + \frac{E^2}{4\lambda k_B T}\right]$ in the integral .

The activation energy ΔG^{++} is the height of the barrier of ideal potential contact between metal and semiconductor in the absence of surface state is equal the difference between the metal work function Φ_m and the electron affinity χ of the semiconductor and formulated by

$$\Delta G^{++} = \Phi_B = \frac{(e\Phi_m - e\chi)^2}{4\lambda k_B T} [24].$$

$$K_{et} = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} e^{-\frac{(e\Phi_m - e\chi)^2}{4\lambda k_B T}} \int_0^\infty \left[1 + \exp\left(\frac{E_{CB} - eV_{app} - E_F^\circ}{k_B T}\right)\right]^{-1} |V(k, r)|^2 e^{-\frac{E^2}{4\lambda k_B T}} dE \dots \dots (28)$$

Where E_{CB} , V_{app} , and E_F° are the conduction energy, applied voltage, and Fermi energy. The Fermi-Dirac function in Eq.(28) reduced to the Boltzmann equation when $E_{CB} - E_F \gg k_B T$

$$f(E, E_F)(E_{CB} - E_F \gg k_B T) \approx \exp\left(-\frac{E_{CB} - E_F}{k_B T}\right) \dots \dots \dots (29)$$

The square of the electronic coupling matrix element integrated over the distribution of the electronic state at the given E is [25].

$$H_{DA}(k, r)^2 = \frac{|V(k,r)|^2}{2\pi\delta(E_K - E)} \dots \dots \dots (30)$$

Where $H_{DA}(k, r)$ denotes $\langle \psi_k | H | \psi_A \rangle$ and describes the electronic coupling matrix element between the metal end semiconductor state, and k as the electronic state. The metal density of state $\rho(E)$ can be defined as [17].

$$\rho(E) = \sum 2\pi\delta(E_K - E) \dots \dots \dots (31)$$

By substituting Eq.(31) and Eq.(30) in Eq.(28), we get.

$$K_{et} = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} e^{-\frac{(e\Phi_m - e\chi)^2}{4\lambda k_B T}} \int_0^\infty \sum \exp\left(-\frac{E_{CB} - eV_{app} - E_F^\circ}{k_B T}\right) 2\pi |H_{DA}(k, r)|^2 \delta(E_K - E) e^{-\frac{E^2}{4\lambda k_B T}} dE \dots \dots \dots (32)$$

With recall formulated the above equation.

$$K_{et} = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{eV_{app}}{k_B T}\right) e^{-\frac{(e\Phi_m - e\chi)}{k_B T}} \int_0^\infty f_{(E)} e^{-\frac{E_{CB} - E_F}{k_B T}} |H_{(k,r)}|^2 e^{-\frac{E^2}{4\lambda k_B T}} dE \dots (33)$$

Then the rate constant at semiconductor /metal contact .

$$K_{et}(\text{contact}) = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} \frac{n_{eq}}{N_c \exp\left(\frac{-eV_{bi}}{k_B T}\right)} \int \rho(E) f_0(E) |H_{DA}(k, r)|^2 e^{-\frac{E^2}{k_B T}} dE \dots \dots \dots (34)$$

Then $N_c \exp\left(\frac{-eV_{bi}}{k_B T}\right) = \int_0^\infty \frac{\rho(E) f_0(E)}{V} dE$ is readily evaluated being equal to [11]. where V is the volume of the unit cell of semiconductor.

Then Eq.(34) becomes.

$$K_{et}(\text{contact}) = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} \frac{n_{eq} V}{\int_0^\infty \rho(E) f_0(E) dE} \exp\left(\frac{-(e\Phi_m - e\chi)^2}{4\lambda k_B T}\right) \int_0^\infty \rho(E) f_0(E) |H_{DA}(k, r)|^2 e^{-\frac{E^2}{k_B T}} dE \dots \dots \dots (35)$$

The K_{et} depend exponentially on distance with a decay constant β , the K_{et} becomes [26]

$$K_{et} = \frac{1}{\beta} K_{et}(\text{contact}) \dots \dots \dots (36)$$

The ratio of the term $e^{-\frac{E^2}{4\lambda k_B T}}$ in Eq.(3-86) to $\frac{E}{k_B}$ is $\frac{E}{4\lambda}$, which is very small since $E \approx k_B T$, i.e., 0.025 eV and λ typically is 1 eV that the term $e^{-\frac{E^2}{4\lambda k_B T}}$ can then be ignored [18] yielding

$$K_{et} = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{-(e\Phi_m - e\chi)^2}{4\lambda k_B T}\right) \frac{V \int_0^\infty \rho(E) f_0(E) |H_{DA}(k, r)|^2 dE}{\int_0^\infty \rho(E) f_0(E) dE} \dots \dots \dots (37)$$

The averaged coupling electronic coefficient of matrix element square is given by $|H(E, r)|^2 = \frac{\int_0^\infty \rho(E) f_0(E) |H_{DA}(k, r)|^2 dE}{\int \rho(E) f_0(E) dE}$ [18]. Then the rate constant of electron at metal/semiconductor interface is given by.

$$K_{et} = \frac{2\pi}{\hbar} (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(\frac{-(e\Phi_m - e\chi)^2}{4\lambda k_B T}\right) \frac{V}{\beta} |H(E, r)|^2 \dots \dots (38)$$

Where λ is the reorientation energy, \hbar , is Planck constant, Φ_m is the work function of metal, χ is the work function of semiconductor, and β is the attenuation parameter. The reorganization energy is given by [27].

$$\lambda_s = \frac{(\Delta e)^2}{4\pi\epsilon_0} \left[\frac{1}{2a_s} \left(\frac{1}{n_s^2} - \frac{1}{\epsilon_s} \right) + \frac{1}{2a_m} \left(\frac{1}{n_m^2} - \frac{1}{\epsilon_m} \right) - \frac{1}{4d_s} \left(\frac{n_m^2 - n_s^2}{n_m^2 + n_s^2} \frac{1}{n_s^2} - \frac{\epsilon_m - \epsilon_s}{\epsilon_m + \epsilon_s} \frac{1}{\epsilon_s} \right) - \frac{1}{4d_m} \left(\frac{n_s^2 - n_m^2}{n_s^2 + n_m^2} \frac{1}{n_m^2} - \frac{\epsilon_s - \epsilon_m}{\epsilon_s + \epsilon_m} \frac{1}{\epsilon_m} \right) - \frac{2}{R_{m_s}} \left(\frac{1}{n_s^2 + n_m^2} - \frac{1}{\epsilon_s + \epsilon_m} \right) \right] \dots \dots \dots (39)$$

Where $n_m^2 \epsilon_m$, $n_s^2 R_{m_s}$, a_s , a_m , d_s , and d_m are the dielectric constant for semiconductor and metal, refractive index for semiconductor and metal, distance between metal semiconductor, radii of semiconductor and metal and the distance for semiconductor and metal to electrodes respectively.

Results

Theoretical studies for electron transfer at Au/ ZnSe and Au/ZnS interface system are treated using quantum mechanical theory .We have applied a quantum model results under the weak coupling assumption for the matrix element coupling coefficient to the calculated rate constant of electron transfer at metal/semiconductor interface system using Eq.(38). The evaluate of the rate constant of electron transfer for this system depending on calculation of many parameters, such that: the reorganization free energy λ , the exponent for the decay of the square of the matrix element with distance constant β , the radius a_s, a_m , are the effective radii of both donor and acceptor . The reorganization energy is one of the most important parameters that is calculated using Eq.(39). Substituting in Eq.(39) the values of the static dielectric constant ϵ_m , and ϵ_s for metal , semiconductor and optical dielectric constant , n_m , and n_s from tables(1-2).

Initially of the calculate of rate constant of charge transfer in metal/semiconductor interface system is the reorganization free energy that calculated depending on Marcus– Hush semi classical theory Eq.(39). Inserting the values of a_s , and a_m , are the radii of semiconductor , and metal, and the distance $d_s = a_s + 1, d_m = a_m + 1$, and $R_{m_s} = a_s + a_m$ with values of refractive index and static dielectric constant for semiconductor and metal n_s, n_m, ϵ_s , and ϵ_m respectively. The results are 0.71502218 , 0.670556312, and 0.673663776, there is on agreement with the experimental result[31]. Substituting these values with work function of metal 4.080 [28], and affinity of semiconductor χ_{se} and value of coupling matrix element from table (4) in a Matlab designed program to evaluate the rate constant of charge transfer Eq.(38), results are summarized in table (3-5) for system Au/ ZnSe and Au/ZnS interface systems.

Discussion

A theory of charge transport across metal/semiconductor interface has been derived depending on quantum theory .In our theoretical model, we have been assuming the wave function for transfer of charge from donor to acceptor state describe in Hilbert space, and quantum well. When the metal bring to contact with semiconductor, the Fermi level for two material much be coincident at equilibrium state. The charges upon excitation has to be rapidly transfered into the metal before it can fall back to its ground state .The rate constant of charge transfer have been evaluated for ZnSe and ZnS semiconductors contact with gold Au metal system depending on calculation of many parameters, such that: the reorganization free energy work function of metal, affinity of semiconductor, and the coupling matrix element coefficient in table(3) .The rate constant of charge transfer in tables (3) to (5) for two systems Au/ ZnSe and Au/ZnS interface systems indicate the rate constant dependent on the reorganization energy $\lambda_0(eV)$, and work function $\Phi_m(eV)$, of metal and affinity of semiconductor $\chi_{se}(eV)$.

Consequently the rate of charge transport across metal/semiconductor system has large according with large reorganization energy and vice versa. This indicates the reorganization free energy is large for large dielectric constant for semiconductor .On the other hand the shift in the reorganization free energy is ≈ 0.1 . The ratio of rate indicated the system Au/ZnSe is active media for applied in devices technology according with Au/ZnS system.

Conclusion

A theoretical model for charge transport across metal/semiconductor interface has been derived depending on quantum theory provided a good model that describe the fundamental charge transfer processes. Also the rate constant of charge transfer at two systems Au/ Zn,Se

and Au/ZnS depending on the reorganization free energy that is necessary to alignment and oriented of the configuration system. This energy is limited the ability of transfer.

The rate constant is proportional exponentially with height barrier in $\exp\left[-\frac{(e\Phi_m - e\chi)^2}{4\lambda k_B T}\right]$, for more high, the rate is small. In summary, it can be concluded from the results the Au/ZnSe system are in a good matching as compare with the other system.

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Table No.(1) Properties of semiconductors[29-30]

| Semiconductor Properties | ZnS | ZnSe |
|-----------------------------|-------------|------------|
| Crystal structure | Zinc blend] | Zinc blend |
| Lattice constant(nm) | 0.541 | o.566 |
| Density(g/cm ³) | 4.08] | 5.42 |
| Dielectric constant | 8.3 | 9.2 |
| Refractive index | 2.52226 | 2.62408 |
| Energy gap(eV) | 3.6 | 2.6 |
| Electron affinity(ev) | 3.9 | 4.09 |

Table No.(2) The reorganization energy for Gold metal/semiconductor interface system

| Reorganization energy λ(ev) | | | | |
|-----------------------------|-------------------------|--------------------------|--------------------------|--------------------------|
| System | =a+1.0(A ⁰) | d=a+1.2(A ⁰) | d=a+1.4(A ⁰) | d=a+1.6(A ⁰) |
| Au-ZnS | o.670556312 | o.682074705 | o.69202476 | 0.700700169 |
| Au-ZnSe | o.673663776 | O.685728201 | o.696178713 | o.705299904 |

Table No. (3) The Coupling matrix element $||H_{DA}(k, r)||^2$ for gold (Au)

| $ H_{DA}(k, r) ^2 \times 10^{-11}$ | $ H_{DA}(E, r) ^2 \times 10^{\frac{16(ev)^2}{m^3}}$ | E(ev) |
|--------------------------------------|---|-------|
| 0.4 | 5.889514591 | -1.35 |
| 0.45 | 6.625703913 | -0.90 |
| 0.5 | 7.361893239 | -0.25 |
| 0.55 | 8.098082563 | 0 |
| 0.6 | 8.834271886 | 0.15 |
| 0.65 | 9.57046121 | 0.3 |
| 0.7 | 10.30665053 | 0.5 |
| 0.75 | 11.04283986 | 0.75 |
| 0.8 | 11.77902918 | 1 |

Table No.(4) Rate of electron transfer between Au-ZnS interface

| | | $H(k,E) ^2 * 10^{16} \left(\frac{eV^2}{m^3} \right)$ | | | | | | | | |
|-------------------|--|--|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| | | 5.889514591 | 6.625703915 | 7.361893239 | 8.098082563 | 8.834271886 | 9.57046121 | 10.30665053 | 11.04283986 | 11.77902918 |
| $\beta(A^0)^{-1}$ | Rate of electron transfer K_{et} (m^4/Sec) | | | | | | | | | |
| 0.8 | | 1.142082218E-14 | 1.284842495E-14 | 1.427602773E-14 | 1.57036305E-14 | 1.713123327E-14 | 1.855883604E-14 | 1.998643881E-14 | 2.141404159E-14 | 2.284164436E-14 |
| 0.9 | | 1.015184194E-14 | 1.142082218E-14 | 1.268980242E-14 | 1.395878267E-14 | 1.522776291E-14 | 1.649674315E-14 | 1.776572339E-14 | 1.903470364E-14 | 2.030368388E-14 |
| 1 | | 9.136657745E-15 | 1.027873996E-14 | 1.142082218E-14 | 1.256290439E-14 | 1.370498662E-14 | 1.484706884E-14 | 1.598915105E-14 | 1.713123328E-14 | 1.827331549E-14 |
| 1.1 | | 8.306052496E-14 | 9.344309058E-15 | 1.038256562E-14 | 1.142082218E-14 | 1.245907874E-14 | 1.349733531E-14 | 1.453559186E-14 | 1.557384843E-14 | 1.661210499E-14 |
| 1.2 | | 7.613881454E-14 | 8.565616636E-15 | 9.517351818E-15 | 1.0469087E-14 | 1.142082218E-14 | 1.237255736E-14 | 1.332429254E-14 | 1.427602773E-14 | 1.522776291E-14 |

Table No.(5) Rate of electron transfer between Au-ZnSe interface

| Reorganization energy λ (eV)=0.673663776 eV | | | | | | | | | |
|---|---------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| $H(k,E\epsilon) \left ^2 * 10^{16} \left \left(\frac{eV^2}{m^3} \right) \right. \right.$ | | | | | | | | | |
| $\beta(A^0)^{-1}$ | Rate of electron transfer | | | | | | | | |
| 0.8 | 0.9 | 1 | 1.1 | 1.2 | 1.2 | 1.1 | 1 | 0.9 | 0.8 |
| 5.889514591 | 6.522451996E-12 | 5.870206797E-12 | 5.336551633E-12 | 4.891838997E-12 | 9.783677994E-12 | 8.004827449E-12 | 8.805310194E-12 | 9.539086044E-12 | 1.192385755E-11 |
| 6.625703915 | 7.337758496E-12 | 6.603982646E-12 | 6.003620587E-12 | 5.503318872E-12 | 1.059898449E-11 | 7.337758496E-12 | 8.071534346E-12 | 1.059898449E-11 | 1.192385755E-11 |
| 7.361893239 | 8.153064995E-12 | 7.337758496E-12 | 6.670689542E-12 | 6.114798747E-12 | 1.141429099E-11 | 6.670689542E-12 | 8.071534346E-12 | 1.059898449E-11 | 1.192385755E-11 |
| 8.098082563 | 8.968371495E-12 | 8.071534346E-12 | 7.337758496E-12 | 6.726278621E-12 | 1.141429099E-11 | 7.337758496E-12 | 8.071534346E-12 | 9.783677994E-12 | 1.100663774E-11 |
| 8.834271886 | 9.783677994E-12 | 8.805310194E-12 | 8.004827449E-12 | 7.337758495E-12 | 1.059898449E-11 | 8.004827449E-12 | 8.805310194E-12 | 9.783677994E-12 | 1.100663774E-11 |
| 9.57046121 | 1.059898449E-11 | 9.539086044E-12 | 8.671896404E-12 | 7.94923837E-12 | 1.059898449E-11 | 8.671896404E-12 | 9.539086044E-12 | 1.059898449E-11 | 1.192385755E-11 |
| 10.30665053 | 1.141429099E-11 | 1.027286189E-11 | 9.338965354E-12 | 8.560718241E-12 | 1.141429099E-11 | 9.338965354E-12 | 1.027286189E-11 | 1.141429099E-11 | 1.284107736E-11 |
| 11.04283986 | 1.222959749E-11 | 1.100663775E-11 | 1.000603431E-11 | 9.172198121E-12 | 1.222959749E-11 | 1.000603431E-11 | 1.100663775E-11 | 1.222959749E-11 | 1.375829718E-11 |
| 11.77902918 | 1.304490399E-11 | 1.174041359E-11 | 1.067310326E-11 | 9.783677993E-12 | 1.304490399E-11 | 1.067310326E-11 | 1.174041359E-11 | 1.304490399E-11 | 1.467551699E-11 |

دراسة نظرية لانتقال الشحنة لنظام سطح معدن/ شبه موصل

هادي جبار مجبل العكيلي

محسن عنيد حسوني

مظهر شهاب احمد

رفاه اسماعيل نوري

سراب سعدي جحيل

قسم الفيزياء/ كلية التربية للعلوم الصرفة ابن الهيثم/ جامعة بغداد

استلم البحث في: 24 تشرين الثاني 2013 ، قبل البحث في : 2 شباط 2014

الخلاصة

الوصف الكمي لحركية الانتقال الالكتروني غير الكظيم عند سطحي نظام معدن-شبه موصل أعتمد باستعمال أنموذج مبسط للنظام. افترضنا حالتين كميتين متمركزتين لهذا النظام هما حالة المانح $|D\rangle$ وحالة المستقبل $|A\rangle$ على التتابع. علاقة ثابت معدل الانتقال الالكتروني لنظام سطح معدن-شبه موصل اشتقت تبعاً لانموذج ميكانيك كمي ونظرية الاضطراب للانتقال ما بين حالتى المانح-المستقبل عندما تكون معامل مصفوفة عناصر الازدواج اقل بكثير من $k_B T$. معدل الانتقال الالكتروني حسب مع الطاقة الحرة لاعادة التوصيل باستعمال برنامج ماتلاب. حسابات معدل الانتقال الالكتروني قورنت مع نتائج عملية. وأظهرت تطابقاً جيداً مع نتائج الانموذج.

الكلمات المفتاحية : نظرية الانتقال الالكتروني، سطح معدن /شبه موصل