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Theoretical Study of Probability of Electron Transfer at Nano Electron Device

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Abstract: The focus of this paper is on the study and calculates the transition probability of electron transfer at the metal/semiconductor Nano devices system depending on the quantum consideration. Two localized quantum vector states system l $\varphi_D^{et}\rangle$ and $\varphi_A^{et}\rangle$interacting with each other at interface. The interacting described by the coupling matrix element. The transition probability of the electron transfer can able to election the suitable device using in nanotechnology science applied. Probabilities of transition rate constant have been evaluated due to the reorganization energy using a MATLAB program. Theoretical data for our two systems show that the probability of electron transport is more probable with decreasing the reorganization energy.

Key Word: Probability of Electron Transfer, Nano Electron Device.

INTRODUCTION

The transfer of a single electron from an atom or a molecule to another is considered to be the most elementary Wibrenand Gispen[1] and one of the most ubiquitous and fundamental phenomena in chemistry, physics, and biology.Electron transfer is an integral part of many biophysics, physical chemistry processes and technology, which occurs in a large variety of molecules ranging from small ion pairs up to large biological system Hassooni[2], involves an oxidation of donor state l$\varphi_D^{et}\rangle$ and reduction of an acceptor state l$\varphi_A^{et}\rangle$.Research in the field of nanotechnology is fueled by the possibility of tailoring the fundamental properties of materials with simplification of processing and assembly of devices. The change in properties arises from quantum confinement effects, where the properties of a material become

size dependent. Nano scale materials that have been widely investigated for their properties and application system of Nano rods and nanotubes, biological polymers like deoxyribonucleic acid (DNA) and proteins, thin polymer films, polyelectrolytes (PE) Maheshwari[4].

Since the late 1940s, the field of electron transfer processes has grown enormously, both in chemistry and biology. The development of the field, experimentally and theoretically, as well as its relation to the study of other kinds of chemical reactions been brought together. The early experiments in the electron transfer field were on 'isotopic exchange reactions' (self-exchange reactions) and, later, cross reactions Marcus[4].Around 1950 it became clear that the kinetics of ET reactions strongly vary between different molecular systems. At that time the theoretical description of ET reactions was mainly triggered by Marcus Marcus[4], who was awarded the Nobel Prize in chemistry in 1992 "for his contributions to the theory of electron transfer reactions in chemical systems".

Marcus realized the importance of nuclear configuration changes between reactants and products and the solvent contribution to the ET rateMarcus[4]. Theory of electron transfer reaction is the subject of persistent interest in chemical and biological physics. Over the past several decades, researchers have investigated the transfer of electrons through molecules and solid state structure at molecule/metal interfaces Chun etal[5], and metal /semiconductor interfaces Altered etal[6]. Since the seminal work predicting dynamical of ET reaction in the early 1980's, a great deal of theoretical effort has gone into clarifying the dynamics of the electron transfer Horng[7].The field of electron transfer has been greatly advanced by the detailed analytical theory in the past half century ago depending on the standards Marcus theory and also by the introduction of new technology Jing[8].

In the past time ago, many researchers have studied the kinetics of electron transfer at metal/ semiconductor interface Altered et al[6].They showed that the electron transfer from semiconductor to metal in the bleaching of surface Plasmon band and occur within the time frame of incident pulse laser. In 2009 Prashant and Shanghai[9], Metal semiconductor contact from interfaces that give basic features of many metal /semiconductor devices.To construct the diagram of a metal/ semiconductor contact; we consider the energy band diagram of metal /semiconductor, align with each other these ET systems seen important for 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 to the Fermi level on the two sides are brought into coincidence Krishnan[10].The energy levels in the two materials are rearranged relative to the new common Fermi level. However, the Fermi energy of the metal and semiconductor do not change right away Odell[11].The fundamental aim of this paper is to study the behavior of electron transfer interaction at the metal / semiconductor Nano device interface depending on a quantum theory consideration and Green function with perturbation theory to gate a relationship enables us to study the probability of electron transfer at metal/semiconductor systems. This would be applicable to evaluated the amount of the rate constant of the electron transfer range in metal/semiconductor devices technologically basing on the fact that.

THEORY

The probability of transition rate in steady state can then be written asOdell[11]**.**

$$\Gamma_{ET} = \frac{2\pi}{\hbar}(4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\frac{-1}{2}} \frac{n_{in}V_{sem}}{\sum_0^\infty \rho(E)\mathrm{f}_o(\mathrm{E})}\exp$$
$$-\frac{(\Phi_{met}-\chi_{sem})}{\mathrm{k_B T}}\pi k_B T\sum|\overline{T_{DA}(E)}|^2\mathrm{f}_o(\mathrm{E})\rho_{(E)}\left[[\pi\mathrm{k_B T}-\frac{1}{4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T}}\left(\frac{(\pi\mathrm{k_B T})^3}{4}\right)\right.$$
$$+\frac{1}{32\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}2}\mathrm{k_B}^2T^2}\left(\frac{5(\pi\mathrm{k_B T})^5}{16}\right)-\frac{1}{384\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}3}\mathrm{k_B}^3T^3}\left(\frac{61(\pi\mathrm{k_B T})^7}{64}\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$\left.+\frac{1}{\mathrm{n!}\,(4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\mathrm{n}}}(\propto(\pi\mathrm{k_B T})^{2\mathrm{n}+1})\right] \qquad \ldots(1)$$

where T_{DA} is the probability of electron tunneling from "donor" to "acceptor" contacts , and $F_{(E)}$ is the Fermi Dirac distribution ,n_{in} is the density of concentration at interface, V_{sem} is the volume of unit cell,$\rho_{(E)}$ is the density of state ,T is the temperature and $\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}$ is the reorganization energy

The total coupling matrix elements $\overline{\Lambda(E)}$ are given byAl-Aagealy, and Hassooni[12]

$$\langle\left|\overline{\Lambda(E)}\right|^2\rangle = \frac{\sum|\overline{T_{DA}(E)}|^2\mathrm{f}_o(\mathrm{E})\rho_{(E)}}{\sum_0^\infty \rho(E)\mathrm{f}_o(\mathrm{E})} \qquad \ldots(2)$$

Then the probability of electron transfer in Eq. (1), with Eq. (2)Is given by

$$\Gamma_{ET} = \frac{2\pi}{\hbar}(4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\frac{-1}{2}} n_{in}V_{sem}\exp$$
$$-\frac{(\Phi_{met}-\chi_{sem})}{\mathrm{k_B T}}\pi k_B T\langle\left|\overline{\Lambda(E)}\right|^2\rangle\left[[\pi\mathrm{k_B T}-\frac{1}{4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T}}\left(\frac{(\pi\mathrm{k_B T})^3}{4}\right)\right.$$
$$+\frac{1}{32\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}2}\mathrm{k_B}^2T^2}\left(\frac{5(\pi\mathrm{k_B T})^5}{16}\right)-\frac{1}{384\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}3}\mathrm{k_B}^3T^3}\left(\frac{61(\pi\mathrm{k_B T})^7}{64}\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$\left.+\frac{1}{\mathrm{n!}\,(4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\mathrm{n}}}(\propto(\pi\mathrm{k_B T})^{2\mathrm{n}+1})\right] \qquad \ldots(3)$$

For a $\langle\left|\overline{\Lambda(E)}\right|^2\rangle$ replaced by $\langle\left|\overline{\Lambda(0)}\right|^2\rangle$ to study state, then is, as already noted thatShachi[13].

$$\langle\left|\overline{\Lambda(E)}\right|^2\rangle$$
$$= \pi k_B T\,\langle\left|\overline{\Lambda(0)}\right|^2\rangle \qquad \ldots(4)$$

Then the results of rate become

$$\Gamma_{ET} = \frac{2\pi}{\hbar}(4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\frac{-1}{2}} n_{in}V_{sem}\exp-\frac{(\Phi_{met}-\chi_{sem})}{\mathrm{k_B T}}\langle\left|\overline{\Lambda(0)}\right|^2\rangle \qquad \ldots(5)$$

But the probability of electron transfer at metal/semiconductor are depends exponentially on distance with a decay constant, the Γ_{et} becomesGao etal[14]

$$\Gamma_{et} = \frac{1}{\beta}\Gamma_{ET}\ldots\ldots\ldots. \qquad \ldots(6)$$

Where β petration factor and the coupling matrix element coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$ for metal and semiconductor.

Then

$$\Gamma_{et} = \frac{2\pi}{\hbar}(4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\frac{-1}{2}}\frac{n_{in}V_{sem}}{\beta}\exp - \frac{(\Phi_{met}-\chi_{sem})}{\mathrm{k_B T}}\langle|\overline{\Lambda(0)}|^2\rangle\left[\pi\mathrm{k_B T} - \frac{1}{4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T}}\left(\frac{(\pi\mathrm{k_B T})^3}{4}\right) + \frac{1}{32\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}2}\mathrm{k_B}^2T^2}\left(\frac{5(\pi\mathrm{k_B T})^5}{16}\right) - \frac{1}{384\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}3}\mathrm{k_B}^3T^3}\left(\frac{61(\pi\mathrm{k_B T})^7}{64}\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots + \frac{1}{\mathrm{n!}\,(4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}\mathrm{k_B T})^{\mathrm{n}}}(\propto(\pi\mathrm{k_B T})^{2\mathrm{n}+1})\right] \quad \ldots(7)$$

Now the electron can be transport from donor state to an acceptor state when a light is incident on the donor acceptor system, and the energy or driving force energy that needed to drive an electron to transfer is given by Al-Aagealyand Hassooni[15].

$$\Delta V^{\circ} = E_{abs} - \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} = h\mathrm{f} - \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \quad \ldots(8)$$

WhereE_{abs}Is the absorption energy by electron,h is Planck constant, f is the frequency,$f = \frac{c}{\lambda}$ Where c is the velocity of light, λ is the wwavelengthand $\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}$ is the reorientation energy. The reorientation energy $\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}$arises from the reorientation of the electron in the system dependent on the radius of the donor and acceptor site, on its distance (d), and on the dielectric properties of the metal and the semiconductor. It is given byGarol[16].

$$E_{semi.}^{met} = \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2R_{met}}\left(\frac{1}{n_{met}^2}-\frac{1}{\varepsilon_{met}}\right)+\frac{1}{2R_{semi}}\left(\frac{1}{n_{semi}^2}-\frac{1}{\varepsilon_{semi}}\right)-\frac{1}{4D_{semi}}\left(\frac{n_{met}^2-n_{semi}^2}{n_{met}^2+n_{semi}^2}\frac{1}{n_{semi}^2}-\frac{\varepsilon_{met}-\varepsilon_{semi}}{\varepsilon_{met}+\varepsilon_{semi}}\frac{1}{\varepsilon_{semi}}\right)-\frac{1}{4D_{met}}\left(\frac{n_{semi}^2-n_{met}^2}{n_{semi}^2+n_{met}^2}\frac{1}{n_{met}^2}-\frac{\varepsilon_{semi}-\varepsilon_{met}}{\varepsilon_{semi}+\varepsilon_{met}}\frac{1}{\varepsilon_{met}}\right)-\frac{1}{R_{met-semi}}\left(\frac{1}{n_{met}^2+n_{semi}^2}-\frac{1}{\varepsilon_{semi}+\varepsilon_{met}}\right)\right] \quad \ldots(9)$$

Where R_{met} and R_{semi} are the radius of metal and semiconductor, $D_{semi} = R_{semi} + 1A^{\circ}$,$D_{met} = R_{met} + 1A^{\circ}$, and $R_{met-semi} = R_{met} + R_{semi}$ are the distance between semiconductor ,metal to interface and metal-semiconductor, n_{met} , ε_{met} are the optical and statistical dielectric constant and n_{semi} and ε_{semi} are the optical and statistical dielectric constant for semiconductor. The radius of the molecule can be estimated from the apparent molar volume using a spherical approachAl-Aagealy and Hassooni[15]

$$R = \left(\frac{3M}{4\pi N\rho}\right)^{\frac{1}{3}} \quad \ldots(10)$$

Where M is the molecular weight, N is Avogadro's number, and ρ is the mass density.

RESULT

Theoretical description and investigation of the transmission probability rate of electron transfer at metal/semiconductor Nano devices system are depending on many important parameters, one of these important parameters is the reorientation energy $E_{met}^{sem}(eV)$. The reorientation energy $E_{met}^{sem}(eV)$ is the energy required to reorientation of the system before transfer, to initial transfer process. One of the elementary steps to calculation of the reorganization energy $E_{met}^{sem}(eV)$) , that's must be evaluated radius for donor state Ag metals and TiO_2 ,and ZnO for acceptor semiconductor state using spherical approach expression in Eq.(10) . By inserting the values of Avogadro's constant $N = 6.02 \times 10^{23}\ \frac{Molecule}{mol}$,molecular weight M, and density masses ρ for all TiO_2 ,and ZnO semiconductors and Ag metalfromtables (1) in Eq.(10), we can evaluate the values of radii for two semiconductors and metal respectively, data of the evaluation are shown in table (1).

Table 1: Common properties of Ag metal, TiO2 and ZnO semiconductor.

Properties	Ag	TiO_2	ZnO
Atomic weight	107.87 Patnaik[17]	79.866 Cotton etal[19]	81.38
Crystal structure	Cubic Patnaik[17]	Tetragonal rutile	Wurtzite Ruzyllo[22]
Density (g/cm^3)	10.43 Patnaik[17]	4.23 Cotton etal[19]	5.66 Ruzyllo[22]
Refractive index		2.609 Cotton etal[19]	2.00337 Edward[23]
Dielectric constant	16.0	102 Cotton etal[19]	8.5 Ruzyllo[22]
Effective density of states in conduction band, N_C (cm^{-3})		1.163×10^{19}Perevalov[20]	2.22*10^24
Energy gap (eV) at 300K		3.02 Shipra and Manoj[21]	3.4 Ruzyllo[22]
Lattice constant (Å)	4.09 Marvin[18]	a = 4.5936 c =2.9587 Cotton etal[19]	a=0.32495, c=o. 5206 Ruzyllo[22]
Melting point (ºC)	961.93 °C	1.843°C Cotton etal[19]	1975°C
Calculated Radius(Å)	1.44	1.95612	3.8025
work function or Electron affinity, (eV)	94.26	4.2 Perevalov[20]	4.5 Ashok and Durger[24]

Depending on radii data result and properties of metal and the semiconductor in table (1),we can be calculate the reorientation energy of metal / semiconductor system for Ag metals donor with TiO_2 ,and ZnO Nano devices interface systems using Marcus– Hush in Eq.(9) with a Matlab program and substituting the values of donor and acceptor ,R_{met} and R_{semi} radius for metal and semiconductor, distance from interface to metal $D_{met} = R_{met} + 1A^{\circ}$, and semiconductor $D_{semi} = R_{semi} + 1A^{\circ}$ with$R_{met-semi} = R_{met} + R_{semi}$ are the distance between metal-semiconductor interface , the statically ε_{met} , ε_{semi} optical dielectric constant n_{met}, and n_{semi} For metal and semiconductor from tables (4-

1) and(4-2) respectively . Knowing that$\frac{e^2}{8\pi\epsilon} = 7.2\ eV$, results of data for reorientation energies have been summarized in tables (2) and (3) for Ag /TiO_2, and Ag /ZnO interface system respectively.

Table 2: Results of the reorganization energy $E_{met}^{sem}(eV)$ for electron transfer at Ag metal / TiO_2 semiconductor interface system.

energy for Ag Marvin [18]	n for Ag Marvin [18]	k for Ag Marvin [18]	$\epsilon_m$for Ag Marvin [18]	$E_{met}^{sem}(eV)$ for Ag-TiO_2
2	0.27	4.18	17.545	48.6415
2.5	0.24	3.09	9.6057	61.3176
3	0.23	2.27	5.2058	66.4438
3.25	0.23	1.86	3.5125	66.1172
3.5	0.21	1.42	2.0605	78.7054
3.6	0.23	1.13	1.3298	64.4699
3.8	0.73	0.3	0.6229	1.4376
3.9	1.3	0.36	1.8196	0.6094
4	0.326	0.33	0.2126	0.6138

Table 3: Results of the reorganization energy $E_{met}^{sem}(eV)$) for electron transfer at Ag metal/ZnO semiconductor interface system.

for AgenergyMarvin [18]	n for Ag Marvin [18]	for Ag Marvin [18]	$\epsilon_m$for Ag Marvin [18]	$E_{met}^{sem}(eV)$ for Ag $-$ ZnO)
2	0.27	4.18	17.5453	48.6493
2.5	0.24	3.09	9.6057	61.2987
3	0.23	2.27	5.2058	66.3954
3.25	0.23	1.86	3.5125	66.0515
3.5	0.21	1.42	2.0605	78.6211
3.6	0.23	1.13	1.3298	64.373
3.8	0.73	0.3	0.6229	1.294
3.9	1.3	0.36	1.8196	0.4326
4	1.61	0.6	2.9521	0.4254

A theoretical studies of electron transfer probability due to interface of the metal/semiconductor system have been depending on the calculation of the unit cell volume of TiO_2, and ZnO semiconductors. Volume of unit cell of TiO2, and ZnO semiconductors have been calculated by using the volume equation $(m^3) = A.|B \times C|$, where A, B, and C are the lattice parameters. Results of volume unit cell are $6.2432*10^{-29}$ and $5.498*10^{-29}$ for TiO_2, and ZnO semiconductors.

To calculate the rate constant of electron transfer, we must estimate the electronic coupling coefficient $\overline{\Lambda(0)}$ for the overlapping wave function for metal and semiconductor. The coefficient of coupling $\overline{\Lambda(0)}$For the metal/semiconductor system was estimated with a typical value from experimental results $\langle|\overline{\Lambda(0)}|^2\rangle = 0.4,0.45,0.5,\ 0.55,\ 0.6,\ 0.65,\ 0.7,\ 0.75,$ and $0.8\text{x}10^{-11}(\ eV)^2$depending on literature data in Shachi[13] and exchange to $\overline{\Lambda(0)}(\text{cm}^{-1})$ using transform parameter,and the results are shown in **Table (4).**

Table 4: Data of the coupling coefficient overlapping between metal and semiconductor interface.

Coupling $\text{x}10^{-11}(\ eV)^2$	Coupling (cm^{-1})
0.4	0.01613
0.45	0.017109
0.5	0.018030
0.55	0.018915
0.6	0.019750
0.65	0.020560
0.7	0.01339
0.75	0.022088
0.8	0.022813

A theoretical description and studies of electron transfer at metal/semiconductor interface system is depending on the probability of rate constantΓ_{ET} results. Our expression in Eq.(7) have been applied to known the behavior of electron transfer across interface metal/semiconductor, we have been evaluated of the probability of electron transition at metal/semiconductor interface is dependent on the calculation of the many important parameters such that; reorientation energy E_{met}^{sem}, potential highest barrier ,work function of metal Φ_{met}, affinity of semiconductor χ_{sem},concentration of electron n_{in},volume of unit cell for semiconductor V_{sem},penetration factor β, temperature T(K) and the electronic coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$.

The rate constant of ET can be calculated using expression in Eq.(73-86) enable gate all information about all electrical properties of metal/semiconductor interface devices through knowing the values of rate constant for Ag /TiO_2 and Ag /ZnO systems.

A MATLAB version 6.5 program has been used for calculations the probability of transmission of electron ET at metal/semiconductor interface system using Eq.(7) and inserting the reorientation energies$E_{met}^{sem}(eV)$ data from tables (2-3) for Ag /TiO_2 and Ag /ZnO systems, concentration of electron n_{in},volume of unit cell for semiconductor V_{sem},penetration factor β=$1 \times 10^{-10}\ m^{-1}$, and the coupling matrix element coefficient$\langle|\overline{\Lambda(0)}|^2\rangle$and work function of metalΦ_{met} and affinity of semiconductorχ_{sem}

Results data of calculation are listed in tables (5), (6) for Ag /TiO_2 and Ag /ZnO systems.

Table 5: Data of the rate constant calculation for electron transfer at Ag /TiO_2semiconductor interface with variety coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$,at 300 K

Rate constant of electron transfer Γ_{ET}(Sec − 1)Ag- TiO_2									
$E_{met}^{sem}(eV)$	*Couplingmatrixelement* $\langle|\overline{\Lambda(0)}|^2\rangle$ x10^{-11}($eV)^2$								
for Ag- TiO_2	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
48.6415	5.052E+08	5.683E+08	6.314E+08	6.946E+08	7.577E+08	8.209E+08	8.840E+08	9.472E+08	1.010E+09
61.3176	4.500E+08	5.062E+08	5.624E+08	6.187E+08	6.749E+08	7.312E+08	7.874E+08	8.437E+08	8.999E+08
66.4438	4.323E+08	4.863E+08	5.403E+08	5.944E+08	6.484E+08	7.024E+08	7.564E+08	8.105E+08	8.645E+08
66.1172	4.333E+08	4.875E+08	5.417E+08	5.958E+08	6.500E+08	7.041E+08	7.583E+08	8.125E+08	8.666E+08
78.7054	3.972E+08	4.468E+08	4.965E+08	5.461E+08	5.958E+08	6.454E+08	6.951E+08	7.447E+08	7.943E+08
64.4699	4.388E+08	4.937E+08	5.485E+08	6.034E+08	6.582E+08	7.131E+08	7.679E+08	8.228E+08	8.776E+08
1.4376	2.909E+09	3.272E+09	3.636E+09	3.999E+09	4.363E+09	4.726E+09	5.090E+09	5.454E+09	5.817E+09
0.6094	4.407E+09	4.958E+09	5.509E+09	6.059E+09	6.610E+09	7.161E+09	7.712E+09	8.263E+09	8.814E+09
0.6138	4.392E+09	4.941E+09	5.489E+09	6.038E+09	6.587E+09	7.136E+09	7.685E+09	8.234E+09	8.783E+09

Table 6: Data of the rate constant calculation for electron transfer at Ag /Zno semiconductor interface with variety coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$,at 300 K

Rate constant of electron transfer Γ_{ET}(Sec − 1) zno –Ag									
$E_{met}^{sem}(eV)$	*Couplingmatrixelement* $\langle|\overline{\Lambda(0)}|^2\rangle$ x10^{-11}($eV)^2$								
for zno -Ag	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
48.6493	1.382E+13	1.555E+13	1.727E+13	1.9E+13	2.073E+13	2.246E+13	2.418E+13	2.591E+13	2.764E+13
61.2987	1.231E+13	1.385E+13	1.539E+13	1.693E+13	1.847E+13	2.001E+13	2.155E+13	2.309E+13	2.462E+13
66.3954	1.183E+13	1.331E+13	1.479E+13	1.627E+13	1.775E+13	1.922E+13	2.07E+13	2.218E+13	2.366E+13
66.0515	1.186E+13	1.334E+13	1.483E+13	1.631E+13	1.779E+13	1.927E+13	2.076E+13	2.224E+13	2.372E+13
78.6211	1.087E+13	1.223E+13	1.359E+13	1.495E+13	1.631E+13	1.767E+13	1.903E+13	2.039E+13	2.174E+13
64.373	1.201E+13	1.352E+13	1.502E+13	1.652E+13	1.802E+13	1.952E+13	2.103E+13	2.253E+13	2.403E+13
1.294	8.378E+13	9.425E+13	1.047E+14	1.152E+14	1.257E+14	1.361E+14	1.466E+14	1.571E+14	1.676E+14
0.4326	1.418E+14	1.595E+14	1.772E+14	1.949E+14	2.127E+14	2.304E+14	2.481E+14	2.658E+14	2.835E+14
0.4254	1.429E+14	1.607E+14	1.786E+14	1.965E+14	2.143E+14	2.322E+14	2.501E+14	2.679E+14	2.858E+14

DISCUSSION

Theoretical models have been used for describing and investigation electron transfer depending on the calculated the probability of electron transitions across metal/semiconductor Nano devices system according on the quantum consideration transport theory. We have been assuming the wave function for transmission of electron from donor to acceptor state describe in Hilbert space, and transmission of electron can happened due to the tunneling to transfer of electron happened across interface ,when the metal bring to interface with semiconductor, the Fermi level for tow material much be coincident at equilibrium state and describe by Fermi distribution function .Probability of electron transport $\boldsymbol{\Gamma_{ET}(Sec^{-1})}$by the tunneling due to the interface created between metal and semiconductor in Ag /TiO_2 and Ag /ZnO systems in Eq.(7) describe the behavior of electron transport at interface.

Due to Eq. (7) the electron transfer has been occurring by tunneling region at the overlap of the wave functions for the acceptor metal state and donor semiconductor state. At the interface of the metal / semiconductor interface, the wave functions for donor and acceptor overlap. In spite of the electron tunneling between metal and semiconductor occurs, the electronic states for donor and acceptor should have alignment energies. For this reason, one assumes the two material energy levels state are continuum for system because, the semiconductor electron state structures are different of electron state in metals, and also its electronic density on various metal surfaces has more than in conduction band of semiconductor. The probability of electron transfer rate constant $\boldsymbol{\Gamma_{ET}(Sec^{-1})}$ in Eq.(7) indicates that the transition of electron rate depending on the reorientation energy, potential barrier height e$(\Phi_{met} - \chi_{sem})$, coupling coefficient matrix element$\langle\left|\overline{\Lambda(0)}\right|^2\rangle$, concentration of electron n_{in},volume of unit cell for semiconductor V_{sem}, penetration factor β, and temperature T(K) .On the other hand, the simplicity and different physical natures for metal, and semiconductor interface appear to predict correctly the typical order of the magnitude of the values observed for the reorganization energies $E_{met}^{sem}(eV)$ and rate constant $\Gamma_{ET}(\text{Sec})^{-1}$of electron transfer. The coupling matrix element coefficient $\left|\overline{\Lambda(0)}\right|$(eV), have controlled the mechanism of electron transfer between the metal and semiconductor system. The electronic properties of semiconductor are markedly affected by the proximity of metal surfaces, depending on the strength of the metal–semiconductor interaction. Electronic coupling is evidently reflected that the capability to transfer electron is determined by the alignment of the levels state of semiconductor with respect to the metal Fermi energy.

Hence, the coupling coefficient of matrix element $\left|\overline{\Lambda(0)}\right|(\text{cm}^{-1})$ have been used in the range from $(0.017- 0.022)(\text{cm}^{-1})$ depending on the typical results of experimental data .The resultant data of the probability rate constant of electron transition $\Gamma_{ET}(Sec^{-1})$ That is calculated theoretically using Eq. (7) are listed in tables (5-6) for Ag/ TiO_2 and Ag/ ZnO system . As expected, the data results according to our theoretical models give a good idea for the behavior of transition for electron. Rate constant of electron become increasing when the coupling coefficient matrix element between metal and semiconductor system will be increasing that's shown from data in tables (5 to 6). The present data for the probability of electron transfer that occurs in a metal/semiconductor system with lest reorientation energies for both Ag/semiconductor system for example $\Gamma_{ET}(\text{Sec}-1) = 5.052\text{E}+08$when $E_{met}^{sem}(eV) = 48.6415$ for Ag/ TiO_2 compared with $\Gamma_{ET}(\text{Sec}-1) = 4.392\text{E}+09$more reorientation energy such that that have the reorganization energy $E_{met}^{sem}(eV) = 0.6138$. The reorganization energy $E_{met}^{sem}(eV)$ is depending on the polarity function, this indicates that the transfer of electron is more probable in metal /

semiconductor system have more polarity parameter. Not ably the electron transfer in system have large dielectric constant are stronger than system have small dielectric constant.

In summary, the number of electron transfer across interface of metal/semiconductor depending on the reorganization energy and energy has to drive to cross from donor to acceptor state. From calculation of the transition of electron differential conductance of these devices depending on potential barrier, we observe direct tunneling features that are consistent with vibration excitations of the semiconductor with metal contact that's shown in figure (1). Decreasing potential barrier height leads to increase the probability of electron transfer due the metal/ semiconductor interface and an increase of the driving force energies.

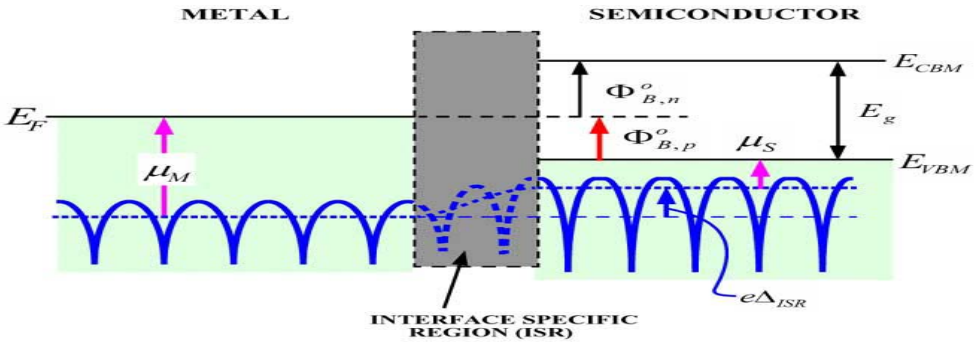

Figure 1: Schematic illustration tunneling processOdell[11].

CONCLUSION

Probability of rate constant for electron transfer in metal/semiconductor system has been studies theoretically depending on quantum consideration. According to the present results that have been discussed, several conclusions can be mentioned follows:-

1. A model that derived depending on experimental consideration successfully to described the behavior of electron which transition across interface from donor to acceptor in metal/semiconductor Nano system
2. The probability of rate constant of electron transfer at metal/semiconductor system results have been enabled us to elaborated and tested the system have its advantage to use or not in many applied.
3. Reorganization energy $E_{met}^{sem}(eV)$of the electron transfer should be effected on the quantum transport probabilities of rate constant $\boldsymbol{\Gamma_{ET}(Sec^{-1})}$ at metal/semiconductor system and the rate constant $\boldsymbol{\Gamma_{ET}(Sec^{-1})}$are large for system with lest polarity function and increases with decreases of the reorganization energy.
4. Probability to transfer of electron depends on the coupling coefficient scale of the overlapping between of the wave functions for both metal and semiconductor state that limited the transfer across tunneling created between metal and semiconductor.
5. In order to achieve a system with a high degree of probability of transition, it was important to choose systems with weak potential barrier to enable to good transfer behavior between metal and semiconductors

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