Theory of electron transmission probability at metal/semiconductor Interface system

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المستخلص

ركزنا في هذا البحث على الوصف النظري لاحتمالية الانتقال الإلكتروني عند السطح الفاصل في وصلة معدن / شبه موصل اعتمادا على نظرية الكم و دالة كثافة لاحتمالية. تعتمد تكنولوجيا النبائط الإلكترونية إلى حد كبير على السطوح الفاصلة لانظمة معدن / أشباه الموصلات، و التي تكون احتمالية الانتقال الإلكتروني فيها معتمدة على معلمات من اهمها مثل: الطاقة الحرة لاعادة التوجيه ، ارتفاع حاجز الجهد $\Delta\mathbb{V}^*(eV)$، دالة الشغل Φ_{met}، الالفة الالكترونية لشبه الموصل ، ومعامل الازدواج لمصفوفة العناصر المتفاعلة $\langle\left|\overline{\xi(E)}\right|^2\rangle$، والتركيز الإلكتروني ، وحجم خلية لوحدة لشبه الموصل V،ومعامل الاختراق β ، ودرجة الحرارة (K) T . تم احتساب احتمالية معدل الانتقال الإلكتروني لنظامي Au/ Ge و Au/Si ، و عند السطح الفاصل وتم فحص الانتقال اعند السطح . استخدم برنامج الماتلاب لحساب ثابت معدل الانتقال الإلكتروني و جميع معلمات الانتقال من خلال حل الصيغ الرياضية المناسبة . اظهرت بيانات النتائج المحسوبة أن احتمالية معدل ثابت الانتقال الإلكتروني تزداد مع زيادة معامل الازدواج الالكتروني ودرجة الحرارة ، وانخفاض الطاقة الحرة لاعادة التنظيم.

Abstract

We focus in this review on the theoretical description of the probability of electron transmission at metal/semiconductor at the interface depending on the quantum theory and density functional theory .Electronic devices technology largely rely on metal/ semiconductor system interfaces, whose most important coefficient parameters for the probability of electron transmission such that :reorientation free energy , potential barrier height $\Delta\mathbb{V}^*(eV)$,work function Φ_{met},affinity of semiconductor χ_{sem},coupling coefficient matrix element $\langle\left|\overline{\xi(E)}\right|^2\rangle$, concentration of electron n_{in},volume of unit cell for semiconductor V_{sem},petration factor β, and temperature T(K) . The probability of electron transport rate constant in Au/ Ge ,and Au/Si interface system has been calculated and the transmission through interface is examined .A Mat lab program has been used to calculate the rate constant of electron transfer and all parameters of transmission by solvingthe suitable formulas .Our results data show that the probability of the rate constant for electron transfer increases with the increasing of the coupling coefficient and temperature, and decreasing of the reorganization energy

Key word: Theory of Electron Transmission Probability, Metal/Semiconductor Systems

Introduction

Electron transfer (ET) is one of the most fundamental processes in chemistry, physics, and biology. Indeed, electron transfer plays a central role in many biochemical and environmental processes (e.g., corrosion, enzymatic activity, photosynthesis, mineral precipitation, and dissolution) (1). Theoretical investigations of ET processes typically start from a two-site model for the electronic degrees of freedom at the donor and acceptor sites which are coupled via a tunneling matrix element (2). The process of electron transfer however, has always had fundamental significance. Many chemical situations involve electron transfer and consequently much work was performed with the aim of understanding these processes. The main theoretical framework to emerge for studying charge transfer is known as Marcus Theory (3). Theoretical interest in charge transfer processes has not diminished since the first theories were successfully tested. In fact, the increasing complexity of the systems considered and the greater breath and accuracy of experiments have revealed a number of situations where the conventional approach does not fully account for the experimental observations, calling for improvement and generalization of the original theoretical models(4). Quantum electron transport through metal semiconductor interfaces is of strong current interest because of the miniaturization of devices both in semiconductor technology as well as in molecular electronics (5). One of crucial factors that govern the quantum transport is the position of the Fermi leve with respect to the local semiconductor band gap i.e. the height of the barrier forming at the metal-semiconductor interface   (6). The tails of metal states penetrating into the semiconductor as first shown by first-principles calculations . If the metal density of states does not vary significantly across the band gap, the distribution of MIGS is only a conseuence of intrinsic features of the bulk semiconductor (6). Thus FLP results when MIGS-induced metallic screening ominates the charge rearrangement at the interface inolved with the alignment of the Fermi level. Such a role of metal induced gap state   in Fermi level pining has been demonstrated experimentally or narrow-gap semiconductors such as GaAs (7). On the other hand, no FLP has been obtained for wide-gap semiconductors as   well as for insulators (8). This is because the penetration of MIGS into the semiconductor or insulator is strongly reduced owing to the stronger decay of evanescent states. In many of the technological applications that surface systems have been put to use in, the transport of electrons plays an important role. It can form part of the system's function directly, for example the charge transport along nanowires or the charge separation or recombination in artificial solar cells. And can also be important indirectly, for example determining how strongly a nanostructure may bind to a surface. Studying and harnessing the transport of electrons through nano-structures has been termed the (9).

Theoretical model

The probability for electron transfer at metal/semiconductor interface is depending on the coupling of the localized states for donor vector basis $|\alpha_D^{et}\rangle$ interacting with an acceptor localized state vector basis $|\alpha_A^{et}\rangle$ of electron in Hilbert space and given by (10):

$$|\theta(\mathrm{r})\rangle = \sum_n \gamma_i \alpha_n(\vec{r})\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where γ_i is the expansion coefficient for basis function $\alpha_n(\vec{r})$. The geometry of the metal/semiconductor quantum system are divided into three regions ,namely donor and acceptor regions, and interface region. For these reason, we can adapt the Tight Binding Energy Hamiltonian to describe the electron transfer dynamics and can be described by (11)

$$\mathbb{H}_{EL} = \bar{\epsilon}_o c^\dagger c + \sum_{k\epsilon_{D,A}} c^\dagger_k c + \sum_{k\epsilon_{D,A}}(V_k c^\dagger_k c + H.c) = \widehat{\mathbb{H}}_{MET} + \widehat{\mathbb{H}}_{SE} + \widehat{\mathbb{H}}_{ME-T_{SE}}\ldots(2)$$

Where $c^\dagger$,and c are creation and annihilation operators for single electronic state with energy ϵ_o , $c^\dagger_k$ and c are creation and annihilation operators for electrons in the energy ϵ_k and V_k are couplings of the single electronic state in donor to the electrons state of acceptor ,while $\widehat{\mathbb{H}}_{MET}$, $\widehat{\mathbb{H}}_{SE}$ and $\widehat{\mathbb{H}}_{MET-SE}$ are the metal , semiconductor and the couplings between metal state and semiconductor state Hamiltonian operators .The $\widehat{\mathbb{H}}_{MET}$, and $\widehat{\mathbb{H}}_{SE}$ must be satisfied the Schrödinger equation (12):

$$\begin{cases} \widehat{\mathbb{H}}_{MET}|\alpha_A^{et}\rangle \\ \widehat{\mathbb{H}}_{SE}|\alpha_D^{et}\rangle \end{cases} = \begin{cases} = \frac{-\hbar^2}{2m}\nabla^2|\alpha_A^{et}\rangle + V_A(r)|\alpha_A^{et}\rangle = \epsilon_A I|\alpha_A^{et}\rangle \\ = \frac{-\hbar^2}{2m}\nabla^2|\alpha_D^{et}\rangle + V_D(r)|\alpha_D^{et}\rangle = \epsilon_D I|\alpha_D^{et}\rangle \end{cases}\ldots\ldots\ldots\ldots\ldots(3)$$

Let us rewrite these equations by scattering operator (13).

$$\begin{cases} (\epsilon_A I - \widehat{\mathbb{H}}_{MET} + i\eta)|\alpha_A^{et}\rangle \\ (\epsilon_D I - \widehat{\mathbb{H}}_{SE} + i\eta)|\alpha_D^{et}\rangle \end{cases} = \begin{cases} = |\zeta_A^{et}\rangle \\ = |\zeta_D^{et}\rangle \end{cases}\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

The transmission probability can be evaluated in terms of a scattering matrix $|\zeta_D^{et}\rangle$ and $|\zeta_A^{et}\rangle$,then the total matrix element of the scattering operator is given by.

$$|\zeta_{AD}^{et}\rangle = \langle\alpha_D^{et}|\alpha_A^{et}\rangle - 2\pi i \mathcal{H}_{DA}\delta(\epsilon_A - \epsilon_D) = -i\lim_{\eta\to 0_+}[G_{DA}(\epsilon + i\eta) - G_{DA}(\epsilon - i\eta)]\ldots(5)$$

This quantity gives the probability at a given energy ϵ of removing a particle from donor with quantum numbers while leaving the remaining N −1,particle system at an energy $\epsilon_D^- = \epsilon_A^+ - \epsilon$.

$$|\zeta_{AD}^{et}\rangle(\epsilon) = -\frac{1}{\pi}Im G_{DA}(\epsilon) = \sum_D |\langle\alpha_A^{et}|c_D^\dagger|\alpha_D^{et}\rangle|^2 \delta(\epsilon - (\epsilon_A^{et} - \epsilon_D^{et})\ldots\ldots\ldots\ldots(6)$$

The current of electrons cross interface of metal /semiconductor system is describe by the Green's functions expression is defined as [14] :

$$G_{DA}(\tau) = G_{DA}(t - t^*) = \begin{cases} -i\langle\Psi(\vec{r})|c_A(t)c_D^\dagger(t^*)|\theta(\mathrm{r},t)\rangle & t > t^* \\ +i\langle\Psi(\vec{r})|c_D^\dagger(t^*)c_A(t)|\theta(\mathrm{r},t)\rangle & t \le t^* \end{cases}\ldots\ldots(7)$$

here $c_A(t)$ and $c_D^\dagger(t^*)$ are the same annihilation and creation operator in Eq.(7), τ is the time ordering operator. If we add a particle in state $|\alpha_A^{et}\rangle$ at a given time t^*, the one-body propagator for $t > t^*$ gives the probability that we find the system still in its state if we remove a particle in state $|\alpha_D^{et}\rangle$ at time t and vice versa. The effect of interactions between the single-particle states is represented by the diagonal elements of the single-particle propagator (14):

$$G_{DA}(\epsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iw\tau}\, G_{DA}(\tau)d\tau =$$

$$\int_{-\infty}^{\infty}\frac{d\epsilon\zeta(DA,\epsilon)}{2\pi(\epsilon_D^{et}-\epsilon_A^{et})} = \sum_A \frac{\langle\alpha_D^{et}|C_A|\alpha_A^{et}\rangle\langle\alpha_A^{et}|C_D^{\dagger}|\alpha_D^{et}\rangle}{\epsilon-(\epsilon_A^{et}-\epsilon_D^{et})++i\eta} + \sum_D \frac{\langle\alpha_A^{et}|C_D^{\dagger}|\alpha_D^{et}\rangle\langle\alpha_D^{et}|C_A|\alpha_A^{et}\rangle}{\epsilon-(\epsilon_D^{et}-\epsilon_A^{et})-i\eta} + \sum_A \frac{\langle\alpha_D^{et}|C_A|\alpha_A^{et}\rangle\langle\alpha_A^{et}|C_D^{\dagger}|\alpha_D^{et}\rangle}{\epsilon-\epsilon_A^{+}+i\eta} +$$

$$\sum_D \frac{\langle\alpha_A^{et}|C_D^{\dagger}|\alpha_D^{et}\rangle\langle\alpha_D^{et}|C_A|\alpha_A^{et}\rangle}{\epsilon-\epsilon_D^{-}-i\eta}\ \dots\dots\mathbf{(8)}$$

The current flow of electron through a metal /semiconductor system has to include the effects of the donor source and acceptor. In the donor and acceptor, the electrons are in equilibrium with the potentials V_D , and V_A respectively. We consider the transfer of electrons through the interface region from donor to acceptor under the potential voltage drop $V = (V_D - V_A)/q$, is obtained using the Laudauer-Buttiker expression(15).

$$I = \int d\epsilon\frac{q}{\pi\hbar}\{\mathcal{H}_{DA}(\epsilon,V)f_A(\epsilon,V_A)[1-f_D(\epsilon,V_D)] - \mathcal{H}_{AD}(\epsilon,V)f_D(\epsilon,V_D)[1-f_A(\epsilon,V_A)]\}\dots\mathbf{(9)}$$

where $\mathcal{H}_{DA}$ and $\mathcal{H}_{AD}$ are probabilities of electron tunneling from "donor" to "acceptor" and vice versa, $f_A(\epsilon,V_A)$ and $f_D(\epsilon)$ are the Fermi Dirac distribution function for the donor and acceptor electrons and given by (16).

$$f_i(\epsilon) = [1 + e^{\frac{(\epsilon_i-\mu_i)}{k_B T}}]^{-1}\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\mathbf{(10)}$$

At equilibrium $V = 0$, $f_A(\epsilon,V_A) = f_D(\epsilon,V_D)$, and $\mathcal{H}_{DA} = \mathcal{H}_{AD}$, one obtains

$$I(V) = \frac{2q}{h}\int \mathcal{H}_{DA}(\epsilon,V)[f_A(\epsilon,V_A) - f_D(\epsilon,V_D)]d\epsilon\dots\dots\dots\dots\dots\dots\mathbf{(11)}$$

But(15).

$$\mathcal{H}_{DA}(\epsilon,V) = \frac{-1}{2\pi}Im\left[Tr\left(\frac{\Omega_D\Omega_A}{\Omega_D+\Omega_A}\right)G(\epsilon)\right]\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\mathbf{(12)}$$

Then Eq(11) may be written as .

$$I(V) = \frac{-2q}{\hbar}\int\frac{d\epsilon}{2\pi}[f_A(\epsilon,V_A) - f_D(\epsilon,V_D)]Im[Tr(\frac{\Omega_D\Omega_A}{\Omega_D+\Omega_A}G(\epsilon))]\dots\dots\dots\dots\mathbf{(13)}$$

The current and rate are both fluxes, related by $\Gamma_{ET} = \frac{I}{q}$, and the transition probability rate .

$$\Gamma_{ET} = \frac{-2}{\hbar}\int\frac{d\epsilon}{2\pi}(\frac{\Omega_D\Omega_A}{\Omega_D+\Omega_A})Im[\,G(\epsilon)]\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\mathbf{(14)}\text{'}$$

But the coupling will be much stronger than the discrete initial statecoupling so that

$$\frac{\Omega_D\Omega_A}{\Omega_D+\Omega_A} \approx \Omega_{A,D} = 2\pi|\mathcal{H}_{A,D}|^2\delta(\epsilon - \epsilon_{AD})\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\mathbf{(15)}$$

Then Eq.(14) for transition probability rate can then be written as

$$\Gamma_{ET} = \frac{-2}{\hbar}\int\frac{d\epsilon}{2\pi}2\pi|\mathcal{H}_{A,D}|^2\delta(\epsilon - \epsilon_{AD})Im[\,G(\epsilon,\epsilon_o)]\dots\dots\dots\dots\dots\dots\dots\mathbf{(16)}$$

By considering the imaginary part of this Green function, we obtain the local density of states at the defect(13).

$$D(\epsilon,\epsilon_o) = \frac{-1}{\pi}\int d\epsilon\, ImG(\epsilon,\epsilon_o)[f_A(\epsilon,V_A) - f_D(\epsilon,V_D)]\dots\dots\dots\dots\dots\mathbf{(17)}$$

Then the probability of electron transfer rate constant may be written as .

$$\Gamma_{ET} = \frac{2\pi}{\hbar} \int |\mathcal{H}_{DA}|^2 D(\epsilon)\delta(\epsilon - \epsilon_{AD})d\epsilon \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (18)$$

But $\int_{-\infty}^{+\infty} F(m-n)\delta(m-n-\epsilon)d\epsilon = F(m-n) \quad (17)$

The probability of transition with Eq.(18) is replaced to .

$$\Gamma_{ET} = \frac{2\pi}{\hbar} \int |\mathcal{H}_{DA}(\epsilon)|^2 D(\epsilon)d\varepsilon \dots\dots\dots\dots (19)$$

The probability density of electrons state for system is $\widehat{D}(\epsilon) = \sum_i |\alpha_n\rangle D_n \langle\alpha_n|$, and (D_n) evidently satisfies the $o \geq D_n \leq 1$, $\sum_n D_n = 1$ conditions(18).

When $|\alpha_D^{et}\rangle e^{\frac{-iE_D t}{\hbar}}$ and $|\alpha_A^{et}\rangle e^{\frac{-iE_A t}{\hbar}}$, are a complete set orthonormal for donor and acceptor state we may expand a basis set for $||\theta(r,t)\rangle$ (19).

$$|\theta(r,t)\rangle = \sum_n \beta_n^i \; |\alpha_n\rangle \; e^{\frac{-iE_n t}{\hbar}}, \dots\dots\dots\dots\dots\dots (20)$$

We can also find the relation between Green function and total density of states (13).

$$\widehat{D}(\varepsilon) = -\frac{1}{\pi} Tr[Im G_{DA}(\epsilon)] \dots\dots\dots\dots\dots\dots\dots\dots (21)$$

The density of states is non-negative. This is consistent with the fact that the imaginary part of the Green function has to be non-positive $Im G_{DA}(\epsilon) \leq 0$ .The retarded Green function in time vanishes for t < 0. This is in accordance with the poles lying on the lower half of the complex energy plane (15). The expectation value for $\widehat{D}(\varepsilon)$ can be written.

$$< \widehat{D}(\epsilon) > = <\theta(r,t)|\widehat{D}(\epsilon)|\theta(r,t) > = \sum_D \sum_A <\theta(r,t)|\alpha_D^{et}> < \alpha_D^{et}|\widehat{D}(\epsilon)|\alpha_A^{et}>< \alpha_A^{et}|\theta(r,t) > \dots\dots\dots\dots\dots\dots\dots (22)$$

The density operator can given by $\widehat{D}(\varepsilon) = e^{\frac{\epsilon}{K_B T}} D \; e^{\frac{-\epsilon}{K_B T}}$. Then Eq(22) with $\widehat{D}(\varepsilon)$, results.

$$< \widehat{D}(\varepsilon) > = \sum_D \sum_A <\theta(r,t)|\alpha_D^{et}> < \alpha_D^{et}|e^{\frac{\epsilon}{K_B T}} D \; e^{\frac{-\epsilon}{K_B T}}|\alpha_A^{et}>< \alpha_A^{et}|\theta(r,t) > =$$
$$\sum_D \sum_A D_{DA} \; e^{\frac{-(\epsilon_D - \epsilon_A)}{k_B T}} \dots (23)$$

Such that $D_{(DA)} = < \alpha_D^{et} | \theta(r,t) >^* < \alpha_A^{et} | \theta(r,t) > = N\langle\theta(r,t)|\theta(r,t)\rangle (10)$. This may be enable to write the density of state of electron Eq.(23) in expression .

$$<\widehat{D}(\varepsilon) > = N \sum e^{\frac{-(\epsilon_D - \epsilon_A)}{k_B T}} < \theta(r,t) | \theta(r,t) > \dots\dots\dots\dots (24)$$

This lead to write Eq.(24)

$$\widehat{D}(\varepsilon) = N e^{\frac{-(\epsilon_D - \epsilon_A)}{k_B T}} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (25)$$

For the electron transfer in metal/semiconductor system, The energy difference $\epsilon_D - \epsilon_A$ is the height barrier energy $\Delta\mathbb{V}^* = \epsilon_D - \epsilon_A$.

Substituting $\Delta\mathbb{V}^*$ in Eq.(25),results.

$$\widehat{D}(\epsilon) = Ne^{\frac{-\Delta\mathbb{V}^*}{k_B T}} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\text{(26)}$$

The sum of all the diagonal elements is given by (12).

$$\text{Tr}\,\widehat{D}(\epsilon) = \text{Tr}Ne^{\frac{-\Delta\mathbb{V}^*}{k_B T}} = N\text{Tr}e^{\frac{-\Delta\mathbb{V}^*}{k_B T}} = 1 \dots\dots\dots\dots\dots\text{(27)}$$

Yield $N = (4\pi\varepsilon_{\text{met}}^{\text{sem}}k_B T)^{\frac{-1}{2}}$.

Then the probability of rate constant for ET can them be written as.

$$\Gamma_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} |\mathcal{H}_{DA}(\epsilon)|^2 (4\pi\epsilon_{\text{m-S}} k_B T)^{\frac{-1}{2}} exp\frac{-(\epsilon_{\text{m-S}}+\Delta\mathbb{U})^2}{4\epsilon_{\text{m-S}}k_B T}\ d\epsilon \dots\dots\text{(28)}$$

Where ΔV is a free energy driving force of reaction where the donor state in the metal electrode is at the interface Under the prevailing conditions of temperature T, metal electrode- semiconductor potential difference (ΔV) is related to (E) by $\Delta V = \Delta\mathbb{U}^\circ - \epsilon(20)$. Here $(\Delta\mathbb{U}^\circ)$ is the free energy of the reaction where the donor state in the metal electrode is at the interface.The electron transfer rate constant for of the semiconductor acceptor relation to the metal donor can then be further written as .

$$\Gamma_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} |\mathcal{H}_{DA}(\epsilon)|^2 (4\pi\epsilon_{\text{m-S}}k_B T)^{\frac{-1}{2}} exp\frac{-(\epsilon_{\text{m-S}}+\Delta\mathbb{U})^2}{4\epsilon_{\text{m-S}}k_B T} F_{(\epsilon)}d\epsilon \dots\dots\text{(29)}$$

For a theoretical description, we must be consider the electron properties of a metal in greater. Electrons state in all metal form energy bands. Bands are filled up to a highest level (Fermi level) at $T = 0$. Levels are filled below the Fermi energy, while empty at above.The excitation energy raised more electrons from below the Fermi level to above empty level at finite temperatures near equilibrium, the exchange of electron scan occurs mainly near the Fermi level, but a reduced species can denate an electron to any empty level on the metal . When an electron transfer to above the Fermi level with an energy E, the free energy$\Delta\mathbb{U}$for this process is reduced by $\Delta\mathbb{U}^\circ - \epsilon$, resulting to the energy of activation is (20).

$$\Delta\mathbb{V}^* = \frac{(\epsilon_{\text{m-S}}+\Delta\mathbb{U})^2}{4\epsilon_{\text{m-S}}} = \frac{(\epsilon_{\text{m-S}}+\Delta\mathbb{U}^\circ-\epsilon)^2}{4\epsilon_{\text{m-S}}} \dots\dots\dots\dots\dots\dots\dots\text{(30)}$$

Inserting Eq.(30) ,and Eq.(10)in Eq.(29) results

$$\Gamma_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} |\mathcal{H}_{DA}(\epsilon)|^2 (4\pi\epsilon_{\text{m-S}}k_B T)^{\frac{-1}{2}} exp\frac{-(\epsilon_{\text{m-S}}+\Delta\mathbb{U}^\circ-\epsilon)^2}{4\epsilon_{\text{m-S}}k_B T} \frac{1}{1+exp^{\frac{E}{k_B T}}}d\epsilon \dots\dots\text{(31)}$$

The first exponent of the factor inside integral in the Eq(31) can be written as .

$$exp \frac{-(\epsilon_{m-S}+\Delta\mathbb{U}°-E)^2}{4\epsilon_{m-S}k_BT} = \exp - \frac{(\epsilon_{m-S}+\Delta\mathbb{U}°)^2}{4\epsilon_{m-S}k_BT}\exp + \frac{2E(\epsilon_{m-S}+\Delta\mathbb{U}°)}{4\epsilon_{m-S}k_BT} \quad \exp - \frac{E^2}{4\epsilon_{m-S}k_BT}\ldots\ldots\ldots(32)$$

The first term $\exp - \frac{(\epsilon_{m-S}+\Delta\mathbb{U}°)^2}{4\epsilon_{m-S}k_BT}$ is independent (E) that can be removed out of integral, yielding.

$$\Gamma_{ET} = \frac{2\pi}{h}\exp - \frac{(\epsilon_{m-S}+\Delta\mathbb{U}°)^2}{4\epsilon_{m-S}k_BT}\int_{-\infty}^{\infty}|\mathcal{H}_{DA}(E)|^2(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp + \frac{2(\epsilon_{m-S}+\Delta\mathbb{U}°)E}{4\epsilon_{m-S}k_BT}\exp - \frac{E^2}{4\epsilon_{m-S}k_BT}\frac{1}{1+exp^{\frac{E}{k_BT}}}dE\ldots\ldots\ldots\ldots\ldots(33)$$

The term $(\exp + \frac{2(\epsilon_{m-S}+\Delta\mathbb{U}°)E}{4\epsilon_{m-S}k_BT})$ varies much more slowly with (E) than (E/k_BT) in the exponent of the third term in the integral Eq.(32)when$\epsilon_{m-S} \cong -\Delta\mathbb{U}°$ can then ignore yielding.

$$\Gamma_{ET} = \frac{2\pi}{h}\exp - \frac{(\epsilon_{m-S}+\Delta\mathbb{U}°)^2}{4\epsilon_{m-S}k_BT}\int_{-\infty}^{\infty}|\mathcal{H}_{DA}(E)|^2(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp(-\frac{E^2}{4\epsilon_{m-S}k_BT}\frac{1}{1+exp^{\frac{E}{k_BT}}})dE\ldots\ldots\ldots(34)$$

Where the$(|\mathcal{H}_{DA}(E)|^2)$ is an averaged coupling electronic matrix elements square of ,the all the electronic states which is given by (21).

$$\langle|\mathcal{H}_{DA}(E)|^2\rangle = \pi k_B T \sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\delta(E_D - E_A)\ldots\ldots\ldots\ldots\ldots(35)$$

Then the probability of electron transfer at system in Eqز (34) reduced to

$$\Gamma_{ET} = \frac{2\pi}{h}(4\pi\epsilon_{m-s}k_BT)^{\frac{-1}{2}}\exp - \frac{(\epsilon_{m-S}+\Delta\mathbb{U}°)^2}{4\epsilon_{m-S}k_BT}\int_{-\infty}^{\infty}\pi k_BT\sum\sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\delta(E_D - E_A) \exp - \frac{E^2}{4\epsilon_{m-S}k_BT}\frac{1}{1+exp^{\frac{E}{k_BT}}}dE\ldots\ldots\ldots\ldots\ldots\ldots\ldots(36)$$

Where the$\sum|\overline{\mathcal{H}_{DA}(E)}|^2$ are an averaged coupling electronic matrix elements square of the all the electronic states, but the exponential out of integral describe barrier height $\Delta\mathbb{V}^* = \Phi_{met} - \chi_{sem}$ (22). Then the Eq (36) become:

$$\Gamma_{ET} = \frac{2\pi}{h}(4\pi\epsilon_{m-s}k_BT)^{\frac{-1}{2}}\exp - \frac{(\Phi_{met}-\chi_{sem})}{k_BT}\int_{-\infty}^{\infty}\pi k_BT\sum\sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\delta(E_D - E_A) \exp - \frac{E^2}{4\epsilon_{m-S}k_BT}\frac{1}{1+exp^{\frac{E}{k_BT}}}dE\ldots\ldots\ldots\ldots\ldots(37)$$

Also ,we can write the function of distribution of electron in system by $\frac{1}{1+exp^{\frac{E}{k_BT}}} =$

$$\frac{\exp\frac{-E}{2k_BT}}{\exp\frac{-E}{2k_BT}+\exp\frac{E}{2k_BT}}$$

That may to write Eq (37) by

$\Gamma_{ET} = \frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp -\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\int_{-\infty}^{\infty}\pi k_BT\sum\sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\delta(E_D - E_A)\exp -$

$\frac{E^2}{4\epsilon_{m-S}k_BT}\frac{\exp\frac{-E}{2k_BT}}{\exp\frac{-E}{2k_BT}+\exp\frac{E}{2k_BT}}dE)....(38)$

The minus exponential $e^{\frac{-E}{2k_BT}}$ pull out of distribution function to gate

$\Gamma_{ET} = \frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp -\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\int_{-\infty}^{\infty}\pi k_BT\sum\sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\exp\frac{-E}{2k_BT}\delta(E_D -$

$E_A)\frac{\exp-\frac{E^2}{4\epsilon_{m-S}k_BT}}{\exp\frac{-E}{2k_BT}+\exp\frac{E}{2k_BT}}dE..................................(39)$

Let we assume integration $I(E,\epsilon_{m-S}) = \int_{-\infty}^{\infty}\frac{\exp-\frac{E^2}{4\epsilon_{m-S}k_BT}}{\exp\frac{-E}{2k_BT}+\exp\frac{E}{2k_BT}}dE$ .Exponential

factors $(\exp-\frac{E^2}{4\epsilon_{m-S}k_BT})$ in Eq.(39) reduce to .

$\exp-\frac{E^2}{4\epsilon_{m-S}k_BT} = 1-\frac{E^2}{4\epsilon_{m-S}k_BT}+\frac{E^4}{32\epsilon_{m-S}^2k_B^2T^2}-\frac{E^6}{384\epsilon_{m-S}^3k_B^3T^3}.....+\frac{E^{2n}}{n!(4\epsilon_{m-S}k_BT)^n}.....(40)$

Substituting in Eq.(40) , in $I(E,\epsilon_{m-S})$,the results

$I(E,\epsilon_{m-S}) = \int_{-\infty}^{\infty}\frac{\left(1-\frac{E^2}{4\epsilon_{m-S}k_BT}+\frac{E^4}{32\epsilon_{m-S}^2k_B^2T^2}-\frac{E^6}{384\epsilon_{m-S}^3k_B^3T^3}.....+\frac{E^{2n}}{n!(4\epsilon_{m-S}k_BT)^n}\right)}{\exp\frac{-E}{2k_BT}+\exp\frac{E}{2k_BT}}dE......(41)$

The results of integral calculation in Eq.(41)is given

$I(E,\epsilon_{m-S}) =$
$\left[[\pi k_BT-\frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)+\frac{1}{32\epsilon_{m-S}^2k_B^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right)-\frac{1}{384\epsilon_{m-S}^3k_B^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)............+\right.$
$\frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto (\pi k_BT)^{2n+1})])..(42)$

By substituting integration results in Eq.(39) ,the rate become

$\Gamma_{ET} = \frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp -\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\pi k_BT\sum\sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\exp\frac{-E}{2k_BT}\delta(E_D - E_A)\left[[\pi k_BT-\right.$

$\frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)+\frac{1}{32\epsilon_{m-S}^2k_B^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right)-\frac{1}{384\epsilon_{m-S}^3k_B^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)............+$

$\frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto (\pi k_BT)^{2n+1})]...(43)$

And the exponential factors in Eq.(43) is reduced to Boltzman equation when

$E = E_{C.B} - E_f \gg k_BT$,then $\exp\frac{-E}{2k_BT} = \exp\frac{E_f-E_{C.B}}{2k_BT}$.where $E_{C.B}$is the conduction

band at semiconductors,and E_f is the Fermi energy at metals .The Fermi energy at

metals is $E_f = V_{ap(D,A)} + E_f^o$ (94),and the density of electrons state as $\rho_{(E)} = \sum_{D,A}\delta(E_D - E_A)$ (95), then the rate constant of electron transfer in Eq.(43) became.

$\Gamma_{ET} =$

$\frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp\frac{V_{ap(D,A)}}{2k_BT}\exp-\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\pi k_BT\sum\sum_{D,A}|\overline{\mathcal{H}_{DA}(E)}|^2\exp\frac{E_f^O-E_{C.B}}{2k_BT}\rho_{(E)}\left[\pi k_BT-\right.$

$\frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)+\frac{1}{32\epsilon_{m-S}{}^2k_B{}^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right)-\frac{1}{384\epsilon_{m-S}{}^3k_B{}^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)\dots\dots\dots\dots\dots\dots+$

$\left.\frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto(\pi k_BT)^{2n+1})\right]\dots\dots(44)$

For two face $V_{ap(D,A)}\approx 2V_{app}$ then $\exp\frac{V_{ap(D,A)}}{2k_BT}=\exp\frac{V_{app}}{k_BT}$, and at applied potential $eV_{app}\approx zero$,the occupancy state of electron at interface is$f_o(E)=\exp\frac{E_f^O-E_{C.B}}{2k_BT}$ .And results

$\Gamma_{ET}=\frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\exp\frac{eV_{app}}{k_BT}\exp-\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\pi k_BT\sum|\overline{\mathcal{H}_{DA}(E)}|^2f_o(E)\rho_{(E)}\left[[\pi k_BT-\right.$

$\frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)+\frac{1}{32\epsilon_{m-S}{}^2k_B{}^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right)-\frac{1}{384\epsilon_{m-S}{}^3k_B{}^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)\dots\dots\dots\dots\dots\dots+$

$\left.\frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto(\pi k_BT)^{2n+1})\right]\dots.(45)$

But the density of concentration at interface is $n_{in}=N_{eff}exp^{\frac{-V_n}{k_BT}}$ is defined as , where N_{eff} is the effective density of state in the metal side and conduction band ,and

$V_n=V_{bi}-V_{app}$ (23). Where V_{bi} is the built drop potential .On the other hand the evaluated of $N_{eff}exp^{\frac{-V_{bi}}{k_BT}}$ is readily to$N_{eff}exp^{\frac{-V_{bi}}{k_BT}}=\frac{\sum_0^\infty\rho(E)f_o(E)}{V_{sem}}$ (23). Then the probability of electron transfer across interface of metal/ semiconductor system in Eq.(45) may be write with as.

$\Gamma_{ET}=\frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\frac{n_{in}V_{sem}}{\sum_0^\infty\rho(E)f_o(E)}\exp-\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\pi k_BT\sum|\overline{\mathcal{H}_{DA}(E)}|^2f_o(E)\rho_{(E)}\left[[\pi k_BT-\right.$

$\frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)+\frac{1}{32\epsilon_{m-S}{}^2k_B{}^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right)-\frac{1}{384\epsilon_{m-S}{}^3k_B{}^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)\dots\dots\dots\dots\dots\dots+$

$\left.\frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto(\pi k_BT)^{2n+1})\right]\dots\dots(46)$

But the total coupling matrix elements $\overline{\xi(E)}$ are given by (24).

$\langle|\overline{\xi(E)}|^2\rangle=\frac{\sum|\overline{\mathcal{H}_{DA}(E)}|^2f_o(E)\rho_{(E)}}{\sum_0^\infty\rho(E)f_o(E)}\dots\dots\dots\dots\dots\dots\dots\dots..(47)$

Then the probability of electron transfer in Eq.(46) ,with Eq. (47)is given by .

$\Gamma_{ET}=\frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}n_{in}V_{sem}\exp-\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\pi k_BT\langle|\overline{\xi(E)}|^2\rangle\left[[\pi k_BT-\frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)+\right.$

$\frac{1}{32\epsilon_{m-S}{}^2k_B{}^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right)-\frac{1}{384\epsilon_{m-S}{}^3k_B{}^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)\dots\dots\dots\dots\dots\dots+\frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto$

$\left.(\pi k_BT)^{2n+1})\right]\dots\dots(48)$

For a $\langle|\overline{\xi(E)}|^2\rangle$ replaced by $\langle|\overline{\xi(0)}|^2\rangle$ to stady state , then is, as already noted that $\langle|\overline{\xi(E)}|^2\rangle=\pi k_BT\langle|\overline{\xi(0)}|^2\rangle$.But the probability of electron transfer at

metal/semiconductor are depends exponentially on distance with a decay $\Re$ constant $\Gamma_{et} = \frac{1}{\Re}\Gamma_{ET}$, the Γ_{et} becomes

$$\Gamma_{et} = \frac{2\pi}{h}(4\pi\epsilon_{m-S}k_BT)^{\frac{-1}{2}}\frac{n_{in}V_{sem}}{\Re}\exp-\frac{(\Phi_{met}-\chi_{sem})}{k_BT}\langle|\overline{\xi(0)}|^2\rangle\left[\pi k_BT - \frac{1}{4\epsilon_{m-S}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right) + \right.$$

$$\left.\frac{1}{32\epsilon_{m-S}^2k_B^2T^2}\left(\frac{5(\pi k_BT)^5}{16}\right) - \frac{1}{384\epsilon_{m-S}^3k_B^3T^3}\left(\frac{61(\pi k_BT)^7}{64}\right)\dots\dots\dots\dots\dots\dots\dots + \frac{1}{n!(4\epsilon_{m-S}k_BT)^n}(\propto\right.$$

$$\left.(\pi k_BT)^{2n+1})\right]\dots(49)$$

The reorientation energy ϵ_{m-S} arises from the reorientation of the charge in the system .Its magnitude 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 . Its due to the electron transfer reaction for metal/semiconductor interface is given by (25).

$$\epsilon_{m-S} =$$
$$\frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2R_{met}}\left(\frac{1}{n_{met}^2} - \frac{1}{\varepsilon_{met}}\right) + \frac{1}{2R_{semi}}\left(\frac{1}{n_{semi}^2} - \frac{1}{\varepsilon_{semi}}\right) - \frac{1}{4D_{semi}}\left(\frac{n_{met}^2-n_{semi}^2}{n_{met}^2+n_{semi}^2}\frac{1}{n_{semi}^2} - \frac{\varepsilon_{met}-\varepsilon_{semi}}{\varepsilon_{met}+\varepsilon_{semi}}\frac{1}{\varepsilon_{semi}}\right) - \right.$$
$$\left.\frac{1}{4D_{met}}\left(\frac{n_{semi}^2-n_{met}^2}{n_{semi}^2+n_{met}^2}\frac{1}{n_{met}^2} - \frac{\varepsilon_{semi}-\varepsilon_{met}}{\varepsilon_{semi}+\varepsilon_{met}}\frac{1}{\varepsilon_{met}}\right) - \frac{1}{R_{met-semi}}\left(\frac{1}{n_{met}^2+n_{semi}^2} - \frac{1}{\varepsilon_{semi}+\varepsilon_{met}}\right)\right]\dots\dots(50)$$

Where R_{met} and R_{semi} are the radius of metal and semiconductor , $D_{semi} = R_{semi} + 1A^°$, $D_{met} = R_{met} + 1A^°$, and $R_{met-semi} = R_{met} + R_{semi}$ are the distance between semiconductor ,metal to interface and metal-semiconductor , $n_{met}, \varepsilon_{met}$ 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 spherical approach (26).

$$R = (\frac{3MW}{4\pi N_A\rho})^{\frac{1}{3}}\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \textbf{(51)}$$

Where MW is the molecular weight, N_A is Avogadro's number, and ρ is the mass density.

Results

A result of rate constant according on the theoretical model based on the quantum system have been used to the investigation; and the understanding of the probability of electron transfer at the metal/semiconductor interface. Our model have been applied to known the behavior of the probability of electron transfer at metal/semiconductor interface depending on calculation of the probability of rate of electron transfer Γ_{ET} due to the reorientation energy $\epsilon_{m-S}(eV)$ that is the most important coefficient effect on the probability of transmission due to interface .The reorientation energy $\epsilon_{m-S}(eV)$ is the energy required to reorientation of the system

before transferto initial transfer process.   It is an important to evaluate the transmission probability rate constant of electron transfer at metal/semiconductor interface system, the driving force energy $\Delta V°$ (eV) and the potential barrier height. It can be calculated theoretically using the Marcus Hush equation before transfer in Eq. (50). To calculate the reorientation energy $\epsilon_{m-S}(eV)$) , that's must be evaluation radius for donor state Au metal and Ge,and Si for acceptor semiconductor state using Eq.(51) . Inserting the values of molecular weight MW, and density masses ρ for all Ge and Si semiconductors and Aumetal fromtables (1) in Eq.(51) with Avogadro's constant $N_A = 6.02 \times 10^{23} \frac{Molecule}{mol}$, we can evaluated the   values of radii for two metals and for molecules respectively., data of the evaluation are shown in the table (2).

Table (1): Common properties of semiconductor (27)

Properties	Ge	Si
Atomic weight	72.60	28.09
Crystal structure	Diamond	Diamond
Density (g/cm^3)	5.3267	2.328
Refractive index	4.0	3.3
Dielectric constant	16.0	11.9
Effective density of states in conduction band, N_C (cm^{-3})	1.04x 10^{19}	2.8x 10^{19}
Effective density of states in valence band,N_v (cm^{-3})	6.0x 10^{18}	1.04x 10^{19}
Energy gap (eV) at 300K	0.66	1.12
Lattice constant (Å)	5.6575	5.4310
Melting point (ºC)	937	1415
Radius(Å)	1.7547	1.920
Electron affinity, (eV)	4.0	4.05

Table (2): Calculated results of radii of metals and semiconductor material

Properties	Metal material	Semiconductor material	
	Au	Ge(27)	Si(27)
Atomic weight	26.982(27)	72.60	28.09
Crystal structure	Cubiccrystal(27)	Diamond	Diamond
Density (g/cm^3)	2.70 (28)	5.3267(27)	2.328(27)
Radii	1.43(29)	1.7547	1.920

Depending on radii data result ,and properties metal and semiconductor in tables(2) ,we can be calculate the reorientation energy for metal / semiconductor   system for Au metal donor with Ge, and Sian acceptor semiconductors interface systems using an expression of Marcus– Hush in Eq.(50) with a Matlab program and substituting the values of donor and acceptor ,R_{met} and R_{semi} radius for   metal and semiconductor,and   distance from interface to metal $D_{met} = R_{met} + 1A°$, and semiconductor$D_{semi} = R_{semi} + 1A°$ with $R_{met-semi} = R_{met} + R_{semi}$ are   the distance between metal-semiconductor interface , and the statical ε_{met} , ε_{semi} and optical dielectric constant n_{met}, and n_{semi} for metal and semiconductor from tables (1 and2) respectively .Data for reorientation   energies have been summarized in tables (3 to 4) for Au /Ge,and   Au /Sifor metal/semiconductor interface system respectively.

Table (3): Results of the reorientation energy $\epsilon_{m-S}(eV)$ for electron transfer at Au metal /Ge +semiconductor interface system

Energy for Au(28)	n for Ag	k for Au	ϵ_m for Au(28)	$\epsilon_{m-S}(eV)$ for Au-Ge
2.4	0.5	1.86	3.7096	13.1597
2.6	1.24	1.54	3.9092	1.3978
2.8	1.46	1.77	5.2645	0.9926
3	1.54	1.8	5.6116	0.8667
3.2	1.54	1.8	5.6116	0.8667
3.4	1.56	1.76	5.5312	0.8193
3.6	1.62	1.73	5.6173	0.7234
3.8	1.63	1.79	5.861	0.7335

Table (4): Results of the reorientation energy $\epsilon_{m-S}(eV)$ for electron transfer at Au metal / Si semiconductor interface system

energy for Au(28)	n for Au(28)	k for Au(28)	ϵ_m for Au(28)	$\epsilon_{m-S}(eV)$ for Au-Si
2.4	0.5	1.86	3.7096	13.1969
2.6	1.24	1.54	3.9092	1.4297
2.8	1.46	1.77	5.2645	1.0246
3	1.54	1.8	5.6116	0.8984
3.2	1.54	1.8	5.6116	0.8984
3.4	1.56	1.76	5.5312	0.8507
3.6	1.62	1.73	5.6173	0.7543
3.8	1.63	1.79	5.861	0.7646

The evaluated of the probability of rate constant for electron transfer for metal /semiconductor interface system depending on the calculation of unit cell volume of Si, and Ge semiconductors. Probability of transmission of electron at metal/semiconductor is proportional due to the volume according on the expression in Eq.(49). Volume of unit cell of Si, and Ge semiconductors have been calculated by using the volume equation $V(m^3) = A.|B \times C|$,where A,B,and C are the lattice parameters .Results of volume unit cell are summarized in table(5).

Table (5): Results of unit cell volume $V(m^3)$ for Si, and Ge semiconductors

Semiconductor type	Lattice parameters (Å)	Unit cell volume $V(m^3)$
Ge	5.6575(27)	$1.81081*10^{-28}$
Si	5.4310(27)	$1.6019*10^{-28}$

Probability of rate constant of electron transfer Γ_{ET} can be evaluated depending on relation in Eq.(49) the results of our model derived according on continuum levels state of Au metal and Si,and semiconductors corporation with quantum postulate.

Our model 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 $\epsilon_{m-S}(eV)$ 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},petration factor β, temperature T(K) and the electronic coupling coefficient $\langle|\overline{\overline{\xi(E)}}|^2\rangle$.

The rate constant of ET can be calculated by using Eq.(3-70) enable gate all information about all electrical properties of metal/semiconductor interface devices through knowing the values of rate constant for Au /Ge, and Au/ Si 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.(49)and inserting the reorientation energies $\epsilon_{m-S}(eV)$ data from tables(3)to (4) for

two Au /Si, and Au/ systems ,concentration of electron n_{in}, volume of unit cell for semiconductor V_{sem} from table(4-17) ,penetration factor $\beta=1 \times 10^{-10}\,m^{-1}$, and the coupling matrix element coefficient$\langle|\overline{\overline{\xi(E)}}|^2\rangle = 0.4, 0.45, 0.5, 0.55, 0.6, 0.65, 0.7, 0.75,$ and $0.8\text{x}10^{-11}(eV)^2$for metal ,semiconductor and calculation of height barrier from table(4-16)through values of work function of metalΦ_{met} and affinity of semiconductorχ_{sem} .for twelve   systems. Results data of calculation are listed in tables (6) and (7) for Au/Ge ,and Au /Si systems .

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

$\epsilon_{m-S}(eV)$ for Ag-Ge	Rate constant of electron transfer $\Gamma_{ET}(\text{Sec}^{-1})$Au-Ge								
	Coupling matrix element $\langle|\overline{\overline{\xi(E)}}|^2\rangle$x$10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
208.2286	5.433E-10	6.112E-10	6.791E-10	7.470E-10	8.149E-10	8.829E-10	9.508E-10	1.019E-09	1.087E-09
13.1597	2.159E-09	2.429E-09	2.698E-09	2.968E-09	3.238E-09	3.508E-09	3.778E-09	4.048E-09	4.318E-09
1.3978	6.560E-09	7.380E-09	8.200E-09	9.020E-09	9.840E-09	1.066E-08	1.148E-08	1.230E-08	1.312E-08
0.9926	7.752E-09	8.721E-09	9.690E-09	1.066E-08	1.163E-08	1.260E-08	1.357E-08	1.453E-08	1.550E-08
0.8667	8.278E-09	9.313E-09	1.035E-08	1.138E-08	1.242E-08	1.345E-08	1.449E-08	1.552E-08	1.656E-08
0.8667	8.278E-09	9.313E-09	1.035E-08	1.138E-08	1.242E-08	1.345E-08	1.449E-08	1.552E-08	1.656E-08
0.8193	8.506E-09	9.569E-09	1.063E-08	1.170E-08	1.276E-08	1.382E-08	1.489E-08	1.595E-08	1.701E-08
0.7234	9.031E-09	1.016E-08	1.129E-08	1.242E-08	1.355E-08	1.468E-08	1.580E-08	1.693E-08	1.806E-08
0.7335	8.971E-09	1.009E-08	1.121E-08	1.234E-08	1.346E-08	1.458E-08	1.570E-08	1.682E-08	1.794E-08

Table (7): Data of the rate constant calculation for electron transfer at Au /Si semiconductor interface with variety coupling coefficient$\langle|\overline{\overline{\xi(E)}}|^2\rangle$, at 300 K

$\epsilon_{m-S}(eV)$ for Ag-Si	Rate constant of electron transfer $\Gamma_{ET}(\text{Sec}^{-1})$Au-Si								
	Coupling matrix element $\langle|\overline{\overline{\xi(E)}}|^2\rangle$x$10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
48.2318	9.560E-09	1.076E-08	1.195E-08	1.315E-08	1.434E-08	1.554E-08	1.673E-08	1.793E-08	1.912E-08
60.8942	3.794E-08	4.268E-08	4.742E-08	5.216E-08	5.691E-08	6.165E-08	6.639E-08	7.113E-08	7.588E-08
66.0072	1.142E-07	1.285E-07	1.427E-07	1.570E-07	1.713E-07	1.855E-07	1.998E-07	2.141E-07	2.284E-07
65.6736	1.343E-07	1.511E-07	1.679E-07	1.847E-07	2.015E-07	2.183E-07	2.351E-07	2.519E-07	2.687E-07
78.2542	1.432E-07	1.611E-07	1.790E-07	1.969E-07	2.148E-07	2.327E-07	2.506E-07	2.685E-07	2.863E-07
64.0144	1.432E-07	1.611E-07	1.790E-07	1.969E-07	2.148E-07	2.327E-07	2.506E-07	2.685E-07	2.863E-07
0.9839	1.470E-07	1.654E-07	1.837E-07	2.021E-07	2.205E-07	2.389E-07	2.572E-07	2.756E-07	2.940E-07
0.1756	1.558E-07	1.752E-07	1.947E-07	2.142E-07	2.337E-07	2.531E-07	2.726E-07	2.921E-07	3.115E-07
0.1932	1.548E-07	1.741E-07	1.934E-07	2.128E-07	2.321E-07	2.515E-07	2.708E-07	2.902E-07	3.095E-07

Discussion

A theoretical model have been used to describing and investigation of electron transfer depending on the calculation the probability of electron transitions due to metal/semiconductor devices system according on the quantum consideration transport theory. Due on this model, 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 of transfer of electron happened across interface .When the metal bring to interface with semiconductor; the Fermi level for two material much be coincident at equilibrium state and described by Fermi distribution function.

Many parameters influence of these transfer such that: as reorientation energy, potential barrier height $\Delta\mathbb{V}^*(eV) = e(\Phi_{met} - \chi_{sem})$, coupling coefficient matrix element$\langle\left|\overline{\xi(E)}\right|^2\rangle$, concentration of electronn_{in},volume of unit cell for semiconductor V_{sem},petration factor β, and temperature T(K) . Probability of electron transport $\boldsymbol{\Gamma_{ET}}(\textbf{Sec}^{\textbf{-1}})$ by the tunneling due to the interface created between metal and semiconductor in Au /Si, and Au/Ge systems in Eq.(49) describe the behavior of electron transport at interface . Due to this model, the transition of electron.(49) has been occurs by tunneling region at the overlap of the wave functions for the acceptor metal state and donor molecule state **.**

At interface of 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. These electronic states are brought into resonance by fluctuations of wave function of metal and semiconductor system, and this resonance is the transition state of electron transfer reaction.

The most important of all the calculation of electron transfer parameters requires us to define a theoretical model as the reorientation energy$\epsilon_{m-S}(eV)$. It which is enables us to calculate the rate constant of electron parameters for metal/semiconductor system. It is calculated according to continuum semi classical Marcus-Hush theory. From the simple Marcus model, it has already evaluated the reorientation energies follows that an electron state at donor and acceptor are oriented in metal and semiconductors leads to transfer of electron between two states in these devices.

Marcus classical theory approaches is modeled in the sense of the physical concepts such as optical dielectric constant related to refractive index, and static dielectric constant beside the radii for donor -acceptor system. For all calculations the optical and statically dielectric constants of materials were taken from experimental data sheet in literature. Depending on the literature to introduce the molecular parameters in the model have assigned reasonable values and the theoretical results were compared qualitatively with experimental data.

On the other hand, the simplicity and different physical natures for metal, and semiconductor interface appear to predict correctly the typical order of magnitude values observed for the reorientation energies $\epsilon_{m-S}(eV)$ and rate constant $\Gamma_{ET}(Sec^{-1})$ of electron transfer. Consequently, interface effects compete with the metals properties gave us good image about scenario of potential barrier at interface. The interface interactions of electron transfer at metal/semiconductor system should be effected by the properties of polarity for the system, since these metal and semiconductor have static dielectric constant and optical dielectric constant properties. Taking into account information of polarity from investigations of the reorientation energy by semi classical Marcus-Hush model, the simplest possible expression description is given by this model.

However the most important factor in the probability rate expression is the transmission matrix element coefficient $\langle|\overline{\xi(E)}|^2\rangle$ that has been used to study the two type of electron transfer adiabatic and non-adiabatic. The coefficientmatrix element $\langle|\overline{\xi(E)}|^2\rangle$ of the electron transfer reaction process is proportional to the square of the electronic matrix element $\langle|\overline{\xi(E)}|^2\rangle$. The coupling matrix element coefficient $\langle|\overline{\xi(E)}|^2\rangle$ have controled 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 $\langle|\overline{\xi(E)}|^2\rangle$ has been used in the range from $(0.017 - 0.022)eV$ depending on the typical results of experimental data (21).

Furthermore, the Marcus -Hush model have been applied for metal/semiconductor system reactions makes it possible to evaluation the most one of an important parameters of electron transfer that's reorientation energy $\epsilon_{m-S}(eV)$ in relatively under the action of oxidants or reductions state.

Reorientation energy $\epsilon_{m-S}(eV)$ of the electron transfer should be affected on the probabilities of rate constant $\Gamma_{ET}(Sec^{-1})$ at metal/semiconductor system. The reorientation energy for electron transfer should be considered as starting points for studies the behavior of electron transition at metal/semiconductor interface devices. We present evidence of the probability of electron transfer in this system at several interface and propose the electron transfer to be related to coupling coefficient and reorganization energy governed by interface dipole formation on the respective metals.Electron transfer interactions at metal/semiconductor interface system should be effected by polarity parameter for the metal and semiconductor through depending on the reorganization energy in Eq.(50).Results of the reorganization energy in tables (3-4) for Au/Si and Au/Ge systems are be effected by polarity parameter for the metal and semiconductor . The reorientation energy $\epsilon_{m-S}(eV)$ is large for large polarity parameter and vice versa. This indicates that the reorganization energies $\epsilon_{m-S}(eV)$ are dependent on the polarity parameter for metal.

The probability of electron transfer $\Gamma_{ET}(\text{Sec}^{-1})$ across the interface created between metal and semiconductor in system depends and proportional on the reorganization energy $\epsilon_{m-S}(eV)$ that provided support to electron transfer. Reorganization energy $\epsilon_{m-S}(eV)$ of the electron transfer have been limited the values of these probabilities of rate constant $\Gamma_{ET}(\text{Sec}^{-1})$ at metal/semiconductor system. Since the rate constant $\Gamma_{ET}(\text{Sec}^{-1})$ values are large for system with less polarity function and increases with decreases of the reorganization energy. This indicates that for Au/Ge are more reactive electron transfer compare with Au/Si, and ET occur activity with less polarity parameters. That means when the polarity function is large lead to large reorganization energy and vice versa ,and the reorganization energy $\epsilon_{m-S}(eV)$ values for metal / semiconductor system increasing with the increase of the dielectric constant and polarity function for the system and leads to decreases in probability of transition rate as compared with the system that have small reorganization energy $\epsilon_{m-S}(eV)$ because the system has small value of reorganization energy $\epsilon_{m-S}(eV)$ more orient to transfer of electron. On the other hand the 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 (6-7). The present data for the probability of electron transfer that occurs in a metal/semiconductor system with lest reorientation energies for all Au/Ge , and Au/Si respectively system for example $\Gamma_{ET}(\text{Sec}^{-1})$ =1.470 $\times 10^3$ when $\epsilon_{m-S}(eV) =$ 0.9839 for Au/Si compared with $\Gamma_{ET}(\text{Sec}^{-1}) = 7.752\text{E} - 09$ to more reorientation energy such that that have *the reorganization energy* $\epsilon_{m-S}(eV) = 0.9926$. The reorganization energy $\epsilon_{m-S}(eV)$ is large for more polarity function metal and small for less polarity function for metal, 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.

Also the ability of the transition of electron across metal/semiconductor interface system depends on the potential barrier height $\Delta\mathbb{V}^*(eV)$ that is created between two material interfaces (metal and semiconductor). At this point, it is tempting to study the effect of potential barrier on the transition electron rate at metal/semiconductor devices. At the metal/semiconductor interface, due to energy level difference the potential barrier $\Delta\mathbb{V}^*(eV)$ is formed depending on the properties of metal and semiconductor system and impedance and decreases the electron transport. These interface metal/semiconductor serve as a control to identify possible spurious effects from properties of metal and semiconductor. Transport probability calculations of metal/semiconductor devices interfaces prepared and tested as actual devices .These interface allow us to compare the transport behavior from devices made with our semiconductor of interest and metal whose transport characteristics are well documented. These control devices are expected to act essentially like tunnel interfaces. The potential barrier height $\Delta\mathbb{V}^*(eV)$ isrelated withreorganization energy and the driving force energy. The probability for electron transition in metal/semiconductor systems is dependent on the potential barrier height $\Delta\mathbb{V}^*(eV)$

for the tunneling between metal and semiconductor interface.The potential barrier height $\Delta\mathbb{V}^*(eV)$ for the electron transfer at metal/semiconductor interface system was calculated depending on the results of the work function $\varphi_m(eV)$,of metal and affinity of semiconductor$\chi_{se}(eV)$. The electron transfer creates a potential barrier at the metal/semiconductor interface that modifies significantly the conduction band of semiconductor states depending on the corresponding electron density distribution for metal. For all semiconductors, the metal Fermi level is found to lie closer to the conduction band level in the system gap for both semiconductors is due to the metal-gap states arising from the hybridization of the metal surface states with the occupied conduction band states. 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.

Conclusion

We can concluded depending on data results of the probability of rate constant for electron transfer in metal/semiconductor system the probability of transfer at metal/semiconductor interface system depending on: the reorientation energy, potential barrier height $\Delta\mathbb{V}^*(eV)$, 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},petration factor β, and temperature T(K). A theoretical model successfully to investigate and studythe behavior of electron transition across interface from donor to acceptor in metal/semiconductor system, and enable us to study the electron transition mechanism. 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 physical.

probabilities of rate constant $\mathbf{\Gamma_{ET}(Sec^{-1})}$ at metal/semiconductor systemand the rate constant $\mathbf{\Gamma_{ET}(Sec^{-1})}$are depending on the energies of reorganization for system with polarity function and increases with decreases of the reorganization energy.

The coupling coefficient is an important scale of the probability to transfer of electron due to tunneling created between metal and semiconductor. Rate constant $\mathbf{\Gamma_{ET}(Sec^{-1})}$ increases with the increasing of the coupling coefficient.

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