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Investigation on the Theoretical formulations of electron transfer cross section at metal - semiconductor interface

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Abstract

A theoretical studies and calculation the cross-section for electron transfer at metal/semiconductor interfaces material depending on quantum description. Cross sections of charge transfer for Ag with Si, TiO2, and ZnO have carried out using simplified models of the system at the Multi driving force energy at interaction in the devices interface. Investigation and evaluation of the cross section for electron transfer σ_{ET} at metal/semiconductor system is depending on the coefficient; driving force energy (ϑ) , transfer energy orientation energy, wave number ϑ, mean refractive index n , amplitude of electronic coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle$ and the lifetime of electron transfer τ_{ET}. The cross section for electron transfer σ_{ET} at metal/semiconductor system evaluated using MATLAP program. The result shows that the increasing of cross section along with the increasing of the driving force energy and coupling coefficient and vice versa.

***Keywords*:** Electron transfer, Cross section, Metal -Semiconductor**.**

Introduction

Many researchers have been studies and investigation of the movement of electron through metal/semiconductor interface in the past years ago. The treatment of electron transition theoretically cross-interfaces of two different materials played an important role in much more emerging fields, Electron Transfer (ET) is the basic and simple interaction. The transfer of an electron between a donor and acceptor states without creation or breaking any chemical bonds [1]. The investigated of the electronic transtion process in collision has a big great important not only in fundamental collision of atomic physics, it understands the interactions of charged particles with each other , but also in such diverse fields as; development of x-ray laser , electronic devices controlled-thermonuclear-fusion research and astrophysics[2]. The transfer of a single electron from an atom or a molecule to another is considered to be the most elementary [3], and one of the more fundamental and ubiquitous phenomena in physics, chemistry, biology processes and technology [1], involves an oxidation of donor state and reduction of an acceptor state. In such process , more electrons will simultaneously transition to upper excite state with significantly not small cross section and the ionic produced finally were stability due to emission of electron(s) or photon(s) or both [2]. The field of electrons transfer have extended enormously in late 1940s. These field was developed in both theoretically and experimentally as well as to the studied much more other types of reactions been brought together. The self-exchange reactions, the isotopic exchange reactions and cross section reactions are early experiments in field of electronic transition process [4]. Electron transfer cross section was investigate and studied using classical barrier model (CBM) [5]. Around 1950, the theoretical investigated and described reactions of ET were generally triggered by Rudy Marcus, he is awarded the Nobel Prize in 1992 for introduce the main theoretical contributions of electron transition interactions in chemical systems. Rudolph Marcus was realize the important of nuclear configuration change in different system of reactant - product ET rate [6].The electronic transition reaction was the subject of persistent interesting in biological ,chemical and physics. In recent decades, many researchers investigate the transfer of electrons cross the metal /semiconductors interfaces [7]. Metal/ semiconductor contact from interfaces that give basic features of many metal /semiconductor devices in 2009 [8].To construct the diagram of metal contact to semiconductor; we are considering the diagram of energy band for metal contact to semiconductor, align with each other 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 of semiconductor material, which has high energies, the electrons will be flow into other material until the Fermi energy level on the both sides brought into coincidence [9]. The energy levels in both materials have been reformation relative to new common Fermi level. However, Fermi energy of semiconductor and metal do not change right away [10]. Fundamental studies, as performed in these theses were expect to provide guidelines for design of such practically useful ET system in this theses, our main theoretical model can be study of electron transfer at metal/semiconductor interface system. The orientation energy and the probability rate of electron transfer constant were calculates according to this

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model. In this paper, we performed to undertake a theoretical study and calculation the cross section of electron transfer reaction the metal/semiconductor interface system using quantum consideration.

Theoretical Considerations

One of the most important parameter for the study the properties of many material is the cross section that's defined as the number of particles that's pass in a time unit through the area of a beam and may be represented as[11].

$$\sigma_{ET} = \sum_{i=1}^{n} \sigma_{et(i)} \qquad (1)$$

The effective stimulated cross section of electron transfer depended on the lifetime and given by [12].

$$\sigma_{ET} = \frac{E(\vartheta)}{8\pi n^2 c\vartheta^2 \tau_{ET}} \qquad (2)$$

Where $E(\vartheta)$ is driving force energy, ϑ is the wave number $\vartheta = \frac{1}{\lambda}$, n is the mean refractive index, c is the light velocity and $\tau_{ET}$is lifetime for electron transfer. The lifetime of electron transfer is related to the rate of electron transfer is given by [13]

$$\tau_{ET} = \frac{1}{R_{et}} \qquad (3)$$

Where R_{et} is the probability of electronic transition at contact interface of metal and semiconductor that is depending on distance by exponentially with decay constant and may be write [14]

$$R_{et} \approx \frac{2\pi}{\hbar} \frac{N_{in}V_{sem}}{\beta\sqrt{4\pi E_{met}^{sem} k_B T}} exp - \frac{(\Phi_{met} - \chi_{sem})}{k_B T} \langle |\langle \underline{\Lambda(0)} \rangle|^2 \rangle \left[[\pi k_B T - \frac{1}{4E_{met}^{sem} k_B T} \left(\frac{(\pi k_B T)^3}{4} \right) \right] \qquad (4)$$

Here, Φ_{met} is work function of metal, χ_{sem} is affinity of semiconductor, N_{in} consentration of electrons, V_{sem} is the unit cell volume of semiconductor, β the penetration parameter and $\langle \underline{\Lambda(0)} \rangle$ the coupling matrix element coefficient for metal and semiconductor interface. Inserting Eq.(4) in Eq.(3) to give .

$$\tau_{ET} = \frac{1}{R_{et}} = \frac{\hbar}{2\pi} \frac{\beta\sqrt{4\pi E_{met}^{sem} k_B T}}{N_{in}V_{sem}} exp \frac{(\Phi_{met} - \chi_{sem})}{k_B T} (\langle |\langle \underline{\Lambda(0)} \rangle|^2 \rangle)^{-1} \left[[\pi k_B T - \frac{1}{4E_{met}^{sem} k_B T} \left(\frac{(\pi k_B T)^3}{4} \right) \right]^{-1} \qquad (5)$$

Then the cross section of electron transfer would obtained by substituting Eq. (5) in Eq. (2) to get

$$\sigma_{ET} = \frac{N_{in}V_{sem}}{4\hbar n^2 c\vartheta^2} \frac{E(\vartheta)}{\beta\sqrt{4\pi E_{met}^{sem} k_B T}} exp \frac{-(\Phi_{met} - \chi_{sem})}{k_B T} \langle |\langle \underline{\Lambda(0)} \rangle|^2 \rangle \left[\pi k_B T - \frac{1}{4E_{met}^{sem} k_B T} \left(\frac{(\pi k_B T)^3}{4} \right) \right] \qquad (6)$$

Although ,the quantum driving force energy $E(\vartheta)$ satisfy energy that needed to drive an electron to transition from donor state to an acceptor state when a light is incident on donor -acceptor scenario to give by [15]

$$E(\vartheta) = hf - E_{met}^{sem} \qquad (7)$$

h is a Planck constant, f is frequency, $f = \frac{c}{\lambda}$ where c is light velocity, λ is wavelength and the transfer orientation energy E_{met}^{sem} .

The transfer energy orientation E_{met}^{sem} is arising from the reformation of the charge in system. It has quantity depended on the radius of both donor and acceptor matter on its distance "d", the dielectric properties of the semiconductor and metal due to the electronic transfer reaction for metal and semiconductor interface is given by [16]. $E_{semi.}^{met} =$

$$\frac{e^2}{4\pi\varepsilon_0} [\frac{1}{2R_{met}} \left(\frac{1}{n_{met}^2} - \frac{1}{\varepsilon_{met}} \right) + \frac{1}{2R_{semi}} \left(\frac{1}{n_{semi}^2} - \frac{1}{\varepsilon_{semi}} \right) - \frac{1}{4D_{semi}} \left(\frac{n_{met}^2 - n_{semi}^2}{n_{met}^2 + n_{semi}^2} \frac{1}{n_{semi}^2} - \frac{\varepsilon_{met} - \varepsilon_{semi}}{\varepsilon_{met} + \varepsilon_{semi}} \frac{1}{\varepsilon_{semi}} \right) - \frac{1}{4D_{met}} \left(\frac{n_{semi}^2 - n_{met}^2}{n_{semi}^2 + n_{met}^2} \frac{1}{n_{met}^2} - \frac{\varepsilon_{semi} - \varepsilon_{met}}{\varepsilon_{semi} + \varepsilon_{met}} \frac{1}{\varepsilon_{met}} \right) - \frac{1}{R_{met-semi}} \left(\frac{1}{n_{met}^2 + n_{semi}^2} - \frac{1}{\varepsilon_{semi} + \varepsilon_{met}} \right)] \qquad (8)$$

Where R_{met} and R_{semi} are the radii 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 metal and semiconductor to interface and metal-semiconductor , n_{met}^2 , $\varepsilon_{met}$are square of refractive index and square dielectric constant and n_{semi}^2 , ε_{semi} are square refractive index and statistical dielectric constant of semiconductor.

The molecule radius estimates using apparent spherical volume, it's given by [17].

$$R = \left(\frac{3M}{4\pi N\rho} \right)^{\frac{1}{3}} \qquad (9)$$

Where N is Avogadro's number, M is molecular weight, and ρ is mass densities of materials.

Results

Investigation and describe of cross section for electron transfer σ_{ET} at metal/semiconductor device theoretically has depended on many coefficient, one of these important parameters is the driving force energy$E(\vartheta)(eV)$. The driving force energy $E(\vartheta)(eV)$ is the energy required to the electron transfer interaction at the system. It can be evaluated using Eq. (7) with calculated the transfer energy orientation energy using Eq. (8).

The calculation of the transfer energy orientation $E_{met}^{sem}(eV)$) may be fulfilled with estimation the radii of Ag by Eq. (9) with insert values of Avogadro's constant $N = 6.02 \times 10^{23} \frac{Molecule}{mol}$,molecular weight $M = 107.87$ [18] with density masses $\rho = 10.43$ [18] for Ag, the radii results is 1.44 A. The transfer energy orientation $E_{met}^{sem}(eV)$) have been estimation by inserting the radii Ag values 1.44 A with dielectric constant and refractive index for Si, ZnO, TiO_2 using Table (1) in Eq. (8).

The results of transfer energy orientation $E_{met}^{sem}(eV)$) are 0.9839 for Ag / Si, 0.6094 for Ag / TiO_2 and 0.4326 for Ag / ZnO semiconductor interface. The driving force energy $E(\vartheta)(eV)$ evaluated using Eq. (7) with results of the transfer energy orientation 0.9839, 0.4326 and 0.6094 eV for Ag / Si, Ag / ZnO and Ag / TiO_2 system respectively and results shown in Table (2).

Table1. Common properties of semiconductor.

Properties	Values		
Chemical Formula	Si[19]	ZnO[20]	TiO2[21]
Atomic weight	28.09	81.38	79.866
Density (g/cm3)	2.328	5.66	4.23
Crystal structure	Diamond	Wurzite	Tetragonalrutile
Refractive index	3.3	2.0033	2.609
Dielectric constant	11.9	8.5	15.10
Energy gap (eV) at 300K	1.12	**3.44**	3.02
Lattice constant (Å)	5.431	a = 3.249 c =5.206]	a = 4.5936 c =2.9587
Electron affinity (eV)	4.05	4.3	4.2
Calculated Radius(Å)		3.8025	1.95612
Effective density of states N_C m^{-3})	2.8×10^{19}	2.22×10^{24}	1.163×10^{25}

Table2. Results of Driving force energy for Ag metal with Si, TiO_2 and ZnO semiconductor.

System	**Wave length (nm)**				
	400	**500**	**600**	**700**	**800**
Ag / Si	**2.1151**	**1.4951**	**1.0821**	**0.7871**	**0.5651**
Ag / ZnO	**2.6664**	**2.0464**	**1.6334**	**1.3384**	**1.1164**
Ag / TiO_2	**2.4896**	**1.8696**	**1.4566**	**1.1616**	**0.9396**

The probability of cross section for electron transfer σ_{ET} have been evaluated according on Eq.(6) that's a results of a simple model derived due to quantum consideration with continuum state level for Ag metal and Si,$TiO_2$and ZnO semiconductors state levels. Cross section calculates due to the estimate the driving force energy $E(\vartheta)$, transfer energy orientation, wave number, mean refractive index n , amplitude of electronic coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle$and the lifetime of electron transferτ_{ET} coefficients. The lifetime of electron transferτ_{ET} was eva;iated according on the transfer energy orientation energyE_{met}^{sem}, ,work function of metal Φ_{met}, affinity of semiconductor χ_{sem}, electronic concentration n_{in}, unit cell volume of semiconductor V_{sem},penetration parameter β, temperature T(K).

The result of cross section of electron transfer was obtaining by using the Eg. (6), and MATLAB program, formulated to evaluate the probability of cross section for electron transfer at metal/semiconductor interface system. The transfer energy orientation $E_{met}^{sem}(eV)$ data for three Ag /Si, Ag /TiO_2 and Ag /ZnO systems, and electronic concentration n_{in}, unit cell volume of semiconductor V_{sem} from Table(1) was performed along with penetration factor β=$1 \times 10^{-10}\ m^{-1}$. The coupling matrix element coefficient:

$\langle|\underline{\Lambda(0)}|^2\rangle$=0.4, 0.45, 0.5 , 0.55, 0.6, 0.65, 0.7, 0.75, and 0.8x$10^{-11}$$(eV)^2$

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For metal and semiconductor [4].

Results of evaluation listed in Table (3), (4), and (5), for Ag /Si, Ag /TiO_2 and Ag /ZnO systems respectively.

Table3. Results of the cross section for electron transfer $\sigma_{ET} \times 10^{-16}$ at Ag / Si devices due to variety coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle$ at 300 K.

Wave length	coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle \times 10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
400	**1.903**	**2.1415**	**2.3795**	**2.6172**	**2.855**	**3.093**	**3.3313**	**3.570**	**3.8084**
500	**2.101**	**2.3648**	**2.6276**	**2.8901**	**3.152**	**3.4158**	**3.6786**	**3.942**	**4.2055**
600	**2.189**	**2.4633**	**2.7370**	**3.0104**	**3.284**	**3.5580**	**3.8318**	**4.106**	**4.3806**
700	**2.189**	**2.436**	**2.7075**	**2.9780**	**3.248**	**3.519**	**3.7905**	**4.062**	**4.3339**
800	**2.031**	**2.2854**	**2.5360**	**2.7930**	**3.047**	**3.3011**	**3.5551**	**3.810**	**4.0643**

Table4. Results of cross section for electron transfer $\sigma_{ET} \times 10^{-9}$ at Ag / ZnO devices due to variety coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle$ at 300 K.

Wave length	coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle \times 10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
400	**0.9176**	**1.0322**	**1.1467**	**1.2613**	**1.3764**	**1.4910**	**1.6055**	**1.7201**	**1.8346**
500	**1.1004**	**1.2378**	**1.3751**	**1.5125**	**1.6506**	**1.7880**	**1.9254**	**2.0627**	**2.2001**
600	**1.2639**	**1.4216**	**1.5794**	**1.7372**	**1.8958**	**2.0536**	**2.2114**	**2.3691**	**2.5269**
700	**1.4100**	**1.5860**	**1.7620**	**1.9380**	**2.1150**	**2.2910**	**2.4671**	**2.6431**	**2.8191**
800	**1.5368**	**1.7287**	**1.9205**	**2.1123**	**2.3053**	**2.4971**	**2.6889**	**2.8808**	**3.0726**

Table5. Results of the cross section for electron transfe r$\sigma_{ET} \times 10^{-14}$at at Ag / TiO_2 devices due to variety coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle$ at 300 K.

Wave length	coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle \times 10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
400	**1.843**	**2.074**	**2.3045**	**2.5346**	**2.765**	**2.9956**	**3.2261**	**3.456**	**3.6871**
500	**2.573**	**2.8955**	**3.2173**	**3.5385E**	**3.8603**	**4.1821**	**4.5039**	**4.8257**	**5.1475**
600	**2.886**	**3.247**	**3.6085**	**3.9688**	**4.3298**	**4.6907**	**5.0516**	**5.4126**	**5.7735**
700	**3.132**	**3.523**	**3.9155**	**4.3065**	**4.6981**	**5.0897**	**5.4814**	**5.8730**	**6.2646**
800	**3.3106**	**3.724**	**4.1385**	**4.5517**	**4.9656**	**5.3795**	**5.7935**	**6.2074**	**6.6213**

Discussion

A simple model has used to investigate the cross section for electron transfer at Ag /Si, Ag/ZnO and Ag/TiO_2 devices system depending on the quantum theory. Due to this model, we assume the wave function for electron transmission interaction was satisfied all Hilbert space properties. According on this model, the electron transfer interaction has been occurring due to tunnelling region from the overlapping wave functions at interface state.

At the interface ,one assume that materials energy levels state have continuum state for system to alignment energies to happen the electron transfer between two material different structures electronic state in metal. However, the density of electrons on different metal surfaces have more than in conduction band of semiconductor. Although ,the, electronic states must be brought to resonance through the fluctuations of wave functions for both semiconductor and metal in semiconductor system and this resonance is transition state of electronic transfer process. The probability of cross section σ_{ET} in Eq.(6)indicates that the interaction of electron depending on the driving force energy $E(\vartheta)$, wave number ϑ, mean refractive index n , amplitude of electronic coupling coefficient $\langle|\underline{\Lambda(0)}|^2\rangle$and the lifetime of electron transferτ_{ET} that's depending on the transfer energy orientation energy, electronic concentration n_{in}, unit cell volume of semiconductor V_{sem}, penetration factor β, and temperature T(K). First of all the evaluation cross section parameter is required to evaluate the driving force energy $E(\vartheta)$ that's important parameter to enables us to evaluation the cross of section of electron at metal/semiconductor system. The estimation is due to the spectrum of devices and the transfer energy orientation for system. Driving force energy $E(\vartheta)$in Eq. (7) refers to the fundamental physical relations for the eraction of light with the materials in system.

The results of the cross section in Table (3 to 5) for Ag/semiconductor systems were affecting by the driving force energy. The cross section has large for large driving force energy and vice versa, this indicates that cross sections are dependent on driving force energies and its support energy to interaction.

The cross section increases with the increases of the driving force energy, this indicates that Ag/ZnO, are more reactive to electron transfer interaction compare with Ag/ TiO_2 and Ag/Si systems. On the other hand, the factor related to the cross section for electronic transtion is related to coupling coefficient term $|\underline{\Lambda(0)}|$(eV) that has been controlled to the electronic transfer interaction between two materials in system. Electron strength coupling is evidently reflected that the capability to electron transition interaction and determine by alignment energy levels in semiconductor respect to Fermi energy of metal. Hence, the coupling coefficient has used in the range from $(0.4- \ 0.8)(eV)$ depending on the typical results of experimental data [4]. Cross section of electrons become increase when strength coupling parameters matrix element between materials in system will be increasing, it shows from data in tables (3 to 5) for Ag/ZnO, Ag/ TiO_2 and Ag/Si systems.

Afterwards a theoretical analysis of the cross section evaluation data sets has to be performed for the joint determination of the driving force energy, transfer energy orientation, coupling coefficient and life time into the cross section expression in Eq.(6). The probability of cross section σ_{ET} result data have large values for Ag/ZnO system comparing with Ag/Si and Ag/TiO_2 system, this refers that there is Ag is reactive to ZnO semiconductor than TiO_2 and Si and electron transfer reaction occurs.

Conclusions

The cross section for electron transfer in metal/semiconductor system has been studies theoretically depending on quantum consideration and one-can conclusions that simple model was good tool enable us to describe the cross section in the metal, semiconductor interface system. On the other hand, the data results of cross section for electron transfer at metal/semiconductor system enable to elective the system to use or not in different applied physical. Cross section for electron transfer related to the driving force energy and coupling coefficient and the cross section is increases with increases the driving force energy and coupling coefficient and vice versa.

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