Theoretical Treatment and Investigation of the Expectation Electronic Current of Metal-Semiconductor System

Hadi, J.M, Al-agealy[1], Taif Saad Al Maadhede[2]

[1]Department of Physics–College of Education –Ibn Al-Haitham - Baghdad of University

[2]Al-Turath University of college

Abstract: ***The aim of this research is theoretical study and investigation of the electronic properties cross the metal-semiconductor contacts devices depending on the evaluation the expectation values of electronic current transfer. Barrier Potential heights have been characterized the electronic properties cross interface of metal-semiconductor contacts . Continuum energy levels are assume to the metal-semiconductor devices to fulfelment an ideal contacts at interface for the two difrent solid material states. Dipoles effect on the energies of transfer and the barrier potential heights could be presented in real contacts at metal-semiconductor devices . The expectation of electronic current and transfer barrier potential heights have been evaluated by using the theoretical method with transfer energy is given by the optical and statical dielectric constants of the two material . A MATLAB program designed to predict the expectation electronic current transfer.***

Keywords: Electronic Properties, Metal-Semiconductor.

1. Introduction

Electron transfer (ET) in solid phases exceeded the extension structure of the acceptor and donor and, had been focusing over the last decade and a half century ago[1].In the past few decades, there are efforts had been make in order to modulation the band gap that emission or improving luminescent efficiencies in semiconductors. On the other hand , concerntlay had been focused on the metal or surface plasmon induceing local field enhancements. Its believeing that as the surface[2]. Progress had been rested on the donor–acceptor synthetic systems in which electrons were brought to tunneling region across the interface [3]. The theory of electron transfer processes depending on the quantum-mechanical treatment is available, which providesa quantitative description of the effects of configurationally changes[4] . Ideal interfaces, to begin with, are laterally homogeneous, intimate, abrupt, and free of any kind of chemical or structural defects. The band alignment at such ideal interfaces is determined by the continuum of interface-induced gap states[5]. Metal -Semiconductor (M/S) interface contacts have recently solution the problem contact in semiconductor devices. In the Metal -Semiconductor devices, the effect of metal Fermi level pinning leads to the formation potential barriersregion. However, the potential barriers region that alleviate Fermi level pinning also leads to understand the physical mechanisms underlying the reduction of contact[6]. The main purpose of this work is investigation and studies the electric properties at $Fe/TiO_2$and Fe/ZnO system depending on the evaluation the expectation values of electronic current

2. Theory

Depending on the quantum consideration theory, the expectation of electronic current transfer for nonadiabitically processes between donor and acceptor state can be given by [7]:

$$\wp_{D,A} = \frac{2\pi}{\hbar}\sum\left|\Pi_{D,A}^{ET}\right|^2 \mathrm{FC}_{D,A}^{ET}\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where ħ is the Dirac constant, $\mathrm{FC}_{D,A}^{ET}$ is the Franck–Condon ,$\Pi_{D,A}^{ET}$ is the overlap integrals between the nuclear wave functions of oxidation and reduction states and may be estimation depending on Bardeen theorem and may be written as[8] .

$$\Pi_{D,A}^{ET} = \frac{\hbar}{2m_e}\int_S d^2r[\varphi_D{}^*(r)\nabla\varphi_A(r) - \varphi_A{}^*(r)\nabla\varphi_D]\ldots\ldots(2)$$

Where φ_D and φ_A are the wave functions for donor and acceptor respectively. TheFranck–Condon factor $\mathrm{FC}_{D,A}^{ET}$ in Eq.(1) is quite calculatedrelative to effective energy ϵ , transfer energies Δand temperature T and takes the form[9].

$$\mathrm{FC}_{D,A}^{ET} = \left(\frac{1}{4\pi\Delta_{TE}k_BT}\right)^{1/2}exp\left[-\frac{(\epsilon+\Delta_{TE})^2}{4\Delta_{TE}k_BT}\right]\ldots\ldots\ldots\ \ldots\ldots.(3)$$

Where k_B is the Boltzmann constant.Substituting Eq.(3) in Eq.(1) results.

$$\wp_{D,A} = \frac{2\pi}{\hbar}\sum\left(\frac{1}{4\pi\Delta_{TE}k_BT}\right)^{1/2}\left|\Pi_{D,A}^{ET}\right|^2 exp\left[-\frac{(\epsilon+\Delta_{TE})^2}{4\Delta_{TE}k_BT}\ldots(4)\right.$$

The transfer energy Δ_{TE} contribution arises from the transfer of the charge in metal/semiconductor systeminterface is given by [10].

$$\Delta_{TE}(\mathrm{R},n,\varepsilon) = \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2R_m}\left(\frac{1}{n_m^2}-\frac{1}{\varepsilon_m}\right)+\frac{1}{2R_s}\left(\frac{1}{n_s^2}-\frac{1}{\varepsilon_s}\right)-\frac{1}{4D_s}\left(\frac{n_m^2-n_s^2}{n_m^2+n_s^2}\frac{1}{n_s^2}-\frac{\varepsilon_m-\varepsilon_s}{\varepsilon_m+\varepsilon_s}\frac{1}{\varepsilon_s}\right)-\frac{1}{4D_{met}}\left(\frac{n_s^2-n_m^2}{n_s^2+n_m^2}\frac{1}{n_m^2}-\frac{\varepsilon_s-\varepsilon_m}{\varepsilon_s+\varepsilon_m}\frac{1}{\varepsilon_m}\right)-\frac{1}{R_{m/s}}\left(\frac{1}{n_m^2+n_s^2}-\frac{1}{\varepsilon_{semi}+\varepsilon_{met}}\right)\right]\ldots.(5)$$

Where R_m and R_s are the radius of metal and semiconductor and given be $R_{m,s} = (3M/4\pi N\rho)^{\frac{1}{3}}$forthe index M molecular weight, ρ ismass density and N is Avogadro's number, and, $D_s = R_s + 1A^\circ$, $D_m = R_m + 1A^\circ$,and $R_{m/s} = R_m + R_{si}$ are the distance between semiconductor ,metal to interface and metal-semiconductor , n_m , ε_m are the optical and statistical dielectric constant and n_s and ε_s are the optical and statistical dielectric constant for semiconductor. Then we can find the total probability of electronic current

Licensed Under Creative Commons Attribution CC BY

transfer be integration Eq.(4) due to the Fermi-Dirac density of state $F_{(E)}$ and written as .

$$\wp_{D,A} = \frac{2\pi}{\hbar}\int_{-\infty}^{\infty}\left|\mathbf{\Pi}_{D,A}^{ET}\right|^2\left(\frac{1}{4\pi\Delta_{TE}k_BT}\right)^{1/2}exp\left[-\frac{(\epsilon+\Delta_{TE})^2}{4\Delta_{TE}k_BT}\right] \quad F_{(E)}dE \ldots.(6)$$

The effective driving energy for the electron transfer from donor state with energyE to the acceptor is related by [11].

$$\epsilon = \epsilon^{\circ} - E \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

The exponent $exp - (\epsilon + \Delta_{TE})^2/4\Delta_{TE}k_BT$ inside integral in the Eq(6) can be written as .

$$exp - (\epsilon + \Delta_{TE})^2/4\Delta_{TE}k_BT = exp - (\Delta_{TE} + \epsilon^{\circ})^2/4\Delta_{TE}k_BTexp2E(\Delta_{TE} + \epsilon^{\circ})/4\Delta k_BTexp - E^2/4\Delta_{TE}k_BT \ldots\ldots\ldots (8)$$

The first term $exp - (\Delta + \epsilon^{\circ})^2/4\Delta_{TE}k_BT$is independent (E) that can be removed out of integral,the term $exp2E(\Delta_{TE} + \epsilon^{\circ})/4\Delta_{TE}k_BT$ varies much more slowly with (E) than (E/k_BT) in the exponent of the third term in the integral eq (3-52)when$\Delta \cong -\epsilon^{\circ}$) can then ignore and Eq.(6)yielding.

$$\wp_{D,A} = \frac{2\pi}{\hbar}\exp - \left(\frac{(\Delta+\epsilon^{\circ})^2}{4\Delta_{TE}k_BT}\right)\int_{-\infty}^{\infty}\left|\mathbf{\Pi}_{D,A}^{ET}\right|^2\left(\frac{1}{4\pi\Delta_{TE}k_BT}\right)^{1/2}\exp\left(-\frac{E^2}{4\Delta_{TE}k_BT}\right)\left(\frac{1}{1+exp\frac{E}{k_BT}}\right) \ldots.(9)$$

Where the$\left(\left|\mathbf{\Pi}_{D,A}^{ET}\right|^2\right)$ is an averaged coupling electronic matrix elements square the all the electronic states which is given by relative density of state $\rho_{(E)}$ [12].

$$\left\langle\left|\mathbf{\Pi}_{D,A}^{ET}\right|^2\right\rangle = \pi k_BT\sum_{D,A}\left|\overline{\mathbf{\Pi}_{D,A}^{ET}}\right|^2\rho_{(E)} \ldots\ldots\ldots\ldots\ldots\ldots(10)$$

But the exponential out of integral describe barrier height

$$\frac{(\Delta_{TE}+\epsilon^{\circ})^2}{4k_BT} = (\Phi_{met} - \chi_{sem})/4\Delta_{TE} \ldots\ldots\ldots\ldots\ldots(11)$$

Then the probability of electron transfer at system in Eq. (9) with Eq.(10) andEq.(11) reduced to.

$$\wp_{D,A} = \frac{2\pi}{\hbar}\frac{\exp-\frac{(\Phi_{met}-\chi_{sem})}{k_BT}}{(4\pi\Delta_{TE}k_BT)^{1/2}}\int_{-\infty}^{\infty}\pi k_BT\sum_{D,A}\left|\overline{\mathbf{\Pi}_{D,A}^{ET}}\right|^2\rho_{(E)}\exp\left(-\frac{E^2}{4\Delta_{TE}k_BT}\right)\left(\frac{1}{1+exp\ldots}\right) \ldots\ldots\ldots(12)$$

The approximation result of integral.

$$\int_{-\infty}^{\infty}\frac{\exp\left(-\frac{E^2}{4\Delta_{TE}k_BT}\right)}{1+exp\frac{E}{k_BT}}dE \approx \exp - \frac{E}{2k_BT}\left[\pi k_BT - \frac{1}{4\Delta_{TE}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)\right] \ldots.. (13)$$

By substituting above integration results in Eq.(12) ,the rate became .

$$\wp_{D,A} = \frac{2\pi}{\hbar}\exp - (\Phi_{met} - \chi_{sem})/k_BT\left(\frac{1}{4\pi\Delta_{TE}k_BT}\right)^{1/2}\pi k_BT\sum_{D,A}\exp\frac{-E}{2k_BT}\left|\overline{\mathbf{\Pi}_{D,A}^{ET}}\right|^2\rho_{(E)}\left[\pi k_BT - \frac{1}{4\Delta_{TE}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)\right] \ldots\ldots\ldots\ldots(14)$$

Under condition $E = E_{C.B} - E_f \gg k_BT$ and the Fermi energy$E_f = V_{ap\,(D,A)} + E_f^o$ [13]for metal with applied voltage V_{app} the exponential factors in Eq.(14) is reduced for two face $V_{ap\,(D,A)} \approx 2V_{app}$ to.

$$\exp\frac{-E}{2k_BT} = \exp\frac{E_f-E_{C.B}}{2k_BT} = \exp\frac{V_{ap\,(D,A)}+E_f^o-E_{C.B}}{2k_BT} = f_o(E)\exp\frac{V_{app}}{k_BT} \ldots.(15)$$

But the $expV_{app}/k_BT$ is given by[13].

$$\frac{n_{in}}{\frac{\sum_0^{\infty}\rho(E)f_o(E)}{V_{sem}}} = exp^{\frac{V_{app}}{k_BT}} \ldots\ldots\ldots.(16)$$

Then the probability ofelectronic current transfer across interface of metal/ semiconductor system in Eq.(14) may be write with Eq.(16) as;

$$\wp_{D,A} = \frac{2\pi}{\hbar}\frac{\exp-(\Phi_{met}-\chi_{sem})/k_BT}{(4\pi\Delta_{TE}k_BT)^{1/2}}\frac{n_{in}V_{sem}}{\sum_0^{\infty}\rho(E)f_o(E)}\pi k_BT\sum_{D,A}\left|\overline{\mathbf{\Pi}_{D,A}^{ET}}\right|^2\rho_{(E)}\left[\pi k_BT - \frac{1}{4\Delta_{TE}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)\right] \quad ..(17)$$

But thesquarequantum overlapping constant elements $\left|\overline{\mathbf{\Pi}_{D,A}^{ET}}\right|^2$ are given by;

$$\left\langle\left|\Omega_{D,A}^{ET}\right|^2\right\rangle = \pi k_BT\frac{\sum_{D,A}\left|\overline{\mathbf{\Pi}_{D,A}^{ET}}\right|^2\rho_{(E)}}{\sum_0^{\infty}\rho(E)f_o(E)} \ldots\ldots\ldots.(18)$$

Then the expectation ofelectronic current transfer $\wp = \frac{1}{\beta}\wp_{D,A}$ in Eq. (17), with Eq.(18)is given by .

$$\wp(\Delta_{TE}, \Omega_{D,A}^{ET}) = \frac{2\pi}{\hbar}\frac{n_{in}V_{sem}\exp-(\Phi_{met}-\chi_{sem})/k_BT}{\beta(4\pi\Delta_{TE}k_BT)^{1/2}}\left|\Omega_{D,A}^{ET}\right|^2\left[\pi k_BT - \frac{1}{4\Delta_{TE}k_BT}\left(\frac{(\pi k_BT)^3}{4}\right)\right] \ldots(19)$$

3. Results

A theoretical based on the quantum theoryhave been depending to the investigation and evaluation the expectation of electron current in the metal-semiconductor interface devices. Quantum scenario for the transfer of electronic was adapted to the investigation and analysis of the electronic propertiesat the Fe/ZnO and Fe/TiO_2 systems . The electronscurrent transmission from metal to semiconductor have been evaluated using quantumly method expression at Eq. (19) due to the transfer energies Δ_{TE} ,thesquarequantum overlapping constant elements $\left|\Omega_{D,A}^{ET}\right|^2$, work function energy Φ_{met} , electronic affinity χ_{sem} ,penetration depth β ,temperature Tand volume of semiconductor V_{sem} .The transfer energy Δ evaluation ,one can estimation radii of metal and semiconductor $R_{m,s} = (3M/4\pi N\rho)^{\frac{1}{3}}$, . The radii of metalis and the radius of semiconductor are evaluated using the molecular weight M =55.847 [14],79.866 [15],and 81.38[18] and density $\rho = 7.873$[14]`4.23 [15], 5.66 [18] $\frac{gm}{cm^3}$ for Fe ,TiO_2, andZnOalternatively with Avogadro's constant $N = 6.02 \times 10^{23}\,\frac{Molecule}{mol}$,the results of radii are $R_{m,s} = 1.95612$, 3.8025 , and 1.240 A^o for TiO_2 ,ZnO and Fe

Licensed Under Creative Commons Attribution CC BY

Table 1: Common properties of semiconductor

Properties	TiO_2	ZnO
Atomic weight	79.866[15]	81.38[18]
Crystal structure	Tetragonalrutile	Wurtzite[18]
Density (g/cm^3)	4.23[15]	5.66 [18]
Refractive index	2.609[15]	2.00337[18]
Dielectric constant	100[16]	8.5 [18]
Effective density of states in conduction band, N_C (cm^{-3})	1.163×10^{19}[16]	2.22*10^24[18]
Energy gap (eV) at 300K	3.02[17]	3.4[18]
Lattice constant (Å)	a = 4.5936 c =2.9587[15]	a=0.32495,c=o. 5206[18]
Radius(Å)	1.95612	3.8025[18]
Electron affinity, (eV)	4.2[17]	4.4[18]

Next ,the barrier potential hight that's showing in the term $\exp-(\Phi_{met}-\chi_{sem})/k_B T$ can estimation as function of work function and electronic affinity and results are for Fe/TiO2 and Fe/ZnO systems .

In order to calculation the transfer energy for thedonor acceptor interaction at metal–semiconductor can be evaluation using the Eq.(5) and inserted the values of static and optical dielectric constant for metal[14] and semiconductors from table (1),with radii for metal $R_m = 1.240\ A^o$ and semiconductor $R_s = 1.95612$, and $3.8025 A^o$ from table (1) for bothFe/TiO2 and Fe/ZnOsystems .The results of energy transfer are shown in tables (2) and(3) for Fe/TiO2 and Fe/ZnO

Table 2: Theoretical estimation of the transfer energy Δ_{TE} due to static and optical dielectric constant for Fe/TiO2 systems

Energy[14]	Refrective index n	Wave Number	Static Dielectric Constant	Energy Transfer (eV)
2	2.85	3.36	19.412	0.7049
2.4	2.56	3.31	17.51	0.8141
2.6	2.34	3.3	16.366	0.9309
2.8	2.12	3.23	14.927	1.0815
3	1.88	3.12	13.269	1.3094
3.2	1.7	2.96	11.652	1.5376
3.4	1.55	2.79	10.187	1.7867
3.6	1.47	2.63	9.0778	1.9351

Table 3: Theoretical estimation of the transfer energy Δ_{TE} due to static and optical dielectric constant for Fe/ZnO systems

Energy[14]	Refrective index n	Wave Number	Static Dielectric Constant	Energy Transfer (eV)
2	2.85	3.36	19.412	0.5377
2.4	2.56	3.31	17.51	0.6558
2.6	2.34	3.3	16.366	0.7818
2.8	2.12	3.23	14.927	0.9425
3	1.88	3.12	13.269	1.1829
3.2	1.7	2.96	11.652	1.42
3.4	1.55	2.79	10.187	1.6763
3.6	1.47	2.63	9.0778	1.8264

The potential barrier that made at interface between metal and semiconductor have been estimation using Eq.(11) with work function for metal $\Phi_{met} = 4.5\ eV$ [14]and affinity for semiconductor χ_{sem} fro table (1) and the data of transfer energy for tables (2) and (3) for two systems Fe/TiO2 and Fe/ZnO alternatively .results is listed in table (4)for Fe/TiO2 and Fe/ZnO systems .

Table 4: Results of potential barrier estimation for Fe/TiO2 and Fe/ZnO systems

Energy (eV)[14]	Transfer Energy (eV)	Potential barrier for Fe/TiO2 (eV)	Transfer Energy (eV)	Potential barrier for Fe/ZnO(eV)
2	0.7049	0.1063	0.5377	0.004649
2.4	0.8141	0.0921	0.6558	0.003812
2.6	0.9309	0.0805	0.7818	0.0031977
2.8	1.0815	0.0693	0.9425	0.002652
3	1.3094	0.0572	1.1829	0.0021134
3.2	1.5376	0.0487	1.42	0.001760
3.4	1.7867	0.0419	1.6763	0.001491
3.6	1.9351	0.0387	1.8264	0.0013688

The total probability of expectation electronic current values of the electronic transfer from metalto semiconductor interface depending on the potential barrier in table(4) and using quantum consideration at various quantum overlapping constant elements $|\Omega_{D,A}^{ET}| = 0.4, 0.45, 0.5, 0.56, 0.6, 0.65, 0.7, 0.75\ and\ 0.8$. eV[19]is calculation function of using Eq.(19) with inserting the values the thetransfer energy from tables(2) and (3),and results of potential barrier from table(4),the data results are summarized in tables(5) ,and (6)for Fe/TiO_2 and Fe/ZnO systemsat thermal energy .

Licensed Under Creative Commons Attribution CC BY

Table 5: The result of expectation value of electronic current $\wp(\Delta_{TE}, \Omega_{D,A}^{ET})$ in Fe/TiO_2 sytem due to quantum overlapping constant

$Couplingmatrixelement \langle\|\Omega_{D,A}^{ET}\|^2\rangle x10^{-11} (eV)^2$									
re	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	
0.7049	2.784E+05	3.132E+05	3.480E+05	3.828E+05	4.176E+05	4.524E+05	4.872E+05	5.220E+05	5.568E+05
0.8141	2.598E+05	2.922E+05	3.247E+05	3.572E+05	3.896E+05	4.221E+05	4.546E+05	4.871E+05	5.195E+05
0.9309	2.435E+05	2.739E+05	3.043E+05	3.348E+05	3.652E+05	3.956E+05	4.261E+05	4.565E+05	4.869E+05
1.0815	2.264E+05	2.547E+05	2.829E+05	3.112E+05	3.395E+05	3.678E+05	3.961E+05	4.244E+05	4.527E+05
1.3094	2.062E+05	2.320E+05	2.578E+05	2.835E+05	3.093E+05	3.351E+05	3.609E+05	3.866E+05	4.124E+05
1.5376	1.906E+05	2.144E+05	2.383E+05	2.621E+05	2.859E+05	3.097E+05	3.336E+05	3.574E+05	3.812E+05
1.7867	1.771E+05	1.992E+05	2.213E+05	2.435E+05	2.656E+05	2.877E+05	3.099E+05	3.320E+05	3.541E+05
1.9351	1.702E+05	1.915E+05	2.128E+05	2.341E+05	2.554E+05	2.767E+05	2.979E+05	3.192E+05	3.405E+05
2.1449	1.618E+05	1.821E+05	2.023E+05	2.225E+05	2.427E+05	2.630E+05	2.832E+05	3.034E+05	3.237E+05

Table 6: The result of expectation value of electronic current $\wp(\Delta_{TE}, \Omega_{D,A}^{ET})$ in Fe/ZnO sytem due to quantum overlapping constant

Zno									
re	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	
0.5377	8.667E+09	9.750E+09	1.083E+10	1.192E+10	1.300E+10	1.408E+10	1.517E+10	1.625E+10	1.733E+10
0.6558	7.885E+09	8.870E+09	9.856E+09	1.084E+10	1.183E+10	1.281E+10	1.380E+10	1.478E+10	1.577E+10
0.7818	7.247E+09	8.152E+09	9.058E+09	9.964E+09	1.087E+10	1.178E+10	1.268E+10	1.359E+10	1.449E+10
0.9425	6.621E+09	7.448E+09	8.276E+09	9.103E+09	9.931E+09	1.076E+10	1.159E+10	1.241E+10	1.324E+10
1.1829	5.929E+09	6.670E+09	7.411E+09	8.152E+09	8.893E+09	9.634E+09	1.037E+10	1.112E+10	1.186E+10
1.42	5.422E+09	6.100E+09	6.778E+09	7.456E+09	8.133E+09	8.811E+09	9.489E+09	1.017E+10	1.084E+10
1.6763	4.999E+09	5.623E+09	6.248E+09	6.873E+09	7.498E+09	8.123E+09	8.748E+09	9.372E+09	9.997E+09
1.8264	4.792E+09	5.391E+09	5.990E+09	6.589E+09	7.188E+09	7.787E+09	8.386E+09	8.986E+09	9.585E+09
2.0394	4.539E+09	5.106E+09	5.674E+09	6.241E+09	6.808E+09	7.376E+09	7.943E+09	8.511E+09	9.078E+09

4. Discussion

The study of the electronic properties in the Fe/TiO_2 andFe/ZnOsystems was currently interesting of the subject, particulay attention focused a charge transfer theory .The expectation values of electronic current was the one of the important theoretically tolls to studying of the electronic properties at any system . The charge transfer theory is seeking to understand the material properties and the potential at interface of material. It was important to calculate the expectation values of the electronic current for two system, because there are background sources for the electronic properties . The study of electronic properties for metal-semiconductor interface devices depending on exchange the electrons cross interface materials and that causes the transfer charge . The electronic transfer processes due metal-semiconductor system properties depend on the transfer energyΔ_{TE} , square quantum overlapping constant elements $|\Omega_{D,A}^{ET}|^2$, potential hight barrier function to work function energy Φ_{met}, electronic affinity χ_{sem} , penetration depth β,temperature T and volume of semiconductor V_{sem}.. The expectation of electronic current is calculated depending on the assume continuum energy levels for two material system using the formula in Eq.(19) that's relative to perturbation theory in falls off atquantum overlapping two matrix element constant $|\Omega_{D,A}^{ET}| = 0.4, 0.45, 0.5, 0.56, 0.6, 0.65, 0.7, 0.75$ *and* 0.8. eV with transfer energy *from table()*.In order to understanding and calculation the expectation values of the electronic current , the one important coefficient to investigation of the feature of electronic transfer and the electronic properties is transfer energy for the system . Due tocontinuum theory , the transfer energy parameter Δ_{TE} is the scale of the polarity effect on the system that's dependent to expression and discussion the physical properties of transfer at interface of solid solid devices. Electronic current would beinfluenced by polarity coefficient in the metal and semiconductor due to the energy transfer. Tables (2) and (3) , show that the electronic current is effected by polarity parameter for the metal and semiconductor . The transfer energy is large for large polarity parameter and vice versa. The transfer energy $\Delta_{TE}(eV)$ result for two systems increasing with dielectric constant , also it isincreasingpolarity for the two system and leading to decreasing the electronic current as comparing with the system had small transfer energy $\Delta_{TE}(eV)$as a result of the system has small value of transfer energies $\Delta_{TE}(eV)$muchorientation to transfer of electron.

The behavior of electronic transfer interaction depending on the barrier Potential heights that's limited the electronic properties cross interface of metal-semiconductor contacts **.** Barrier Potential heights have been estimation according on the work function of metal and affinity of semiconductor .Since the electrons current have been crossing through thebarrier Potential at the interface by tunneling when the metal wave functions and semiconductor wave functions states are overlapping at interface **.** In spite of that tunneling at interface occurs, the energy level states for metal and semiconductor should be assume alignment

Licensed Under Creative Commons Attribution CC BY

On the other hand, the quantum overlapping two matrix element coefficient $\left|\Omega_{D,A}^{ET}\right|$ (eV), have controlled of the electronic current at metal semiconductor system and affected by the interface of material surfaces according to the strength of the interaction. Since the electronic current for metal-semiconductor systems strongly dependent on the quantum overlapping coefficient. Therefore, the expectation of electronic current increases due to increases of quantum overlapping coefficient, that's showing in tables (5) and (6) respectively. However, we can showing the electronic current increases with decreases the transfer energy, increases the quantum overlapping coefficient and decreases the potential barrier.

5. Conclusion

We can conclusion depending on the present results the expectation values of the electronic current at metal/semiconductor devices system results have supported and enabled us to study the electronic properties.

In summary, it can be concluded that's the electronic current should be effected by transfer energy, the potential barrier and the quantum overlapping coefficient of two matrix element

The electronic current is increases with decreases the transfer energy and potential barrier ,on the other hand its increases with increases the quantum overlapping coefficient.

References

[1] Kuznetsov, A. M. &Ulstrup, J. (1999) *Electron Transfer inChemistry and Biology: An Introduction to the Theory* (Wiley, Chichester, U.K.), in press.

[2] H. Y. Lin and Y. F. Chen ,J. G. Wu, D. I. Wang, and C. C. Chen" Carrier transfer induced photoluminescence change in metal-semiconductor core-shell nanostructures "APPLIED PHYSICS LETTERS Vol.88,PP 161911, 2006.

[3] ESBEN P. FRIIS, JENS E. T. ANDERSEN, YU. I. KHARKATS†, A. M. KUZNETSOV, R. J. NICHOLS, J.-D. ZHANG, and JENS ULSTRUP"An approach to long-range electron transfer mechanisms in metalloproteins: *In situ* scanning tunneling microscopy with submolecular resolution" *Proc. Natl. Acad. Sci. USA,*Vol. 96, pp. 1379–1384, February 1999 ,Biophysics.

[4] Kestner, N. R.; Logan; Jortner, J.,(1974), theory of electron transfer in liquid, J. Phy. Chem., 78, 214.

[5] Winfried Moncha "Electronic properties of ideal and interface-modified metal-semiconductor interfaces"J. Vac. Sci. Technol. B 14(4), Jul/Aug 1996,PP2985-2993.]

[6] Arunanshu Mohan Roy"TUNNELING CONTACTS FOR NOVEL SEMICONDUCTOR DEVICES"PhDThesis , STANFORD UNIVERSITY,2012.

[7] H.J.M.Al-Agealy R.I.N.AL-Obaidi "Charge transfer At Semiconductor / Liquid Interfaces" IBN AL-HAITHAM J. FOR PURE & APPL. SCI VOL.22 (2) 2009.

[8] Pierre Meystre · Murray Sargent III" Elements of QuantumOptics"Book, Fourth Edition, Springer-Verlag Berlin Heidelberg 2007]

[9] Gao, y, Q, and.marcus, R.A."On the theory of charge transfer reactions at semiconductor liquid interface"(2000:_,J.Chem. phys.Vol. 113. No. 15 ,pp 6351-6360.

[10] *Garol C., Bruce S. R.*, and *Sutan N.,2006*" *Interfacial charge transfer absorption " , Am. chem. Soc* .Vol.1,No.1,3425-3436.

[11] Waleed Bdaiwisalih, Hadi J. M. Al-Agealy, Taif S. Murdhi,"Probability of Electron Transfer Rate Constant at Nanoscale Metal/Molecule Interface System "IJAIEMVolume 2, Issue 11, November 2013 .

[12] Shachi S. G., 2002 "Electron Transfer at Metal Surfaces" Ph.D. Thesis, California Institute of Technology Pasadena, California.

[13] Gao.Y.Q., Georgievskii.Y and Marcus. R. A.," on the theory of electron transfers reaction at semiconductor electrode/ liquid interface" J. chem. Phys. 2000, Vol (112), No 7

[14] Pradyot Patnaik "Handbook of inorganic chemical"McGrew Hill Puplishing ,2002.

[15] F.A .Cotton,G. Wilkinson G.,C.A. Murillo, and M .Bochmann..Advanced Inorganic Chemistry, 1999,6thed, p. 697, New York: John Wiley & Sons

[16] T.V.Perevalov, and V.AGritsenko,J.of Experimental and Theoretical Physics,2011, 112,(2), 310-316

[17] G. Shipra and T Manoj, Physical Chemistry, June 2011 Vol.56 No.16: 1639–1657

[18] H. J. M. A-Agealy , H. Kh. Mujbil "Theoretical Calculation of Reorientation Energy in .Metal /Semiconductor Interface "Ibn Al-Haitham Journal for Pure and Applied Science, No.3,Vol.25,2012

[19] Shachi S. G., Ph.D. Thesis, California Institute of Technology Pasadena, California,2002.

Licensed Under Creative Commons Attribution CC BY