Investigate and Calculation Electron Transfer Rate Constant in the N749 Sensitized Dye Contact to ZnSe Semiconductor

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Abstract

The dye–semiconductor interface between N749 sensitized and zinc semiconductor (ZnSe) has been investigated and studied according to quantum transition theory with focusing on the electron transfer processes from the N749 sensitized (donor) to the ZnSe semiconductor (acceptor). The electron transfer rate constant and the orientation energy were studied and evaluated depended on the polarity of solvents according to refractive index and dielectric constant coefficient of solvents and ZnSe semiconductor. Attention focusing on the influence of orientation energies on the behavior of electron transfer rate constant. Differentdata of rate constant was discussion with orientation energy and effective driving energy for N749-ZnSe system. Furthermore, the electron transfer rate constant is increased with less orientation energy at less effective driving energy while the electron transfer rate constant increased with large orientation energy with large effective driving energy, as seen as the electron transfer rate reach to 1.3109×10^{11} with less orientation energy has 0.188708eV at effective driving energy E=0.22eV comparing the rate reach to 9.7207×10^{-96} with driving energy E=1.89eV and same orientation energy. In general, the electron transfer rate constant increases with increases the coupling coefficient of system, its indicate that alignment of energy levels are very good between N749 sensitized metal and ZnSe semiconductor.

Key Words: Electron Transfer Rate Constant, N749 Sensitized Dye, ZnSe Semiconductor.

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Introduction

The processes of electron transfer is the main processes in different science fields; physical, biophysical and chemistry with variety electronic devices technology. These electron transfer processes involvean electron will be transition from initial state called donor to final state called acceptor in different molecule, semiconductor and metal applied fields (Al-Agealy, 2020). Now, the electron transfer fields are fast extended vertically and horizontally in different technologic material andmicroelectronic devices (Al-Agealy, 2019). Organic electronic devices was investigated and studied in different devices such as; solar cell and organic light emission diodes (Otero, R., 2017). The basic concept of electron transfer reaction processes in contact materials with solid is developing by Marcus R., Dogonadeze L and Gerischer (Al-Obaidi, 2020).

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However, the electron transfer reactions are fundamental processes in much more complex systems, it is ranging from atom or molecule to large complex systems. In recent yearcs,the processes of electron transfer become more active search area in applied physics and technological electronic devices especially in molecule contact to semiconductor (Obeed, H.M., 2020). Hadi Al-Agealyetal introduce many theoretical model to study and investigate the electron transfer reaction in different molecule–metal and molecule –semiconductor, system under alignment of the energy levels for materials system with each other (AL-Agealy, H.J., 2020), (Maadhde, T.S.A., 2021). However, the electrons would be transfer from one state in donor material to another acceptor state material would be required that's more alignment of energy levels and closed in complex system (Shi, Y.R., 2019). Furthermore, the potential created between two different materials and the electrons were transfer cross the potential due to gained the enough energy to cross from donor to acceptor (Appelbaum, I., 2005). In this research, the electron transfer process has been occured between N749 sensitized dye and with ZnSe, it most important optoelectronic semiconductor materials and widely bandgap 2.7 eV. ZnSe uses in most solar photovoltaic cells, electronic devices and as a buffer/window material for hetero junction cells applications (Abdalameer, N.K., 2020). The aim of this research is to study and evaluate the electron transfer rate constant for the electron transfer reaction in N749 sensitized with ZnSe semiconductor. The electron transfer rate constant of N749/ ZnSe interface was evaluated and analysis theoretically using MATLAP program.

Theory

The electron transfer reaction rate constant will be investigated with Landau-Zener formula, its written by (Al-Agealy, H.J., 2021).

$$K_{ET} = \frac{2\pi}{\hbar}\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 \delta(E_S - E_D) \quad (1)$$

Where ħ is the Dirac constant, $H_{\frac{S}{D}}(E)$ is coupling coefficient and $\delta(E_S - E_D)$ is the Dirac function for energies semiconductor E_S and dye E_D. We introduce the probability density for electron in Eq.(1) for system to give.

$$K_{ET} = \frac{2\pi}{\hbar}\int\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 \rho_{EL}\delta(E_S - E_D)dE \quad (2)$$

The probability density of state is given by (Obeed, H.M., 2020).

$$\rho_{EL} = \sqrt{\frac{1}{4\pi T_{SD}k_BT}}\, e^{-\frac{(T_{SD}+\Delta E^0)^2}{4T_{SD}k_BT}} \quad (3)$$

Where T_{SD} is orientation energy, k_B is the Boltzman constant, ΔE^0 is effective driving energy and temperature T. Now, Inserting Eq.(3) in Eq.(2) and introduce the Fermi density of state for system to results.

$$K_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{SD}k_BT}}\int \mathrm{F}_{(\mathrm{E})}\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 e^{-\frac{(T_{SD}+\Delta E^0)^2}{4T_{SD}k_BT}}\delta(E_S - E_D)dE \quad (4)$$

For the rate of electron transfer, the activation density of state for semiconductor-liquid system $\rho_{act}(E)$ is (Obeed, H.M., 2019).

$$\rho_{act}(E) = \delta(E_S - E_D) \quad (5)$$

Inserting Eq.(5) in Eq.(4) to results.

$$K_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{SD}k_BT}}\int \mathrm{F}_{(\mathrm{E})}\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 e^{-\frac{(T_{SD}+\Delta E^0)^2}{4T_{SD}k_BT}}\rho_{act}(E)dE \quad (7)$$

The activation density of the electrons is (Al-Obaidi, 2020).

$$\rho_{act}(E) = \rho_S \frac{l_e}{d_a^{2/3}(\frac{6}{\pi})^{1/3}} \quad (8)$$

Where ρ_S is density of electrons in the semiconductor, l_e is length coupling and d_a is the atomic density of semiconductor. The density of electrons in semiconductor ρ_S is given (Simon, S.H., 2013).

$$\rho_S = \frac{3}{2}\left(\frac{N_S(E_f)}{E_f}\right) \quad (9)$$

Where the concentration of electron $N_S(E_f)$ at Fermi level with Fermi energy $\boldsymbol{E_f}$. Inserting Eq.(9) and (8) in Eq.(7) to find.

$$K_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{SD}k_BT}}\frac{l_e}{d_a^{2/3}(\frac{6}{\pi})^{1/3}}\int\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 e^{-\frac{(T_{SD}+\Delta E^0)^2}{4T_{SD}k_BT}}\rho_S(E)\mathrm{F}_{(\mathrm{E})}dE \quad (10)$$

The driving energy of electrons is function of conduction band $\mathrm{E_c}$ and electrochemical potential $\mathrm{qE^o}$ and written as,

$$\Delta E^0 = \mathrm{E_c} - \mathrm{qE^o} \quad (11)$$

The potential created at interface is (Al-Agealy, H.J., 2019).

$$\mathbb{V}_{SD}(\mathrm{E}) = \frac{(T_{SD}+(\mathrm{E_c}-\mathrm{qE^o}))^2}{4T_{SD}} \quad (12)$$

Inserting Eq.(12) in Eq.(10) to results

$$K_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{SD}k_BT}}\frac{l_e}{d_a^{2/3}(\frac{6}{\pi})^{1/3}}\int\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 e^{-\frac{\mathbb{V}_{SD}(\mathrm{E})}{k_BT}}\rho_S(E)\mathrm{F}_{(\mathrm{E})}dE \quad (13)$$

The electron transfer rate is decay with distance by constant β and given by (Saadon, A.K., 2020).

$$K_{et} = \frac{K_{ET}}{\beta} \quad (14)$$

Inserting Eq.(12) and (14) in Eq.(13) reduces to.

$$K_{et} = \frac{2\pi}{\hbar}\frac{1}{\beta}\sqrt{\frac{1}{4\pi T_{SD}k_BT}}\frac{l_e}{d_a^{2/3}(\frac{6}{\pi})^{1/3}}\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 e^{-\frac{(T_{SD}+(E_C-qE^0))^2}{4T_{SD}k_BT}}\int \rho_S(E)F_{(E)}dE \quad (15)$$

The solution integral in Eq.(15) results to (Blakemore, J.S., 1987).

$$\int \rho_S(E)F_{(E)}dE = n_s(E) \quad (16)$$

The electron transfer rate constant in Eq.(15) with Eq.(16) with concentration $n_s(E)$is reduced to

$$k_{et} = \frac{2\pi}{\hbar}\frac{n_s(E)}{\beta}\sqrt{\frac{1}{4\pi T_{SD}k_BT}}\frac{l_e}{d_a^{2/3}(\frac{6}{\pi})^{1/3}}\left|\langle H_{\frac{S}{D}}(E)\rangle\right|^2 e^{-\frac{(T_{SD}+(E_C-qE^0))^2}{4T_{SD}k_BT}} \quad (17)$$

The potential at contact for two materials estimates theoretically by using (Al-agealy, H.J., 2017).

$$\mathbb{V}_{SD}(E) = \frac{hc}{\lambda} - T_{SD} \quad (18)$$

Where $\boldsymbol{c}$ is the velocity of light and λ is the wave length of spectrum for dyes. The orientation energy of the solvent surrounded the system at new equilibrium of system is (AL-Agealy, H.J., 2020).

$$T_{SD}(eV) = \frac{e^2}{8\pi\epsilon_\circ}\left[\frac{1}{D}\left(\frac{1}{n^2}-\frac{1}{\epsilon_{so}}\right) - \frac{1}{2R}\left(\frac{n_S^2-n^2}{n_S^2+n^2}\frac{1}{n^2}-\frac{\epsilon_S^2-\epsilon^2}{\epsilon_S^2+\epsilon^2}\frac{1}{\epsilon^2}\right)\right] \quad (19)$$

Where e is electron charge, $\varepsilon_0$is permittivity D and R are radius of dye and distance between dye and semiconductor, n and ϵ_{so} are the optical and statistical dielectric constant of solvents n_s and ϵ_{sc} are s the refractive index and dielectric constant of the semiconductor. The radius of the dye molecule is (Al-Agealy, H.J., 2017).

$$D(m) = \left(\frac{3}{4\pi}\frac{M}{N\rho}\right)^{\frac{1}{3}} \quad (20)$$

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

Results

The electron transfer rate constant is evalulated theoretically depending on quantum theory and MATLAP program. The rate constant of electron transfer rate in N749 dye contact to ZnSe semiconductor was active effected by orientation energy. It is function of polarity of solvents and semiconductors, dielectric and refractive index. The radues of N749 dye estimates using Eq.(20) by inserting the molecular weight 781.73 $(g.mol^{-1})$ and mass density 0.749 g/cm^3 for N749 dye (Akhtaruzzaman, M., 2013), results and taken Avogadro's constant 6.02 $\times 10^{23}\ \frac{Molecule}{mol}$, results is D =7.45Å for N749. By same Eq. (20), the radi of ZnSe is 2.193 Å. with molecular weight 144.35and mass density 5.42 g/cm^3 from table (1).

Table 1. The main properties of ZnSe semiconductor (Weber, M.J., 2018), (Walker, A.B., 2002).

Properties	**ZnSe**
Molecular Weight	144.35
Crystal Structure	Cubic
Lattice Constant	5.6676 Å
Dielectric Constant	9.2
Band Gap	2.58 eV
Electron Mobility	540 cm^2/Vs
Hole Mobility	28 cm^2/Vs
Heat of Formation	422 kJ/mol
Thermal Expansion Coefficient	720 µm/m°C
Specific Heat Capacity	0.339 J/g°C
Thermal Conductivity	14 W/mK
Density	5.42 g/cm^3
Melting Point	1517°C
Refractive Index	2.89
Radii (Å)	2.193778

However, the evaluation of orientation energy for N749 dye contact to ZnSe System is a function of refractive index and dielectric constant of (chloroform, Morpholine, Acetic acid, Methyl Acetate, N-Methyl-2-Pyrrolldone, Butanol, Methanol Ethyl Ketene, Ethanol and Methyl alcohol) solvents and ZnSe semiconductor. The orientation energy are carried out using Eq.(19) with inserting the refractive index and dielectric constant of solvents from table (2) and refractive index and dielectric constant of ZnSe from table (1), results of orientation energy are listed in table(2).

Table 2. Results data of transition energy for N719/ZnSe system

Solvent type	Refrective index n (Smallwood, I.M. , 1997)	Dielectric constant ε (Smallwood, I.M. , 1997)	$T_{SD}(eV)$for ZnSe
chloroform	1.446	4.81	0.163453
Morpholine	1.4545	7.33	0.221400
Acetic acid	1.372	6.15	0.234680
Methyl Acetate	1.3593	7.3	0.263419
N-Methyl-2-Pyrrolldone	1.4700	32.2	0.315187
Butanol	1.397	17.51	0.320501
Methanol Ethyl Ketene	1.3788	18.8	0.332764
Ethanol	1.359	23.40	0.352563
Methyl alcohol	1.329	32.60	0.379665

On the other hand, for different values of electrochemical potential qE°(eV), we calculated the effected driving energy $\Delta E^0$for N719/ZnSe system using Eq.(11) with two values of conduction band $E_{CB}(ZnSe) = 2.82eV$ and $4.49eV$, results are listed in table (3)

Table 3. Data of the effective driving energy $\Delta E^0$for N719/ZnSe system

Electrochemical potential qE°(eV)	ΔE^0 **(eV) with** $E_{CB}(ZnSe) =$ $\mathbf{2.82}eV$	ΔE^0 **(eV) with** $E_{CB}(ZnSe) =$ $\mathbf{4.49}eV$
3.8	-0.98	0.69
3.6	-0.78	0.89
3.4	-0.58	1.09
3.2	-0.38	1.29
3	-0.18	1.49
2.8	0.02	1.69
2.6	0.22	1.89

Upon the results of effective driving energy in table (3) and orientation energy from table (2) we can using the Eq.(17) to calculate the electron transfer rate constant for N719/ZnSe system with taken the coupling strength $\langle \widehat{H}_{\frac{N3}{Se}} \rangle$ =2×10^{-2}eV/state, 4×10^{-2}eV/state, 6 x10^{-2}eV/ state, 8×10^{-2}eV/ state, 10×10^{-2}eV/ state and 12×10^{-2}eV/ state and 14×10^{-2}eV/ state (Lewis, N.S., 1998), effective length $l_{ecl} = 3A$ (Obeed, H.M., 2020), $n_s(E)$ for ZnSe semiconductor and β contact is and taken the effective driving force energy (ΔE^0(eV) = 0.22., 0.69, 1.29 and 1.89 eV) with using MATLAP program. Results are shown in tables (4) (5) (6) and (7) for taking driving force energy (ΔE^0 = 0.22., 0.69, 1.29 and 1.89 eV respectively.

Table 4. The present calculated of electron transfer rate constant for N719/ ZnSe at effective driving energy = **0.22**

solvent	$\mathbf{T_{\frac{N719}{Sem}}(eV)}$	**The current** $\boldsymbol{J(E)}$**e/ Sec**						
		$\langle \hat{C}_{St}(0) \rangle$**eV/ state**						
		$\mathbf{2\times 10^{-3}}$	$\mathbf{4\times 10^{-3}}$	$\mathbf{6\times 10^{-3}}$	$\mathbf{8\times 10^{-3}}$	$\mathbf{10\times 10^{-3}}$	$\mathbf{12\times 10^{-3}}$	$\mathbf{14\times 10^{-3}}$
chloroform	0.188708	1.3109E+13	2.6218E+13	3.9326E+13	5.2435E+13	6.5544E+13	7.8653E+13	9.1762E+13
Morpholine	0.246608	1.3696E+13	2.7392E+13	4.1088E+13	5.4784E+13	6.8480E+13	8.2176E+13	9.5871E+13
Acetic acid	0.261121	1.3182E+13	2.6365E+13	3.9547E+13	5.2729E+13	6.5912E+13	7.9094E+13	9.2276E+13
Methyl Acetate	0.290099	1.1690E+13	2.3380E+13	3.5070E+13	4.6760E+13	5.8450E+13	7.0140E+13	8.1830E+13
N-Methyl-2-Pyrrolldone	0.34036	8.6117E+12	1.7223E+13	2.5835E+13	3.4447E+13	4.3059E+13	5.1670E+13	6.0282E+13
Butanol	0.346776	8.3069E+12	1.6614E+13	2.4921E+13	3.3228E+13	4.1534E+13	4.9841E+13	5.8148E+13
Methanol Ethyl Ketene	0.359327	7.6242E+12	1.5248E+13	2.2873E+13	3.0497E+13	3.8121E+13	4.5745E+13	5.3370E+13
Ethanol	0.379445	6.5937E+12	1.3187E+13	1.9781E+13	2.6375E+13	3.2969E+13	3.9562E+13	4.6156E+13
Methyl alcohol	0.407018	5.3445E+12	1.0689E+13	1.6034E+13	2.1378E+13	2.6723E+13	3.2067E+13	3.7412E+13

Table 5. The present calculated of electron transfer rate constant for N719/ ZnSe at effective driving energy = **0.69**

solvent	$\mathbf{T_{\frac{N719}{Sem}}(eV)}$	**The current** $\boldsymbol{J(E)}$**e/ Sec**						
		$\langle \hat{C}_{St}(0) \rangle$**eV/ state**						
		$\mathbf{2\times 10^{-3}}$	$\mathbf{4\times 10^{-3}}$	$\mathbf{6\times 10^{-3}}$	$\mathbf{8\times 10^{-3}}$	$\mathbf{10\times 10^{-3}}$	$\mathbf{12\times 10^{-3}}$	$\mathbf{14\times 10^{-3}}$
chloroform	0.188708	4.6907E-03	9.3815E-03	1.4072E-02	1.8763E-02	2.3454E-02	2.8144E-02	3.2835E-02
Morpholine	0.246608	4.6187E+00	9.2375E+00	1.3856E+01	1.8475E+01	2.3094E+01	2.7712E+01	3.2331E+01
Acetic acid	0.261121	1.3265E+01	2.6529E+01	3.9794E+01	5.3058E+01	6.6323E+01	7.9588E+01	9.2852E+01
Methyl Acetate	0.290099	8.5905E+01	1.7181E+02	2.5771E+02	3.4362E+02	4.2952E+02	5.1543E+02	6.0133E+02
N-Methyl-2-Pyrrolldone	0.34036	9.1088E+02	1.8218E+03	2.7327E+03	3.6435E+03	4.5544E+03	5.4653E+03	6.3762E+03
Butanol	0.346776	1.1003E+03	2.2006E+03	3.3010E+03	4.4013E+03	5.5016E+03	6.6019E+03	7.7023E+03
Methanol Ethyl Ketene	0.359327	1.6514E+03	3.3029E+03	4.9543E+03	6.6058E+03	8.2572E+03	9.9086E+03	1.1560E+04
Ethanol	0.379445	2.9395E+03	5.8789E+03	8.8184E+03	1.1758E+04	1.4697E+04	1.7637E+04	2.0576E+04
Methyl alcohol	0.407018	5.6640E+03	1.1328E+04	1.6992E+04	2.2656E+04	2.8320E+04	3.3984E+04	3.9648E+04

Table 6. The present calculated of electron transfer rate constant for N719/ ZnSe at effective driving energy $= \mathbf{1.29}$.

solvent	$T_{\frac{N719}{Sem}}(eV)$	The current $J(E)$e/ Sec $\langle \hat{C}_{St}(0) \rangle$eV/ state						
		2×10^{-3}	4×10^{-3}	6×10^{-3}	8×10^{-3}	10×10^{-3}	12×10^{-3}	14×10^{-3}
chloroform	0.188708	7.8459E-40	1.5692E-39	2.3538E-39	3.1383E-39	3.9229E-39	4.7075E-39	5.4921E-39
Morpholine	0.246608	1.4105E-28	2.8209E-28	4.2314E-28	5.6418E-28	7.0523E-28	8.4628E-28	9.8732E-28
Acetic acid	0.261121	8.4387E-27	1.6877E-26	2.5316E-26	3.3755E-26	4.2193E-26	5.0632E-26	5.9071E-26
Methyl Acetate	0.290099	1.3680E-23	2.7361E-23	4.1041E-23	5.4721E-23	6.8402E-23	8.2082E-23	9.5762E-23
N-Methyl-2-Pyrrolldone	0.34036	2.3908E-19	4.7815E-19	7.1723E-19	9.5630E-19	1.1954E-18	1.4345E-18	1.6735E-18
Butanol	0.346776	5.3950E-19	1.0790E-18	1.6185E-18	2.1580E-18	2.6975E-18	3.2370E-18	3.7765E-18
Methanol Ethyl Ketene	0.359327	3.1739E-18	6.3479E-18	9.5218E-18	1.2696E-17	1.5870E-17	1.9044E-17	2.2218E-17
Ethanol	0.379445	4.1948E-17	8.3897E-17	1.2585E-16	1.6779E-16	2.0974E-16	2.5169E-16	2.9364E-16
Methyl alcohol	0.407018	8.9576E-16	1.7915E-15	2.6873E-15	3.5831E-15	4.4788E-15	5.3746E-15	6.2704E-15

Table 7. The present calculated of electron transfer rate constant for N719/ ZnSe at effective driving energy $= \mathbf{1.89}$

solvent	$T_{\frac{N719}{Sem}}(eV)$	The current $J(E)$e/ Sec $\langle \hat{C}_{St}(0) \rangle$eV/ state						
		2×10^{-3}	4×10^{-3}	6×10^{-3}	8×10^{-3}	10×10^{-3}	12×10^{-3}	14×10^{-3}
chloroform	0.188708	9.7207E-96	1.9441E-95	2.9162E-95	3.8883E-95	4.8603E-95	5.8324E-95	6.8045E-95
Morpholine	0.246608	3.2418E-71	6.4836E-71	9.7254E-71	1.2967E-70	1.6209E-70	1.9451E-70	2.2693E-70
Acetic acid	0.261121	2.5449E-67	5.0899E-67	7.6348E-67	1.0180E-66	1.2725E-66	1.5270E-66	1.7815E-66
Methyl Acetate	0.290099	2.9352E-60	5.8704E-60	8.8056E-60	1.1741E-59	1.4676E-59	1.7611E-59	2.0546E-59
N-Methyl-2-Pyrrolldone	0.34036	7.5294E-51	1.5059E-50	2.2588E-50	3.0118E-50	3.7647E-50	4.5176E-50	5.2706E-50
Butanol	0.346776	4.6355E-50	9.2711E-50	1.3907E-49	1.8542E-49	2.3178E-49	2.7813E-49	3.2449E-49
Methanol Ethyl Ketene	0.359327	2.4464E-48	4.8928E-48	7.3392E-48	9.7856E-48	1.2232E-47	1.4678E-47	1.7125E-47
Ethanol	0.379445	9.7803E-46	1.9561E-45	2.9341E-45	3.9121E-45	4.8902E-45	5.8682E-45	6.8462E-45
Methyl alcohol	0.407018	9.9439E-43	1.9888E-42	2.9832E-42	3.9776E-42	4.9720E-42	5.9664E-42	6.9608E-42

Discussion

The behaviour of electron transfer rate constant have been estimated and discussion theoretically according to the quantum theory. It is more interesting to consider that orientation energy as addition with coupling strength to the electron transfer rate constant in terms of Eq.(17). In that case the orientation energy is limited by the refractive index and dielectric constant for solvents and ZnSe semiconductor in N719/ ZnSe system.

Table (2) show the the orientation energy as function of refractive index and dielectric constant of solvents, it is decreased with increased dielectric constant from 4.81 to 32.60.

On the other hand, the orientation energy in table (2) increases and decreases alternatively upon the increased and decreased the refractive index of solvents . As seen as the orientation energy reach to upper values 0.379eV at dielectric constant 32.6 while has reach to lower values 0.163453 at dielectric constant 4.81. As well as, the electron rate constant in Tables (4), (5) and (6) and (7) for N719/ZnSe system increased with decreased driving energy from (0.22, 0.69, 1.29. and 1.89eV). In this tables, the influence of effective driving energy on electrontransfer rate constant appreciably to decreased largely. It influence the chemical potential of N719 molecule dye in table (3) decrease compare with conduction band of ZnSe semiconductor. The electron transfer rate constant in tables (4),(5),(6) and (7) show that the electron transfer rate constant increases with decreased the orientation energy at low effective driving energy ,this results indicates the system has less orientation energy re configuration the alignment energy levels of N719 dye and ZnSe semiconductor before electron transfer reaction. In fact, the electro transfer rate constant of N719/ZnSe system in Tables 4,5,6 and 7 as well as increases with increase the coupling strength. On the other hand, the electron transfer rate constant begin inversely behaviour when increased the effective driving energy from 0.96 to 1.89 eV, that's means the rate constant for electron transfer decreased with decreased the orientation energy for increased effective driving energy. This indicate the less electrons have large effective driving energy and can transfer from donor to acceptor. This means the electron transfer processes occurred in inverted Marcus region. Furthermore, the electron transfer occurred in normal region for

N719/ ZnSe system with Morpholine solvent while the electron transfer occurred in inverted Marcus region forN719/ ZnSe system with Methyl alcohol solvent.

Conclusion

We concluded the electron transfer rate constant behaviours in N719 contact to ZnSe semiconductor depending on orientation energy, effective driving energy and coupling strength. The orientation energy is force effected on the transfer rate constant according to re-configuration of energy levels of N719 dye and ZnSe semiconductor with each other. Additionally, the coupling strength effected to electron transfer rate increaselly for N719/ZnSe system. The electron transfer rate constant increased with decreased the orientation energy in normal region while the electron transfer rate increased with increased orientation energy in inverted Marcus region. The orientation energy and effected driving energy are limited the rate of electron transfer cross potential as results to effect on electronic density. Increased electronic transfer rate for decreased the effected driving energy in inverted Marcus region.

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