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Theory of Charge Transfer rate At Coumarin–$TiO_2$and Coumarin–SnO_2 systems

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Abstract:*This research aim to study the charge transfer at the coumarin dye-semiconductor interface devices depending on evaluation the electronic transfer rate constant. Quantum theory using here to calculation the reorientation energy, free energy and rate constant at both systems coumarin–$TiO_2$and* ***Coumarin–SnO_2****. Data results discussion to the benefit of using this system in many application on the environmental depending on the electronic transfer rate calculation in system and that's refers to the electric properties of system to using in technological applied and efficiency to using at cleaning electric power sources. Rate constant is evaluated depending on the estimation the reorientation energy , free energy , unit cell volume , penetration coefficient ,square overlapping coefficient, and temperature T using a MATLAB designed program . In two systems coumarin–$TiO_2$and* ***Coumarin–SnO_2*** *systems , the electronic transfer rate are increases with increases the reorientation energy and increases with effective free energy predictions.*

Keywords:*Electronic Transfer, rate constant , coumarin–$TiO_2$and coumarin–* ***SnO_2*** *systems.*

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I. Introduction

Increase problem for energy in many position of the world's and it was expecting to brought an explosive rise nergy consumption. That's lead the researcher to solving these problems be save the energy[1]. A study of this problem due to to electron transfer (ET) fields was essential in physical chemistry and biolo-physics, and in an emerging of electronics molecular field [2]. The electronic transfer nonadiabatically via quantum theory tunneling was characteristic of processing limiting from photosynthesis to conduction band through molecular ,a little knowledge is known about transfer by tunneling process[3]. In contrast, the fundamental theorey cornerstone for condensing phases charge transfer is laid due to Franck and Libby in 1952 . Nextly the description of transfer field had been taken by Rudy Marcus and Hash [4]. Many applied of semiconductor /dye system such that the solar cell that producing from traditional materials and DSSCs that studied alternatively because its low cost production , wide application and flexibility [4-5]. DSSC wasn't limited due to harvesting light ability for semiconductor. On the other hand the sensitization of semiconductors involving interfacial electron transfer following selective excitation of a surface-bound molecular chromophore [6]. The commonly interesting to studied chromophores, that's refers as sensitizers dyes ,its including organic molecules dye and compounds of transition metal coordination [7].

The study of electron transfer rates reactions at the electrode dye solution interface was afundamental basic in electrochemistry. The kinetics information of the reactions at the interface surface of the electrode was great important to understanding of the basic of kinetics heterogeneous electron transfer scenario[8]. A recent alternative embodiment of the DSC concept is the sensitized heterojunction usually with an inorganic wide band gap nanocrystalline semiconductor of n-type polarity as electron acceptor, the charge neutrality on the dye being restored by a hole delivered by the complementary semiconductor, inorganic [9] or organic [10] and of p-type polarity. Electronic transfer is on of the processes in the dye sensitized solar cells, and is of major importance for the overall performance. In this paper, we focus on study and evaluated the electron transfer rate in semiconductor -dye system ; this will be used coumarin–$TiO_2$and **Coumarin–SnO_2** systems.

II. Theory

The electronic transfer rate constant of the semiconductor - dye system state should be refers by probablity according to the quantum theory [11].

$$\mathcal{G}_{S,D} = \frac{4\pi^2}{h}\sum\left|H^{et}_{S,D}\right|^2 \mathcal{F}^{et}_{S,D} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where h is the Planck constant, $\mathcal{F}_{S,D}^{et}$ is the Franck–Condon probaplity ,and $\mathrm{H}_{S,D}^{et}$is the coupling coefficient between the semiconductor and dye states .
The Franck–Condon probaplity $\mathcal{F}_{S,D}^{et}$ in is given by
[12].

$$\mathcal{F}_{S,D}^{et} = \left(\frac{1}{4\pi T_{et}\, k_B T}\right)^{1/2} exp\left[-\frac{(E+T_{et})^2}{4T_{et}\, k_B T}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Where k_B is the Boltzmann constant , E is free energy, T_{et} is transfer energies and temperature T . The transfer energy T_{et} is an orientation energy of the system that's written by [13].

$$T_{et}\,(eV) = \frac{q^2}{8\pi\epsilon_\circ}\left[\frac{1}{D}\left(\frac{1}{n^2} - \frac{1}{\epsilon_{so}}\right) - \frac{1}{2d}\left(\frac{n_{Sc}^2 - n^2}{n_{Sc}^2 + n^2}\,\frac{1}{n^2} - \frac{\epsilon_{Sc}^2 - \epsilon_{so}{}^2}{\epsilon_{Sc}^2 + \epsilon_{so}{}^2}\,\frac{1}{\epsilon_{sc}{}^2}\right)\right] \ldots\ldots\ldots(3)$$

Where $\epsilon_\circ$ is the free permittivity , ϵ is the dielectric constant, n is the optical refractive index of the solvent, n_{Sc} **and** $\epsilon_{sc}$are the optical and static dielectric constant of the semiconductor, D is the rudii of the molecular dye, and d is the distance between the molecule and the semiconductor , and *q* is the charge of electrons. The radii of the dye molecule can be evaluated using [14].

$$D = \left(\frac{3}{4\pi}\,\frac{M}{N\rho}\right)^{\frac{1}{3}} \ldots\ldots\ldots\ldots\ldots\ldots\ (4)$$

Where the molecular weight M, ρ is the density and N is the number of Avogadro,.
Inserting Eq.(2) in Eq.(1) and given by.

$$\mathcal{G}_{S,D} = \frac{4\pi^2}{h}\sum\left|\mathrm{H}_{S,D}^{et}\right|^2\left(\frac{1}{4\pi T_{et}\, k_B T}\right)^{1/2} exp\left[-\frac{(E+T_{et})^2}{4T_{et}\, k_B T}\right] \ldots\ldots\ldots\ldots(5)$$

Due to the unit cell volume of semiconductor and with penetration of electronic transfer at solar cell we can write the rate [15].

$$\mathcal{G}_{S,D} = \frac{4\pi^2}{h}\,\frac{V}{\beta_S}\sum\left|\mathrm{H}_{S,D}^{et}\right|^2\left(\frac{1}{4\pi T_{et}\, k_B T}\right)^{1/2} exp\left[-\frac{(E+T_{et})^2}{4T_{et}\, k_B T}\right] \qquad \ldots\ldots\ldots\ (6)$$

Where the exponential function can be expanding to .

$$exp\left[-\frac{(E+T_{et})^2}{4T_{et}\, k_B T}\right] \approx exp^{-\frac{T_{et}}{4k_B T}}\left[1 - \left(\frac{E}{T_{et}} + 1\right)^2\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

Substituting Eq.(7) in Eq.(5) to results.

$$\mathcal{G}_{S,D} = \frac{4\pi^2}{h}\,\frac{V}{\beta_S}\sum\left|\mathrm{H}_{S,D}^{et}\right|^2\left(\frac{1}{4\pi T_{et}\, k_B T}\right)^{1/2} exp^{-\frac{T_{et}}{4k_B T}}\left[1 - \left(\frac{E}{T_{et}} + 1\right)^2\right] \ldots\ (8)$$

Where [11]

$$E = h\frac{c}{\lambda} - T_{et} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(9)$$

where $h = 6.6\mathrm{x}10 - 34\mathrm{J.sec}$ is Planck constant , c is the light velocity (3x 10^8m/sec), and ν is the frequency and equall to $\nu = \frac{c}{\lambda}$, λ is wave length for absorption spectra .

The coupling by coefficient matrix element is estimated by using [16].

$$\mathrm{H}_{S,D}^{et} = \mathrm{H}_{S,D}^{et}(0)\left(\frac{I_{sc}}{d_{sc}^{2/3}\left(\frac{6}{\pi}\right)^{1/3}}\right)^{\frac{1}{2}} \ldots\ldots\ldots\ldots\ldots\ldots\ (10)$$

Where I_{sc} is the effective coupling length, d_{sc} is the density of the atom that contributes to the density of states in the bond of concern, and $H_{DA}$is electronic parameter.

III. Results

Electronic transfer at solar cell have been studied a theoretically depending on calculation the electronic transfer rate for coumarin-TiO$_2$ and coumarin- SnO$_2$ sensitized dye solar cell systems . Reorientation energy,effective free energy and overlapping coupling constant are active coefficients controlling on the electronic transfer in sensitized dye solar cell. The electronic transfer as fulfillment to evaluation the reorientation energy for coumarin-TiO$_2$, coumarin- SnO$_2$ systems by using Eq.() and the physical properties for semiconductor and solvent in table (1) and (2) that are using in the present evaluation .

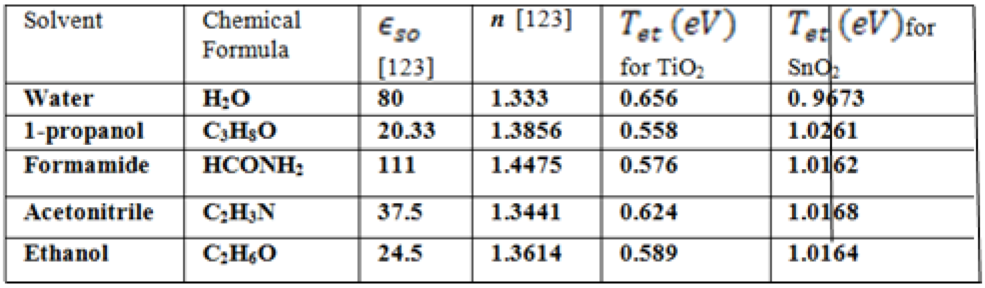
Table(1) The solvent properties

Solvent	Chemical Formula	Static dielectric constant ϵ_{so} [17]	Refrective index *n* [17]
Water	**H_2O**	**80**	**1.333**
1-propanol	**C_3H_8O**	**20.33**	**1.3856**
Formamide	**$HCONH_2$**	**111**	**1.4475**
Acetonitrile	**C_2H_3N**	**37.5**	**1.3441**
Ethanol	**C_2H_6O**	**24.5**	**1.3614**

Table (2) Common properties of semiconductor.

Semiconductor	Dielectric constant ϵ_{sc}	Refractive index n_{sc}	Energy gab (eV)	Lattice constant (nm)	Crystal structure
TiO_2	100[18]	2.609[19]	3.02[20]	*a* = 4.5936 *c* =2.9587[19]	Tetragonalrutile [19]
SnO_2	4.175 [21]	1.94[21]	3.45[21]	a=0.32495,c=o. 5206[21]	Wurtzite [21]

To estimation the transtion energies for dye-TiO$_2$, and dye-ZnO systems, one must initially evaluate the values of the radii of coumarin dye from Eq.(). Inserting of molecular weights $M_{co=}$334.35 [22], and densities ρ_{co}= 1.326 g/cm^3 [22], the values of the radii is $R_{Com} = 4.6423A^o$.Inserting the value of dielectric constant ϵ_{so} and refractive index *n* for variety solvent, and the dielectric constant $\epsilon_{sc}$and refractive index n_{Sc} for semiconductor in equation (2), with value of radii of dye and the distance between the molecule dye and semiconductor $d = R_{Com} + 1A^o$, the results have been summarized in table (3) for coumarin-TiO$_2$, coumarin-ZnO systems system.



Solvent	Chemical Formula	ϵ_{so} [123]	*n* [123]	$T_{et}\,(eV)$ for TiO$_2$	$T_{et}\,(eV)$for SnO$_2$
Water	**H_2O**	**80**	**1.333**	**0.656**	**0. 9673**
1-propanol	**C_3H_8O**	**20.33**	**1.3856**	**0.558**	**1.0261**
Formamide	**$HCONH_2$**	**111**	**1.4475**	**0.576**	**1.0162**
Acetonitrile	**C_2H_3N**	**37.5**	**1.3441**	**0.624**	**1.0168**
Ethanol	**C_2H_6O**	**24.5**	**1.3614**	**0.589**	**1.0164**

Table (3): The transfer energies $T_{et}\,(eV)$value for donor coumarin dye and acceptor semiconductor TiO$_2$ and Zn

Next , the parameter of the electronic transfer rate is effective driving energy E(eV) .It is supplied the solar cells by power according on the absorption of light. The effective driving energy EeV) is energy that's taking the electrons to cross interface from the molecule of dye state to the semiconductor state. It can be estimation by using Eq.(10), where the wave length for coumarin is taken (400–800) nm [23] and the reorentation energy taken account from table (3). The results of E(eV) for coumarin–TiO$_2$, and coumarin–SnO$_2$ system are listed in Tables (4), and (5) respectively

Table (4) Effective free energy E(eV) of the electronic transfer in coumarin–TiO$_2$ system for variety in solar cell.

SOLVENT	Effective free energy E(eV)				
	Wave length (nm)				
	$400\,nm$	$500\,nm$	$600\,nm$	$700\,nm$	$800\,nm$
Water	**-2.3944**	**-1.8270**	**-1.4134**	**-1.11802**	**-0.8964**
1-propanol	**-2.4544**	**-1.9236**	**-1.5100**	**-1.2146**	**-0.9930**
Formamide	**-2.5163**	**-1.9059**	**-1.49229**	**-1.1968**	**-0.9752**
Acetonitrile	**-2.4698**	**-1.8577**	**-1.4441**	**-1.1487**	**-0.9271**
Ethanol	**-2.4929**	**-1.8927**	**-1.4791**	**-1.1837**	**-0.9621**

Table (5) Effective free energy E(eV) of the electronic transfer in coumarin– SnO_2 system for variety in solar cell.

SOLVENT	Effective free energy E(eV)				
	Wave length(nm)				
	$400\ nm$	$500\ nm$	$600\ nm$	$700\ nm$	$800\ nm$
water	**-2.3881**	**-1.7677**	**-1.3540**	**-1.0586**	**-0.8370**
1-propanol	**-2.4895**	**-1.8691**	**-1.4555**	**-1.1600**	**-0.9385**
formamide	**-2.4721**	**-1.8517**	**-1.4381**	**-1.1427**	**-0.9210**
Acetonitrile	**-2.4199**	**-1.7995**	**-1.3859**	**-1.0905**	**-0.8690**
Ethanol	**-2.4568**	**-1.8364**	**-1.4228**	**-1.1273**	**-0.9058**

However ,the transfer rate is function of the unit cell volume of semiconductor that's shown in Eq.(10). The lattice constant for TiO_2 is a =b= 4.5936, c =2.9587[19] and a=b=3.2469 $\mathring{A}$ and c=5.2069 $\mathring{A}$ [122] lattice constant for ZnO semiconductor . The volume of TiO_2 is $V_{TiO_2} = 6.242 \times 10^{-23} cm^3$and for ZnO is $V_{ZnO} = 4.753 \times 10^{-23} cm^3$.

The electronic transfer rate constant could be calculation using Eq.(8) for coumarin–TiO_2 and coumarin–ZnO for variety solvents by substituting the reorientation energy$\Delta_{TE}\ (eV)$, effective free energy E (ev), unit cell , volume V(m^3), penetration coefficient β(m^{-1}) . A MATLAB soft ware programming have been used to calculation the electronic transfer rate constant for Tio_{2-} coumarin and ZnO- coumarin using Eq.(8), the results are tabulated in tables (6) and (7) for Tio_{2-} coumarin and ZnO- coumarin respectively.

Table (6) Electronic transfer rate constant $g_{S,D}\left(\frac{cm^4}{sec}\right)$ for coumarin–TiO_2 solar cell system. with variety solvents at coupling coefficient V_{DA} =4.032421511×$10^{-4}\ eV$

Solvent	Electronic transfer rate constant $g_{S,D}\left(\frac{cm^4}{sec}\right)$				
	Water	**1-propanol**	**Formamide**	**Acetonitrile**	**Ethanol**
λ =**400nm**	**1.006** $\times 10^{-42}$	**4.603** $\times 10^{-52}$	**4.551** $\times 10^{-50}$	**2.540** $\times 10^{-45}$	**1.098** $\times 10^{-48}$
λ =**500nm**	**1.6179** $\times 10^{-30}$	**7.048** $\times 10^{-36}$	**1.026** $\times 10^{-34}$	**5.521** $\times 10^{-32}$	**6.494** $\times 10^{-34}$
λ =**600nm**	**3.2278** $\times 10^{-24}$	**2.038** $\times 10^{-26}$	**1.049** $\times 10^{-27}$	**4.532** $\times 10^{-26}$	**3.207** $\times 10^{-27}$
λ =**700nm**	**8.0314** $\times 10^{-23}$	**1.019** $\times 10^{-24}$	**2.802** $\times 10^{-42}$	**2.646** $\times 10^{-23}$	**5.520** $\times 10^{-22}$
λ =**800nm**	**8.7429** $\times 10^{-22}$	**7.782** $\times 10^{-23}$	**1.423** $\times 10^{-22}$	**5.010** $\times 10^{-22}$	**2.112** $\times 10^{-22}$

Table (7) Electronic transfer rate constant $g_{S,D}\left(\frac{cm^4}{sec}\right)$ for coumarin–ZnO solar cell system. with variety solvents at coupling coefficient V_{DA} =4.032421511×$10^{-4}\ eV$

Solvent	**Water** $k_{ET}(cm^4/sec)$	**1-propanol** $k_{ET}(cm^4/sec$	**Formamide** $k_{ET}(cm^4/sec)$	**Acetonitrile** $k_{ET}(cm^4/sec$	**Ethanol** $k_{ET}(cm^4/sec)$
$\lambda =$**400nm**	**1.394** $\times 10^{-40}$	**1.769** $* 10^{-48}$	**6.666** $* 10^{-46}$	**9.422**$\times 10^{-42}$	**1.338**$\times 10^{-45}$
$\lambda =$**500nm**	**2.746** $\times 10^{-29}$	**1.074**$\times 10^{-33}$	**8.489**$\times 10^{-33}$	**1.789**$\times 10^{-30}$	**4.623**$\times 10^{-32}$
$\lambda =$**600nm**	**5.013**$\times 10^{-24}$	**1.541**$\times 10^{-27}$	**5.213** $\times 10^{-26}$	**1.118**$\times 10^{-25}$	**1.398**$\times 10^{-26}$
$\lambda =$**700nm**	**2.950** $\times 10^{-22}$	**1.260** $\times 10^{-24}$	**2.555**$\times 10^{-23}$	**1.382**$\times 10^{-23}$	**4.468**$\times 10^{-23}$
$\lambda =$**800nm**	**1.260** $\times 10^{-22}$	**2.969** $\times 10^{-22}$	**4.318** $\times 10^{-22}$	**9.554**$\times 10^{-22}$	**5.723**$\times 10^{-22}$

IV. Discussion

The kinetic of electronic transport in DSSC have been study according to quantum mechanical to transfer cross interface region at dye / semiconductor contact. At interface , the both wave functions are overlapping to enable more electron to transfer at interface. Due to transition theory postulate, the levels states of dye and semiconductor are brought to resonance state due to fluctuations of polarity medium surrounding dye /semiconductor system. Thats resonance is transition state of electronic reaction.

The rate constant $\mathcal{G}_{S,D}(\frac{cm^4}{sec})$ at interface of dye/semiconductor system in Eq.(8) refers to ability to electric transfer at solar cell system . The electrons cross over potential at interface when the the dye and semiconductor could be alignment in energy levels as result to different structures state and electronic density at dye surfaces and semiconductor conduction band. For both systems with more polar media like water and Acetonitrile , the transtion energy was large for more polar compare to less polar solvents have small values, this indicates that transition energy dependent on the polarity function . Tables (3) show that transition energy was lower in less polar media for coumarin–semiconductor system. Consequently ,the transfer occurs most probable in polar media like Water, Acetonitrile and Formamide, one of the most polar solvents $\epsilon_{so} = 111$ give small transition energy for both systems as compared with other solvents media that have less than dielectric constant, this indicates that Formamide have large refrective index $n = 1.4475$ a compared to other media. This is a reason for less transtion energy and low value electronic rate constant for dye /semiconductor system that's shown in tables (6-7). The transition energy were agreement to experimental value of $T_{et}\,(eV) = 0.7\ eV and\ 0.8\ eV$ [12], and $T_{et}\,(eV) = 0.5\ eV$ [24]. On the other hands, the transfer overlapping $\mathrm{T}_{Dye/Sem}$ are a controls coefficient to transition processes between dye/semiconductor system and its limited the type of transfer that's means a non adiabatic electronic transition reactions. However , the electronic rate constant was large for dye/semiconductor system have polar solvent and its higher for coumarin-ZnO comparing with coumarin-TiO_2 dye and electronic transfer occurs activity with polar media.

Tables (4) to (5) show negative results for driving free energies ,this refers to the driving free energies was a part of the work which could be broken to reorientation the system to transfer. The tables (4) to (5) and Eqs. (1-9) show that driving force dependent on the transition energies and absorption spectrum . Tables (6) to (7) show that the electronic rate constant increases with decrease of the driving force energy and vice versa. Upon this energy, the electrons would be transfer at dye /semiconductor system until the energy equals Fermi energy.

V. Conclusion

In summary, we conclusion that SC system has a good conversion solar energy into electric power without any effect on the environmental . Solar cell system is a tool of energy technology devices to voiding defect in nature. The transition of electronic reactions is strongly depending on the polarity media. For more polar media, the transtion energies is larger than less polarity.The electronic transition rate was large in both systems (dye –semiconductor) with media have large polarity than these less polarity. Electronic transition rate was large in coumarin–ZnO solar cell compare with the other media and indicates the coumarin dye was reactive towards ZnO than TiO_2. This because the different in density of states at semiconductor and proportional with the volume of semiconductor.

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