

Calculate of the Rate Constant of Electron Transfer in TiO_2 – Safranine Dye System

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Abstract

A theoretical calculations of the rate constant of electron transfer (ET) in a dye – semiconductor system with variety solvent are applied on system contains safranineT dye with TiO_2 in many solvents like water, 1-propanol, Formamide, Acetonitrile and Ethanol.

A matlab program has been written to evaluate many parameters such that, the solvent reorganization energy, effective free energy, activation free energy, coupling matrix element and the rate constant of electron transfer.

The results of the rate constant of electron transfer calculated theoretically are in a good agreement with experimental and theoretical values of other research.

Key Words: electron transfer, dye-semiconductor, quantum mechanical theory

Introduction

Electron transfer (ET) reactions represented a simple process which occurs in donor-acceptor system molecules. The transfer of a single electron from an atom or a molecule to another is considered to be the most elementary chemical and biological reaction. In general, reactions which involve the transfer of an electron are called redox reactions. It should be noted that the particle that is actually transferred in redox reactions need not always be just a single electron. Electron transfer forms the basis of conventional color photography; the absorption of light by an organic dye placed on a small silver halide semiconductor crystal induces the transfer of an electron from the dye to the crystal [1]. Electron transfer can be optically or /and thermally activated and triggers photosynthesis, metabolism, polymerization reactions, electrochemical reaction, etc. Several theories for ET at different levels of sophistication have been developed. The most generally useful theoretical frame work for thinking about electron transfer is Marcus theory [2]. The field of ET has grown enormously since both in the experimental and theoretical sphere. A substantial amount of work had been devoted to the photoinduced ET step in photosynthetic reaction centra of several organisms. Many studies have also been conducted on

photoinduced ET in compounds that are much simpler than the active part of biological reaction centra. A relatively new field in which ET plays a role is molecular electronics . This subject has evolved during the 1980's as scientists and technologists have become aware of the potential applications of organic materials. One may think of electrically conducting wires, memories, electronic switches, rectifiers, light –sensitive detectors, electroluminescent device and photoconductors [1].

In our research we have calculated the rate constant of electron transfer in safranin dye with TiO_2 semiconductor system in variety solvent like water, 1-propanol, Formamide, Acetonitrile and Ethanol, by using a theoretical model that derived on this system depending on quantum mechanical and golden rule expression model applied theoretically system with many solvents like water, 1-propanol, Formamide, Acetonitrile and Ethanol.

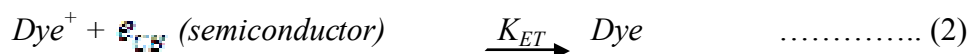
Theoretical model

The dye should absorb light and upon excitation .This photo excitation of dye leads to well defined change in their redox.



Where h is plank constant , ν_f is frequency

Photoexcitation of dye molecules dispersed on the surface of band gap semiconductor, results in ejection of electrons from the excited dye (Dye^*) to the conduction band or energetically accessible surface electronic state of semiconductor.



Where the e_{CB} represents the electron ejected from the excited dye molecule to the conduction band. In addition, the dye should be located close to the semiconductor, otherwise luminescence or nonradiative decay takes place instead of electron injection from the excited molecule [3].

A dye couple to semiconductor is an excellent model for processes that occur in the ET fields. The dye should absorb light promotes an electron from the ground state of the dye located in the semiconductor energy gap into an excited state that is in resonance with the conduction band (CB). Typically, the dye excited state is well inside the conduction band [4].

Light excites the dye molecules from the ground state, which is located energetically in the semiconductor band gap, to an excited state resonant with the TiO_2 conduction band, Figure (1) shows the energy level Jobloniske diagram [4].

We have applied the theoretical model that suggested for ET on the dye and metal oxide which are the main focus in this research.

Under this discussion the Hamiltonian of the acceptor /donor system is given by [5]

$$\hat{H} = \hat{H}_D + \hat{H}_A + \hat{H}_{DA} \quad \dots\dots\dots (3)$$

This operator obeys the Schrodinger equation [6]

$$i\hbar \frac{\partial}{\partial t} |\psi, t\rangle = \hat{H} |\psi, t\rangle \quad \dots\dots\dots (4)$$

The probability of transfer is [7]

$$k_{ET} = \frac{P_{tr}(t)}{t} = \frac{2\pi}{\hbar} |V_{DA}|^2 \rho(E) \quad \dots\dots\dots (5)$$

Where $P_{tr}(t)$ is the probability of ET, t is the time, V_{DA} is the Coupling coefficient of ET, $\rho(E)$ is the density of state.

We consider a donor ($|D\rangle$) or acceptor ($|A\rangle$) are a continuum levels the rate constant for ET can then be written as [8]

$$k_{ET} = \frac{4\pi^2}{\hbar} \frac{v}{\beta_S} \frac{1}{\sqrt{4\pi\lambda k_B T}} e^{-\frac{(\lambda + \Delta G^\circ)^2}{4\lambda k_B T}} \int \frac{(|V_{(E,r)}|^2) e^{-\frac{-(E-E^\circ)^2}{k_B T}}}{\rho(C) f_{(C)} dC} \rho(E) dE \quad \dots(6)$$

where, $\hbar$ is Planck constant, λ is reorganization energy, ΔG° is the effective free energy, k_B is Boltzman constant, T is the absolute temperature, $V_{(E,r)}$ is Coupling coefficient, $f_{(E)}$ is Fermi energy, β_S is the decay constant, v is volume of unit cell. The reorganization energy can be derived by treating the solvent as a dielectric continuum and given by [9].

$$\lambda_{out} = \frac{1}{2} \frac{q^2}{4\pi\epsilon_0} \left[\frac{1}{D} \left(\frac{1}{n^3} - \frac{1}{\epsilon} \right) - \frac{1}{2R} \left(\frac{n_{sc}^2 - n^2}{n_{sc}^2 + n^2} \frac{1}{n^3} - \frac{\epsilon_{sc}^2 - \epsilon^2}{\epsilon_{sc}^2 + \epsilon^2} \frac{1}{\epsilon^3} \right) \right] \quad \dots\dots\dots (7)$$

Where ϵ_0 is the vacuum permittivity, ϵ is the static dielectric constant of solvent, n is the refractive index of the solvent, n_{sc} is the refractive index of the semiconductor, ϵ_{sc} dielectric constant of the semiconductor, D is the radius of the molecular dye, and R is the distance between the complex and the semiconductor, and q is the charge of electron. The radius of the dye molecule can be evaluated from the apparent molar volumes using spherical approach [10].

$$\frac{4}{3}\pi D^3 = \frac{M}{N_A \rho} \quad \dots\dots\dots (8)$$

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

Where $(|V_{(E,r)}|^2)$ is an averaged coupling electronic matrix elements square [11]

$$\langle |V_{(E,r)}|^2 \rangle = \frac{|V_{(E,r)}|^2 \int f_{(E)} \rho(E) dE}{\int f_{(C)} \rho(C) dC} \quad \dots\dots\dots (9)$$

$$k_{ET} = \frac{4\pi^2 \nu}{h \rho_s} \frac{1}{\sqrt{4\pi\lambda k_B T}} e^{-\frac{(\lambda + \Delta G_s)^2}{4\lambda k_B T}} (|V_{(sr)}|^2) \quad \dots\dots\dots (10)$$

Where ΔG_s effective free energy is given by[7]

$$h\nu_f - \lambda - \Delta G_s \quad \dots\dots\dots (11)$$

The volume of unit cell for semiconductor v is given by [12]

$$v = abc \quad \dots\dots\dots (12)$$

Where a, b, and c are lattice constant of semiconductor.

The coupling electronic matrix elements can be evaluated by the expression [13]:

$$H_{DA} = H_{DA} \sqrt{\frac{I_{sc}}{d_{sc}^2 \epsilon (\frac{\epsilon_s}{\epsilon_0})^{1/2}}} \quad \dots\dots\dots (13)$$

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 the electronic parameter.

The average of the square of the coupling which is then multiplied by the volume to yield the total coupling coefficient that's mean.

$$V_{(sr)} = V_{DA} = H_{DA} v = H_{DA} \sqrt{\frac{I_{sc}}{d_{sc}^2 \epsilon (\frac{\epsilon_s}{\epsilon_0})^{1/2}}} v \quad \dots\dots\dots (14)$$

Results

The ET rate constant is determined theoretically, using quantum mechanical theory and the Golden Rule by many parameters; the value of the reorganization energy of the electron donor (D) and acceptor (A) required upon ET, activation free energy ΔG^* , the effective free energy ΔG_s , and the coupling coefficient matrix element of ET, V_{DA} between two sites donor and acceptor. One initial we have been evaluated the reorganization energy for the safraninT dye with TiO_2 system by using equation(7) with values of $n_{sc} = 2.438$ [14], $\epsilon_{sc} = 100$ [15], $D = 4.4782 \text{ \AA}$, $R = 5.4782$, and ϵ, n from table (1), the results tabulated in table(1)

The driving force, $\Delta G_s (\text{eV})$ that is provided by the absorption of light in Dye–Semiconductor interface system that is shown from equation (11). The values of the free energy ΔG_s can be calculated for safranin T, TiO_2 system by taking the difference between the reorganization energy (λ) and the absorption energy, where $h\nu$ is the absorption energy were

taken from the absorption spectral of safranin T [16], h , Plank constant ($h=6.626 \times 10^{-34} \text{ J.s}$), ν_f is the frequency that equals (= velocity of light / wave length),

wave length of safranin -T is taken from absorption spectra (400–800) nm [14], The results obtained are summarized in table (2).

The electron is transfer occurs when its energy is sufficient to exceeded the potential barrier represented by the activation free energy $\Delta G^* (\text{eV})$ that is evaluated by inserting the data of the reorganization λ from table (1)[17], and the effective free energy from table (2), in to equation (10), one immediately obtains the values of the activation free energy ΔG^* , the values are listed in table (3), for safranin T– TiO₂ system with variety solvent. Another important quantity that can be calculated theoretically is the electronic coupling term, V_{DA} , which describes the overlap integral of the donor and the acceptor state [18].

For the semiconductor –dye system the coupling matrix element coefficient can be calculated by using equation (14). Inserting the values of $d_{sc} = 3 \times 10^{-8} \text{ cm}$ [13], $I_{sc} = 2.77 \times 10^{22} \frac{\text{photons}}{\text{cm}^2}$ [13], and atypical values of ($H_{DA}=5, 10, 15, 20 \text{ cm}^{-1}$) that assumes in equations (13)and (14), you can evaluate the value of the coupling coefficient, the results are listed in table (4).

The rate constant of ET is depending on the volume of the unit cell through depending on the number of electron density that is proportional with volume by relation [17]. The volume of unit cell is evaluated from equation (12) for any semiconductor with $a= b=4.570 \text{ \AA}$ and $c=2.989 \text{ \AA}$ [19]for TiO₂ semiconductor. The results of the volume of unit cell for TiO₂ is $V_{TiO_2} = 6.242 \times 10^{-23} \text{ cm}^3$

substitution of these parameters as data into a designed program to calculate the rate constant of ET through the solution of the theoretical model equation. These parameters have been calculated theoretically with distance R is taken ($1 \text{ \AA}^{-1}$). A matlab program is written to compute the parameters that's leading to the evaluation of the rate constant of ET in ST– TiO₂ using equation (10), the results are tabulated in tables (4) to (8).

Discussion

The electron transport mechanism in dye –semiconductor has been described in term of a quantum mechanical model to transfer across the tunneling region between dye and semiconductor that is created when the semiconductor is brought to contact with dye. In this region /tunneling, the tail of the wave functions for dye and semiconductor over lap. In order for electron tunneling between dye and semiconductor to occur, the initial and final electronic states should have approximated equal energies that happen when consider the dye–semiconductor system interfaces involves the continuum of electronic states.

According to a fundamental postulate of ET theory, these two states are brought into resonance by fluctuations of polar medium surrounding dye and semiconductor system. This resonance is the transition state of ET reaction.

The transfer matrix element (coupling coefficient) V_{DA} , hence controls the dynamics of transition between the donor and acceptor or dye–semiconductor system and is therefore of our interest, it is this matrix element that enters into the expression for the rate of non adiabatic ET reactions. Hence, the typical of the square values of the coupling coefficient (matrix element) can be expected to be in the range $10^{-6} - 10^{-7} (eV)^2$ for such system.

ET rates were determined by electronic coupling matrix element V_{DA} between the dye molecule and conduction band (CB) of the semiconductor, the driving force energy (effective free energy $\Delta G_0 (eV)$), activation free energy $\Delta G^* (eV)$, volume of the unit cell $v (cm^3)$, and the solvent reorganization energy $\lambda (eV)$.

The rate of ET values that calculated theoretically is listed in tables (4) to (8) for ST–TiO₂/ system with variety solvent like Water, 1– Propanol, Formamide, Acetonitrile, and Ethanol.

From these results ET occurs in system with most polar solvents like water and Acetonitrile. The solvent reorganization energy are large for more polar solvents and small values for less polar solvents, this indicates that the reorganization energy is dependent on the polarity of the solvents. The values of the solvent reorganization energy that were calculated theoretically were fitting the experimental value $\lambda = 0.7 eV$ and $0.8 eV$ [18], and $\lambda = 0.5 eV$ [20].

The rate constant value that is calculated shows large values for dye –semiconductor system with most polar solvent and high value for safranin T–semiconductor system, this indicates that the ST dye is more reactive towards semiconductor than coumarin dye and ET occurs activity with polar solvents. Table (9) shows the results of rate constant which are in a good agreement with the experimental value rate constant .

Conclusion

In summary, it can be concluded from the present results that.

I– theoretical model was suggested for ET in dye –semiconductor interface provides an excellent model for studying the transfer of electron through the results of this model as fitting with experimental value.

II–The reactions of ET strongly depends on the solvent polarity. For more polar solvents, the reorganization energies are large and small values for less polar solvents, this indicates that, the reorganization energy dependent on polarity of the solvent.

III– The rate constant of ET is large in (dye –semiconductor) system with solvent more polar than less polar.

IV– The rate constant of ET is large in safranin T– semiconductor ,this indicates the safranin T dye is more reactive towards semiconductor .

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Table (1): the reorganization energies value for donor ST dye and acceptor semiconductor TiO₂

Solvent	Chemical Formula	ϵ [14]	n [14]	(Our resoult) λ (eV) for TiO ₂
Water	H ₂ O	80	1.333	0.6798942561
1-propanol	C ₃ H ₈ O	20.33	1.3856	0.5795911754
Formamide	HCONH ₂	111	1.4475	0.5978483206
Acetonitrile	C ₂ H ₃ N	37.5	1.3441	0.6480338344
Ethanol	C ₂ H ₆ O	24.5	1.3614	0.6116580688

Table (2): the effective free energy ΔG^*_{eff} (eV) for safranin T–TiO₂ system with variety solvent at wave length (λ) (400–800)nm

SOLVENT	ΔG^*_{eff} for $\lambda = 400nm$	ΔG^*_{eff} for $\lambda = 500nm$	ΔG^*_{eff} for $\lambda = 600nm$	ΔG^*_{eff} for $\lambda = 700nm$	ΔG^*_{eff} for $\lambda = 800nm$
Water	-2.4221656689	-1.8017536839	-1.3881456939	-1.0927114153	-0.8711357064
1-propanol	-2.5224687496	-1.9020567645	-1.4884487745	-1.1930144959	-0.9714387870
Formamide	-2.5042116044	-1.8837996194	-1.4701916294	-1.1747573350	-0.9531816419
Acetonitrile	-2.4540260906	-1.8336141056	-1.4200061156	-1.1245718370	-0.9029961281
Ethanol	-2.4904018562	-1.8699898712	-1.4563818812	-1.1609476026	-0.9393718937

Table (3): The activation free energy ΔG^* (eV) for safranin T–TiO₂ system with variety solvents at wave length (λ) (400–800)nm

SOLVENT	ΔG^* for $\lambda = 400nm$	ΔG^* for $\lambda = 500nm$	ΔG^* for $\lambda = 600nm$	ΔG^* for $\lambda = 700nm$	ΔG^* for $\lambda = 800nm$
water	1.11616977517	0.46278100030	0.18444783679	0.062663423547	0.013448154614
1-propanol	1.62820511577	0.75437450925	0.35629516559	0.162307582500	0.066229679289
Formamide	1.51970861371	0.69150932018	0.31821735641	0.139175781600	0.052798412612
Acetonitrile	1.258270732310	0.54225586105	0.22990358346	0.087606717384	0.025078077622
Ethanol	1.442668052168	0.64717487014	0.29164918917	0.123320122540	0.043895583380

Table (4): The coupling coefficient value that is calculated for semiconductor dye system

V_{DA} (eV)	V_{DA} (eV)	H_{DA} (eV)	V_{DA}^3 (eV ³)	V_{DA}^2 (eV ²)
$V_{DA1} = -3.25244$	$4.032421511 \times 10^{-22}$	5	$V_1 = 3.18586082 \times 10^{-12}$	$1.626042324 \times 10^{-11}$
$V_{DA2} = -6.50486$	$8.064824289 \times 10^{-22}$	10	$V_2 = 6.371721642 \times 10^{-12}$	$6.504139082 \times 10^{-11}$
$V_{DA3} = -9.75730$	$1.209723643 \times 10^{-21}$	15	$V_3 = 9.557582465 \times 10^{-12}$	$1.463431293 \times 10^{-10}$
$V_{DA4} = -13$	$1.612964833 \times 10^{-21}$	20	$V_4 = 1.274344329 \times 10^{-11}$	$2.601655551 \times 10^{-10}$

Table (5): The rate constant of electron transfer at Safranin T-TiO₂ system with variety solvents at coupling coefficient $V_{DA} = 4.032421511 \times 10^{-22}$ eV

Solvent	Water	1-propanol	Formamide	Acetonitrile	Ethanol
400	$8.542250641 \times 10^{-23}$	$1.17833068 \times 10^{-22}$	$8.898357073 \times 10^{-23}$	$2.974730921 \times 10^{-22}$	$1.917267125 \times 10^{-22}$
500	$1.914687409 \times 10^{-22}$	$1.78344521 \times 10^{-22}$	$2.170726702 \times 10^{-22}$	$8.16394338 \times 10^{-21}$	$1.264196539 \times 10^{-21}$
600	$1.30990681 \times 10^{-22}$	$1.46759453 \times 10^{-22}$	$6.627515407 \times 10^{-23}$	$2.177784004 \times 10^{-22}$	$1.896392603 \times 10^{-22}$
700	$1.709433055 \times 10^{-22}$	$3.42944051 \times 10^{-22}$	$8.54321766 \times 10^{-23}$	$6.45601581 \times 10^{-22}$	$1.59958876 \times 10^{-22}$
800	$1.224077414 \times 10^{-22}$	$1.60531287 \times 10^{-22}$	$2.704892721 \times 10^{-22}$	$7.866342259 \times 10^{-22}$	$3.818116749 \times 10^{-22}$

Table (6): The rate constant of electron transfer at Safranine T–TiO₂ system with variety solvents at coupling coefficient $V_{DA} = 8.064824289 \times 10^{-3} \text{ eV}$

Solvent/ λ nm	Water	1-propanol	Formamide	Acetonitrile	Ethanol
400	$3.416884384 \times 10^{-22}$	$4.713300824 \times 10^{-22}$	$3.55932646 \times 10^{-22}$	$1.189886841 \times 10^{-22}$	$7.669038875 \times 10^{-22}$
500	$7.658714059 \times 10^{-22}$	$7.133744944 \times 10^{-22}$	$8.682866877 \times 10^{-22}$	$3.265562184 \times 10^{-22}$	$5.056762667 \times 10^{-22}$
600	$5.239599985 \times 10^{-22}$	$5.870350983 \times 10^{-22}$	$2.650993971 \times 10^{-22}$	$8.71109555 \times 10^{-22}$	$7.585538172 \times 10^{-22}$
700	$6.837700122 \times 10^{-22}$	$1.371769844 \times 10^{-22}$	$3.417271311 \times 10^{-22}$	$2.58237568 \times 10^{-22}$	$6.370325446 \times 10^{-22}$
800	$4.896286913 \times 10^{-22}$	$6.421221659 \times 10^{-22}$	$1.081952113 \times 10^{-22}$	$3.146522287 \times 10^{-22}$	$1.527239605 \times 10^{-22}$

Table (7): The rate constant of electron transfer at Safranine T–TiO₂ system with variety solvents at coupling coefficient $V_{DA} = 1.209723643 \times 10^{-3} \text{ eV}$

Solvent/ λ nm	Water	1-propanol	Formamide	Acetonitrile	Ethanol
400	$7.68989861 \times 10^{-22}$	$1.06492685 \times 10^{-22}$	$8.008484413 \times 10^{-22}$	$2.677245391 \times 10^{-22}$	$1.725532397 \times 10^{-22}$
500	$1.757168651 \times 10^{-22}$	$1.605092612 \times 10^{-22}$	$1.953645018 \times 10^{-22}$	$7.347514911 \times 10^{-22}$	$1.1377716 \times 10^{-22}$
600	$1.178909996 \times 10^{-22}$	$1.32082891 \times 10^{-22}$	$5.964736343 \times 10^{-22}$	$1.959996498 \times 10^{-22}$	$1.706745414 \times 10^{-22}$
700	$1.538482602 \times 10^{-22}$	$3.086482148 \times 10^{-22}$	$7.688860331 \times 10^{-22}$	$5.8103868 \times 10^{-22}$	$1.433323225 \times 10^{-22}$
800	$1.101664555 \times 10^{-22}$	$1.444774873 \times 10^{-22}$	$2.434392216 \times 10^{-22}$	$7.079675143 \times 10^{-22}$	$3.436289111 \times 10^{-22}$

Table (8): The rate constant of electron transfer at Safranine T–TiO₂ system with variety solvents at coupling coefficient $V_{DA} = 1.612964833 \times 10^{-3} \text{ eV}$

Solvent/ λ nm	Water	1-propanol	Formamide	Acetonitrile	Ethanol
400	$1.366753711 \times 10^{-22}$	$1.8853271 \times 10^{-22}$	$1.423730539 \times 10^{-22}$	$4.759547215 \times 10^{-22}$	$3.067613054 \times 10^{-22}$
500	$3.063485527 \times 10^{-22}$	$2.853497888 \times 10^{-22}$	$3.473146642 \times 10^{-22}$	$1.306224833 \times 10^{-22}$	$2.022705003 \times 10^{-22}$
600	$2.095839928 \times 10^{-22}$	$2.348140319 \times 10^{-22}$	$1.060397555 \times 10^{-22}$	$3.484438111 \times 10^{-22}$	$3.03443974 \times 10^{-22}$
700	$2.735508000 \times 10^{-22}$	$5.487079205 \times 10^{-22}$	$1.366908481 \times 10^{-22}$	$1.032957582 \times 10^{-22}$	$2.548130099 \times 10^{-22}$
800	$1.958514703 \times 10^{-22}$	$2.568488583 \times 10^{-22}$	$4.327808314 \times 10^{-22}$	$1.258608897 \times 10^{-22}$	$6.108958229 \times 10^{-22}$

Table (9): compared between our results and experimental and theoretical research for dye -semiconductor

System	Theoretical k_{ET}	Experimental k_{ET}
Si/viologen dye	$1.3-1.6 \times 10^{-16}$ [20]	0.6×10^{-16} [21]
InP/Me ₂ Fe	$0.084-0.086 \times 10^{-16}$ [20]	$1-2 \times 10^{-16}$ [22]
Si/viologen dye	$1.2-1.9 \times 10^{-16}$ [18]	0.6×10^{-16} [18]
Si/ Me ₂ Fe	$0.024-1.7 \times 10^{-16}$ [18]	1×10^{-16} [18]
InP/Me ₂ Fe	$0.017-1.1 \times 10^{-16}$ [18]	
ST– TiO ₂	$1.2 \times 10^{-20}-3.4 \times 10^{-24}$ (our result)	
ST– TiO ₂	1.10166×10^{-20} (our result)	
ST– TiO ₂	1.53848×10^{-21} (our result)	
ST– TiO ₂	1.43332×10^{-22} (our result)	
ST– TiO ₂	3.08648×10^{-23} (our result)	
ST– TiO ₂	1.9599×10^{-24} (our result)	
ST– TiO ₂	3.0344×10^{-25} (our result)	

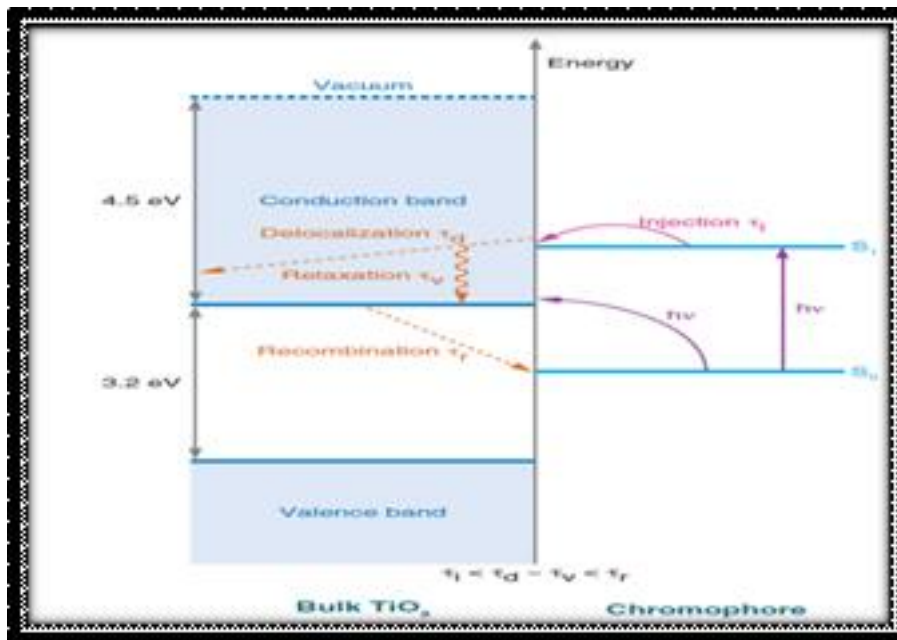


Fig. (1): The energy level Jobloniske diagram [4].

حساب معدل الانتقال الالكتروني في نظام TiO_2 صبغة السافرانين

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استلم البحث في: 28، ايلول، 2009

قبل البحث في: 13، اذار، 2011

الخلاصة

الحسابات النظرية لمعدل الانتقال الالكتروني في نظام صبغة-شبة الموصل لمذيبات مختلفة، طبقت على نظام يحتوي على صبغة السافرانين (ST) و شبة موصل TiO_2 ولمذيبات مختلفة مثل: الماء، و 1-بروبانول، و الفورماميد، و اسيتونترايل، و الايثانول. كُتب برنامج ماتلاب لحساب معاملات مختلفة، مثل: طاقة اعادة الانتظام، و الطاقة الحرة المؤثرة، والطاقة الحرة الفعالة، ومصفوفة العوامل المرتبطة، و معدل الانتقال الالكتروني. النتائج لمعدل الانتقال الالكتروني المحسوبة نظريا كانت ذا تطابق جيد مع نتائج حسابات البحوث العملية والنظرية. الكلمات المفتاحية: الانتقال الالكتروني، صبغة-شبة موصل، نظرية الميكانيك الكمي

