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A Theoretical Investigation of Charge Transfer Dynamics from Sensitized Molecule D35CPDT Dye to SnO_2 and TiO_2 Semiconductor

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Abstract

In this research, the dynamics process of charge transfer from the sensitized D35CPDT dye to tin(iv) oxide(SnO_2) or titanium dioxide (TiO_2) semiconductors are carried out by using a quantum model for charge transfer. Different chemical solvents Pyridine, 2-Methoxyethanol. Ethanol, Acetonitrile, and Methanol have been used with both systems as polar media surrounded the systems. The rate for charge transfer from photo-excitation D35CPDTdye and injection into the conduction band of SnO_2 or TiO_2 semiconductors vary from a $\sim 10^{-26}$ to $\sim 10^{-29}$ for system and from a $\sim 10^{-52}$ to $\sim 10^{-56}$for the system, depending on the charge transfer parameters strength coupling, free energy, potential of donor and acceptor in the system. The charge transfer rate in D35CPDT / SnO_2 the system is larger than the rate in D35CPDT/ TiO_2 a system depending on transition energy and driving energy. However, the charge transfer for both systems to be large is associated with large transition energy, decreasing driving energy and potential, and increasing strength coupling with Methanol solvent.

Keywords: Charge transfer dynamics , Sensitized D35CPDT Dye , SnO_2 , TiO_2.

1. Introduction

Recently, the energy demand becomes increasingly become one of most problems because of the increased requirements in modern life. Photovoltaic and solar cell technology is utilized to convert solar energy to electric energy [1]. The dye-sensitized solar cell DSSC is the main promising renewable device because of the low cost and good conversion efficiency [2]. The molecules electronics are cooperated with solid materials to be used in various devices because they are easily fabricated and cheap [3]. Since O’Regan and Gratzel introduced a work in1990s,dye-sensitized solar cell DSSCs are attracting more attention to convert light to electricity at a low cost [4]. The dye-sensitized had been excitation by light-induced due to absorbed light and the electrons will be transferred from the dye to the conduction band of the semiconductor[5]. The electron transfer process is an important fundamental reaction in different devices and dye-sensitized solar cell devices[6]. It occurs by thermal excitation and photo inducement [6]. A basic classical theory for the charge transfer process was introduced by Rudolph Marcus to describe the transfer between two states donor and acceptor and was awarded Nobel Prize in 1992 [7]. The dye-sensitized had been excited by light-induced due to absorbed light, and the electrons will be transferred from the dye to the semiconductor's conduction band [5]. The electron transfer process is an important fundamental reaction in different devices and dye-sensitized solar cell devices[6]. It occurs by thermal excitation and photo inducement [6]. A basic classical theory for the charge transfer process was introduced by Rudolph Marcus to describe the transfer between two states, donor and acceptor, and awarded Nobel Prize in 1992 [7]. Despite electron transfer theory developments using various tools; analytical theory methods, time-resolved, spectroscopy, and computer simulation [8]. In recent years, many modifications have been proposed to dye-sensitized solar cell DSSC, including the fabrication of indoline organic dyes as sensitizers [9]. The dynamo red dye is a sensitized dye known as D35CPDT dye, as shown in figure (1). It has form 3-{6-{4-[bis(2',4'-dibutyloxybiphenyl-4-yl)amino-]phenyl}-4,4-dihexyl-cyclopenta-[2,1-b:3,4-b'] dithiophene-2-yl}-2-cyanoacrylic acid. It is stable, low cost, and high performance to use in DSSCs devices [10]. SnO_2 and TiO_2 are used to be an acceptor state in two device systems, its conversion of solar energy to electricity and to chemical energy [11]. SnO_2 is one of the n-type used in dye-sensitized solar cells DSSCs [12]. SnO2 is a wide band gap of about 3.6 eV and has chemical and physical steady-state properties at different temperatures [13].

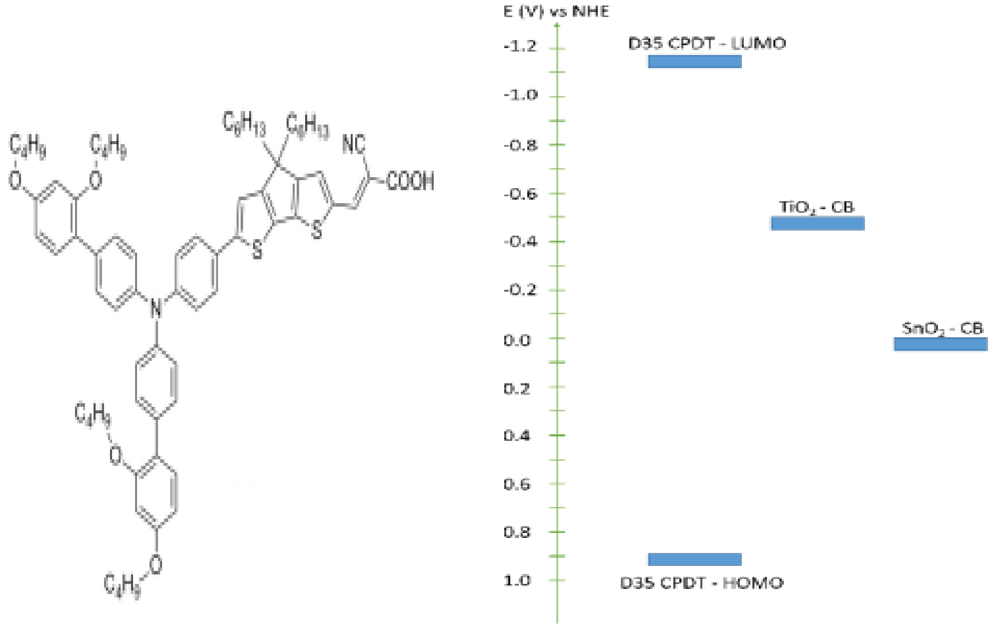

Figure 1. A-Structure of the D35CPDT dye [10] and B- Energy levels for D35CPDT contact to $SnO_2$and TiO_2 [15]

On the other hand, the TiO_2 is an important n-type semiconductor used in solar cell devices. It has a wide energy band gap of about 3.2 eV, is low cost, nontoxic in nature and stable [14].The schematic of energy levels for sensitized D35CPDT dye with SnO_2 and TiO_2 semiconductors is shown in **Figure (1)** [15].

In this paper, we utilize the quantum model to investigate charge transfer dynamics from Sensitized D35CPDT Dye to the conduction band of SnO_2 or/and TiO_2 Semiconductor.

2. Theory

The charge transfer rate (K_{CTR}) is given by Fermi Golden Rule to transfer charge from a donor state to an acceptor state and is given by [16].

$$K_{CTR} = \sum \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 \rho_d(E) \qquad (1)$$

Where h is Planck constant, $\langle C_{CTR}\rangle$ is the charge transfer strength coupling, and $\rho_d(E)$is the active density of electrons. The activation density profile is the function of the effective density of states D_{ES} and effective length l_{el} . It has been determined from the expression [17].

$$\rho_d(E) = D_{ES}\frac{l_{el}}{(\frac{6}{\pi})^{1/3}} \qquad (2)$$

The charge transfer rate in Eq.(1) together with Eq.(2) to reduce:

$$K_{CTR} = \sum \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 D_{ES}\frac{l_{el}}{(\frac{6}{\pi})^{1/3}} \qquad (3)$$

The total effective density of states depends on the density of the state$\langle\hat{\rho}_j\rangle = \frac{e^{-\frac{(\Lambda+\Delta F^0)^2}{4\Lambda k_BT}}}{\sqrt{(4\pi\Lambda k_BT)}}$ for the system and can be described by [18].

$$D_{ES} = \langle\hat{\rho}_j\rangle d_A^{-2/3} = \frac{e^{-\frac{(\Lambda+\Delta F^0)^2}{4\Lambda k_BT}}}{\sqrt{(4\pi\Lambda k_BT)}} d_A^{-2/3} \qquad (4)$$

Whered_A is the atomic density of a semiconductor.

The charge transfer rate in Eq.(1) will be set through Eq.(4) by

$$K_{CTR} = \sum \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 \frac{e^{-\frac{(\Lambda+\Delta F^0)^2}{4\Lambda k_BT}}}{\sqrt{(4\pi\Lambda k_BT)}} d_A^{-2/3} \frac{l_{el}}{(\frac{6}{\pi})^{1/3}} \qquad (5)$$

Introduce the Fermi distribution function $f_{(E)}$ for electrons as a function of the conduction band energy E_C and electronic energy E in the system and may be written [19]:

$$f_{(E)} = \frac{1}{e^{\frac{(E_C-E)}{k_BT}}+1} \qquad (6)$$

We can insert Eq.(6) in Eq.(5) with integration over energy $E(0 \rightarrow E_C$ to obtain:

$$K_{CTR} = \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 \frac{e^{-\frac{(\Lambda+\Delta F^0)^2}{4\Lambda k_BT}}}{\sqrt{(4\pi\Lambda k_BT)}} d_A^{-2/3} \frac{l_{el}}{(\frac{6}{\pi})^{1/3}} \int_0^{E_C} \frac{dE}{e^{\frac{(E_C-E)}{k_BT}}+1} \qquad (7)$$

The corresponding driving energy ΔF^0 in the charge transfer process are obtained as a function of the conduction band energy $E_C$of semiconductor and electrochemical potential ϕ and is computed by [20].

$$\Delta F^0 = E_C - \phi \qquad (8)$$

Inserting Eq.(8) in Eq.(7) to result:

$$\mathrm{K}_{CTR} = \frac{4\pi^2}{h} |\langle C_{CTR} \rangle|^2 \frac{e^{-\frac{(\Lambda+(\mathrm{E_C}-\phi))^2}{4\Lambda k_B T}}}{\sqrt{(4\pi\Lambda k_B T)}} d_A^{-2/3} \frac{l_{el}}{(\frac{6}{\pi})^{1/3}} \int_0^{\mathrm{E_C}} \frac{dE}{e^{\frac{(\mathrm{E_C}-\mathrm{E})}{\mathrm{k_B T}}}+1} \qquad (9)$$

The results solve integral in Eq.(9) reduce to.

$$\int_0^{\mathrm{E_C}} \frac{dE}{e^{\frac{(\mathrm{E_C}-\mathrm{E})}{\mathrm{k_B T}}}+1} = \mathrm{k_B T}[\ln 2 - \ln\left(1 + e^{\frac{-\mathrm{E_C}}{\mathrm{k_B T}}}\right)] \qquad (10)$$

The potential energy is obtained by calculating the driving energy and transition energy and is given as [21].

$$U(\Lambda, \phi) = \frac{\left((\mathrm{E_C}-\phi)+\Lambda\right)^2}{4\Lambda} \qquad (11)$$

Therefore, we insert Eq.(10) and Eq.(11) in Eq.(9) to result:

$$\mathrm{K}_{CTR} = \frac{4\pi^2}{h} |\langle C_{CTR} \rangle|^2 \frac{e^{-\frac{U(\Lambda,\phi)}{k_B T}}}{\sqrt{(4\pi\Lambda k_B T)}} d_A^{-2/3} \frac{l_{el}}{(\frac{6}{\pi})^{1/3}} \mathrm{k_B T}[\ln 2 - \ln\left(1 + e^{\frac{-\mathrm{E_C}}{\mathrm{k_B T}}}\right) \qquad (12)$$

According to the continuum model of donor - acceptor theory, the transition energy Λ(eV) can be obtained[22]:

$$\Lambda(\boldsymbol{eV}) = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{R}[\frac{1}{n^2} - \frac{1}{\epsilon}] - \frac{1}{2D}[(\frac{n_S^2-n^2}{n_S^2+n^2})(\frac{1}{n^2}) - \frac{\epsilon_S^2-\epsilon^2}{\epsilon_S^2+\epsilon^2}\frac{1}{\epsilon^2}]\right] \qquad (13)$$

Where e and $\varepsilon_\circ$ are charge and permittivity, n and n_S are the refractive index of solvent and semiconductor, ϵ and ϵ_S are the dielectric constant of solvent and semiconductor, $\boldsymbol{R}$ is the radius of dye and **D** is the distance between the dye and the semiconductor. The radius is given as a function of molecular weight MW and density ρ_m due to the spherical approach formula [23].

$$R(\,A^o) = (\frac{3}{4\pi})^{\frac{1}{3}}(\frac{MW}{N_A \rho_m})^{\frac{1}{3}} \qquad (14)$$

Where N_A is Avogadro number.

3. Results

To study the charge transfer dynamics from D35CPDT sensitized dye to conduction band SnO_2 or TiO_2 In a semiconductor, we can calculate the rate of the charge transfer process in this system. It can enable us to know the electronic properties. The charge transfer rate at interfaces is calculated depending on the transition energy, driving force, potential at the interface, and strong coupling of charge transfer in the system. Transition energy was calculated depending on the donor-acceptor system with polarity media of solvents. The physical properties of solvents and SnO_2 and TiO_2 semiconductors are shown in **Tables (1) and (2),** respectively.

Table 1. Physical properties of solvents [24].

Solvents	Density g/cm3	Boiling point(C°)	Melting point(C°)	Viscosity (c_p)	Dielectric constant (Ɛ)	Refractive index (n)
Pyridine	0.978	115.4	−41.6	0.88	12.3	1.510
2-Methoxyethanol	0.965	124	-85	1.7	16.90	1.402
Ethanol	0.78945	78.37	-114.1	1.08	24.5	1.3614
Acetonitrile	0.786	82	-45	0.38	37.5	1.3441
Methanol	0.792	64.7	-97.6	0.54	32.7	1.3284

Properties	**SnO_2 [25]**	**TiO_2 [26-27]**
Molecular weight (g/mol)	150.71	79.866
Dielectric Constant	2.19	55
Mass Density (g/cm^3)	6.95	4.23
Density of state N_s /cm^3)	3.5×10^{19}	1.163×10^{25}
Refractive index	1.45	2.609
Lattice constant(Å)	a = b = 4.731 A° and c = 3.189A°	a = 4.5936 ,c =2.9587
Radius(Å)	2.0487	1.9563
Conduction band energy(eV)	3.2 eV	4.05
Electron concentration (1/cm^3)	5×10^{20}cm-3	2×10^{20}cm-3
Electron affinity (eV)	4.5 eV	4.2

Table 2. Physical properties of SnO_2 and TiO_2 semiconductors .

Firstly, we must calculate the radius R of D35CPDT dye and the distance (D) between D35CPDT dye and SnO_2 and TiO_2. Depending on the approach of the spherical formula, the radii of the D35CPDT molecule, SnO_2 and TiO_2 are estimated using Eq.(14), from which we may calculate the association transition energy, driving energy coefficient, the potential at the interface and charge transfer rate of the charge transfer process in both systems.The radii are calculated using the expression in Eq.(14) with inserting the value of molecular weight MW = 1125.58 g/mol [28], 150.71g/ mol [25] and79.866 g/ mol [27] for D35CPDT molecule, SnO_2 and TiO_2 and taking the density ρ_m=1.154 g/cm^3 [28], 6.95 g/cm^3 [25] and 4.23 g/cm^3 [27] for D35CPDT dye, SnO_2 and TiO_2. Results are found to be 7.28404 Å, 2.0487Å and 1.9563 Å for D35CPDT, SnO_2 andTiO_2, respectively. The calculation of the transition energy was carried out using Eq.(13) for D35CPDT / SnO_2 and D35CPDT / TiO_2 by taking the dielectric constant and refractive index for solvents in the table (1) and the dielectric constant with the refractive index for $SnO_2$and TiO_2 in Table(2), and distance is taken D=9.33274Å between D35CPDT dye to SnO_2 and D=9.24034Å from D35CPDT dye to TiO_2.Results are listed in **Table (3).**

Table 3. Results of transition energy for D35CPDT / SnO_2 and D35CPDT / TiO_2.

Solvents	**Chemicals Formula**	**Dielectric constant Ɛ)**	**Refractive index (n)**	**Orientation energy for**	
				D35CPDT/ SnO_2	D35CPDT/ TiO_2
Pyridine	C_5H_5N	12.3	1.510	0.35762	0.27036
2-Methoxyethanol	$C_3H_8O_2$	16.90	1.402	0.43648	0.33614
Ethanol	C_2H_6O	24.5	1.3614	0.47924	0.37318

Acetonitrile	C_2H_3N	**37.5**	1.3441	0.50434	0.39569
Methanol	CH_4O	32.7	1.3284	0.51046	0.40022

We can also calculate the driving energy for the charge transfer process using Eq.(8) as a function of the conduction band of $E_{cb} = 3.2$ eV for SnO_2 , $E_{cb} = 4.05$ eV for TiO_2, and the electrochemical potential energy of D35PCDT are taken in the range ϕ=3.1 eV to 2.5 eV; results are listed in **Table (4).**

Table 4. Results of driving energy as a function of conduction E_{cb} =3.2 eV forSnO_2andE_{cb} =4.05 eV for TiO_2 with electrochemical potential $\phi\ (eV)$ of dye.

Electrochemical potential $\boldsymbol{\phi}$ $(\boldsymbol{eV})$	**The driving energy$\boldsymbol{\Delta F^0 (eV)}$**	
	D35CPDT/ SnO_2	D35CPDT/ TiO_2
3.1	0.1	0.95
3.0	0.2	1.05
2.9	0.3	1.15
2.8	0.4	1.25
2.7	0.5	1.35
2.6	0.6	1.45
2.5	0.7	1.55

Here, we can use values of the transition energy in the table (3) and the driving energy in the table (4) to calculate the potential energy using Eq.(11). Results are listed in the table (5) for D35CPDT / SnO_2 the system with the driving energy $\Delta F^0 (eV) = 0.6$ eV and D35CPDT / TiO_2 system with the driving energy$\Delta F^0 (eV) = 1.25\ eV$, respectively .

Table 5. Data of potential energy $U(\Lambda, \phi)$for D35CPDT/ SnO_2 and D35CPDT/ TiO_2System**.**

Solvent type	**potential barrier $\boldsymbol{U(\Lambda, \phi)}$ (eV)**			
	D35CPDT/ $\boldsymbol{SnO_2}$		D35CPDT/ $\boldsymbol{TiO_2}$	
	$\boldsymbol{\Lambda}$**(eV)**	$\Delta F^0 = 0.6\ eV$.6**eV**	$\boldsymbol{\Lambda}$**(eV)**	$\Delta F^0 = 1.25\ eV$
Pyridine	0.35762	0.6411	0.27036	2.1374
2-Methoxyethanol	0.43648	0.6153	0.33614	1.8711
Ethanol	0.47924	0.6076	0.37318	1.7650
Acetonitrile	0.50434	0.6045	0.39569	1.7111
Methanol	0.51046	0.6039	0.40022	1.7011

To understand the charge transfer properties, it has been pointed to calculate the charge transfer rate (K_{CTR}) associated with the transition energy Λ(eV)of D35CPDT/ SnO_2 and D35CPDT/ TiO_2. We calculate the charge transfer rate using Eq.(12) associated to the transition energy in table (3) for D35CPDT/ SnO_2 using the driving energy ΔF^0=0.6 eV and D35CPDT/ TiO_2 using the driving energy ΔF^0=1.25eV and take the strong coupling $|\langle C_{CTR} \rangle|^2 = 1.25 \times 10^{-1}$,. 2.25×10^{-2}, 3.25×10^{-3}, 4.25×10^{-4} and $5.25\times 10^{-5}(\mathrm{eV/state})^2$ and take the atomic density d_A=6.95 (1)/cm3 [29] for SnO_2 and d_A=4.23 (1)/cm3 for TiO_2 [27-28] with the effective length $l_{el} = 3 \times 10^{-10}\mathrm{m}$ [29]. Results are shown in **Tables (6) and (7)**forD35CPDT/ SnO_2 and D35CPDT/ $TiO_{2,}$ respectively.

Table 6. Results of electrons transfer rate for D35CPDT/ SnO_2at $\Delta F^0 = 0.6eV$.

Solvent	$\boldsymbol{\Lambda}(\mathbf{eV})$	**The charge transfer rate** K_{CTR} **1/ Sec**				
		$|\langle C_{CTR}\rangle|^2(\mathbf{eV/\ state})^2$				
		$\mathbf{1.25\times 10^{-1}}$	$\mathbf{2.25\times 10^{-2}}$	$\mathbf{3.25\times 10^{-3}}$	$\mathbf{4.25\times 10^{-4}}$	$\mathbf{5.25\times 10^{-5}}$
Pyridine	0.35762	1.1877E-26	2.1378E-27	3.0880E-28	4.0381E-29	4.9883E-30
2-Methoxyethanol	0.43648	3.0119E-26	5.4214E-27	7.8310E-28	1.0240E-28	1.2650E-29
Ethanol	0.47924	3.9123E-26	7.0422E-27	1.0172E-27	1.3302E-28	1.6432E-29
Acetonitrile	0.50434	4.3124E-26	7.7623E-27	1.1212E-27	1.4662E-28	1.8112E-29
Methanol	0.51046	4.3922E-26	7.9060E-27	1.1420E-27	1.4934E-28	1.8447E-29

1.1877E-26 **to** 1.8447E-29

Table 7. Results of electrons transfer rate for D35CPDT/ TiO_2at $\Delta F^0 = 1.25eV$.

Solvent	$\boldsymbol{\Lambda}(\mathbf{eV})$	**The charge transfer rate** K_{CTR} **1/ Sec**				
		$|\langle C_{CTR}\rangle|^2(\mathbf{eV/\ state})^2$				
		$\mathbf{1.25\times 10^{-1}}$	$\mathbf{2.25\times 10^{-2}}$	$\mathbf{3.25\times 10^{-3}}$	$\mathbf{4.25\times 10^{-4}}$	$\mathbf{5.25\times 10^{-5}}$
Pyridine	0.27036	1.2631E-52	2.2735E-53	3.2840E-54	4.2945E-55	5.3049E-56
2-Methoxyethanol	0.33614	4.7813E-48	8.6064E-49	1.2431E-49	1.6256E-50	2.0081E-51
Ethanol	0.37318	3.1614E-46	5.6904E-47	8.2195E-48	1.0749E-48	1.3278E-49
Acetonitrile	0.39569	2.6545E-45	4.7782E-46	6.9018E-47	9.0255E-48	1.1149E-48
Methanol	0.40022	3.9436E-45	7.0984E-46	1.0253E-46	1.3408E-47	1.6563E-48

4. Discussion

The transition energy in **Table (3)** for both systems have been calculated in room temperature. It increases upon decreasing the refractive index and increases the dielectric constant (Ɛ) of solvents. Also, the transition energy increases with the decrease of the refractive index and dielectric constant of the semiconductor which is shown in **Table (3). Table (3)** shows the transition energy increasing with SnO_2 which has low dielectric constant 2.19 and a low refractive index 1.45 compared with TiO_2 has a large dielectric constant 55 and large refractive index 2.609.

According the results in **Table (2),** we can find the transition energy for both D35CPDT/ SnO_2 and D35CPDT/ TiO_2 systems has large values with Methanol solvent but the D35CPDT/ TiO_2 system has smaller transition energy than D35CPDT/ SnO_2 that has large transition energy. Table (3) shows the transition energy for D35CPDT / SnO_2 system is larger than the transition energy for D35CPDT / TiO_2 by 0.1 eV with the same solvent; this is because of the effect of dielectric and refrective index of semiconductor. However, the transition energy can be noted to be large; it has about 0.40022eV for D35CPDT /TiO_2 and

0.51046eV for D35CPDT / SnO_2 with Methanol and about 0.39569 eV for D35CPDT / TiO_2 and 0.50434 eV for D35CPDT / SnO_2 Acetonitrile solvents comparing to the low transition energy around 0.27036 eV for D35CPDT / $TiO_2$and 0.35762 eV for D35CPDT / SnO_2 with the Pyridine solvent.**Table (6)** shows the charge transfer rate in range 1.6692E-47 to 4.3922E-26 with the strength $|\langle C_{CTR}\rangle|^2 = 1.25 \times 10^{-1}(\mathrm{eV/\ state})^2$ associated with the transition energy in the range 0.35762 -0.51046eV for D35CPDT /SnO2system. **Table (7)** shows the charge transfer rate in the range 1.2631E-52 to 3.9436E-45with strength $|\langle C_{CTR}\rangle|^2 = 1.25 \times 10^{-1}(\mathrm{eV/\ state})^2$ associated with the transition energy in the range 0.27036-0.40022 eV for D35CPDT /TiO_2system. A large charge transition rate of the D35CPDT/ SnO_2 system is achieved 4.3922E-26 with the transition energy 0.51046 eV and the Methanol solvent. On the other hand, it can be seen that the charge transfer for D35CPDT/ TiO_2 is to be large 3.9436E-45 associated with the transition energy 0.40022eV and the Methanol solvent. It is influenced by the transition energy and increased with the increased transition energy and polarity media with the increased dielectric constant. It decreases the refractive index in both systems. The results of the charge transfer rate found that the charge transfer process depends on the driving force. Hence, in both systems, there are the same values of electrochemical potential ϕ (.1-2.5eV) which are taken with different conduction band energy. **Table (4)** indicates that the driving energy is a function of the electrochemical potential of D5CPDT dye. The driving energy increases with decreases in the electrochemical potential and vice versa in both systems. However, the driving energy is large for D35CPDT / TiO_2 in scale (0.95 to 1.55eV) compared to D35CPDT / SnO_2 in scale (0.1 to 0.7 eV).Further, it is supported by **Table (4)**which indicates its conduction band energy effect. From **Table (4)**, we can see different driving energy values in the inset of **Tables (6) and (7).** The driving energy is $\Delta F^0 \approx 0.6$ eVfor D35CPDT / SnO_2compared to $\Delta F^0 = 1.25$ eV for D35CPDT / TiO_2. **Table (6)** show the charge transfer rate in the range from 1.1877E-26 **to** 1.8447E-29 for D35CPDT / SnO_2**while** the charge transfer rate in the table (7) for D35CPDT / TiO_2 in the range from 1.2631E-52tO3.9436E-.That means the charge transfer rate for D35CPDT / SnO_2 is larger than the charge transfer rate for D35CPDT / TiO_2 .The charge transfer rate was substantially less from 1.1877E-26 at strength coupling $1.25\times 10^{-1}(\mathrm{eV/\ state})^2$ and reach 4.9883E-30 at coupling $1.25\times 10^{-5}(\mathrm{eV/\ state})^2$ in the case of D35CPDT / SnO_2at $\Delta F^0 = 0.6$ eV with Pyridine solvents. Also, we note, that the charge transfer rate is large from4.3922E-26 at coupling $1.25\times 10^{-1}(\mathrm{eV/\ state})^2$to reach 1.8447E-29 at coupling $1.25\times 10^{-5}(\mathrm{eV/\ state})^2$for D35CPDT / SnO_2 with Methanol solvents. However, the charge transfer rate has become minimum at coupling $11.25\times 10^{-5}(\mathrm{eV/\ state})^2$ with Pyridine solvents at $\Delta F^0 = 1.25$eV and to reach to 5.3049E-56 . On the other hand ,charge transfer rate reach to maximum 1.6563E-48 at strength coupling $1.25\times 10^{-5}(\mathrm{eV/\ state})^2$for D35CPDT / TiO_2 with Methanol solvent. The other parameter that is affected and limits the charge transfer process is potential energy. The other parameter that is affected and limits the charge transfer process is the potential energy. It further influences on charge transfer rate. Furthermore, we find the results in **Table (5)** that the potential energy of charge transfer is increased with decreased transition energy. Potential energy reaches to maximum 2.1374eV and 0.6411 eV for D35CPDT / TiO_2 and D35CPDT / SnO_2 with Pyridine solvents while reaching to minimum 1.7011eV and 0.6039 eV for D35CPDT / TiO_2 and D35CPDT / SnO_2 with Methanol solvents, respectively. The greater transfer rate increases for both systems with the coupling $1.25\times 10^{-1}(\mathrm{eV/\ state})^2$and decreases in the charge transfer rate with decreasing of the coupling. It reaches the minimum with the strength coupling $5.25 \times 10^{-5} (\mathrm{eV/\ state})^2$ and reduces to decrease the charge transfer process. The charge transfer rate becomes low with the Pyridine solvent in both systems. It has in range1.1877×10^{-26}-4.9883×10^{-30} for D35CPDT/ $SnO_2$and reaches 1.2631×10^{-52} - $5.3049\mathrm{E} \times 10^{-56}$ for D35CPDT / TiO_2.The D35CPDT / SnO_2 and D35CPDT / TiO_2 systems with Methanol have a charge transfer rate large in range 4.3922×10^{-26}-1.8447×10^{-29} for D35CPDT / $SnO_2$and reaches 3.9436×10^{-45} - $.6563 \times 10^{-48}$ for D35CPDT / TiO_2.Table (5) shows the potential in both systems increasing with the decrease of the transition energy and the charge transfer rate will be increasing tremendously with the decrease of the potential energy. The results in **Table (6)** indicate that D35CPDT contact to SnO_2 with Methanol solvents at driving energy 0.6eV giving us a large rate compared to the results in a table (7) or D35CPDT contact to TiO_2 with Methanol solvent and the D35CPDT / SnO_2 is a good system and can be used in electronic devices.

5. Conclusion

In conclusion, the influence of transition energy in both systems can show the charge transfer rate, the rate increases with the transition energy increase. In contrast, the driving energy in both systems increases with the decreased electrochemical potential and substantially reduces the charge transfer rate. It can be concluded that the charge transfer for both systems increases with decreases in the potential, and the rate is large for D35CPDT / SnO_2 compared to D35CPDT / TiO_2. A large charge transfer rate is observed from a charge donating D35CPDT dye attached to the SnO_2 surface compared to the small rate of charge transfer from D35CPDT dye attached to the TiO_2 surface with the same solvents. The results of the charge transfer rate allow for further systematic analysis of the influence of transfer parameters on the flow of electronic transfer from donor to an acceptor in the device's system and to know the influences on the efficiency of devices

References

1.Saputri, D. G.; Supriyanto, A.; Ahmad, M. K.; Diyanahesa, N. E. H.; Ramadhani, F. Optical properties of dye DN-F05 as a good sensitizer. *Journal of Physics: Theories and Applications,***2019**, *3*(2), 43-49.

2. Liu, P.; Xu, B.; Karlsson, K. M.; Zhang, J.; Vlachopoulos, N.; Boschloo, G.; Kloo, L. (2015). The combination of a new organic D–π–A dye with different organic hole-transport materials for efficient solid-state dye-sensitized solar cells. *Journal of Materials Chemistry A,***2015**, *3*(8), 4420-4427.

3. Obeed, H. M.; Al-Agealy, H. J. Investigation and studied of charge transfer processes at HATNA and HATNA-Cl6 molecules contact with Cu metal. In *AIP Conference Proceedings,***2020**, (Vol. 2292, No. 1, p. 040010). AIP Publishing LLC..

4. Eriksson, S. K.; Josefsson, I.; Ellis, H.; Amat, A.; Pastore, M.; Oscarsson, J.; Rensmo, H. Geometrical and energetical structural changes in organic dyes for dye-sensitized solar cells probed using photoelectron spectroscopy and DFT. *Physical Chemistry Chemical Physics,***2016**, *18*(1), 252-260.

5. Carr, J. M., Allen, T. G., Larson, B. W., Davydenko, I. G., Dasari, R. R., Barlow, S., Rumbles, G. Short and long-range electron transfer compete to determine free-charge yield in organic semiconductors. *Materials Horizons*.**2022.**

6. Al-agealy, H. J. M.; Al-Hakany, J. S. H. (2017). Theoretical Calculations of Rate Constant of Electron Transfer Across N3/TiO2 Sensitized Dye Interface Solar Cell. *Ibn AL-Haitham Journal For Pure and Applied Science*,**2017**, *25*(*2*).

7.Kevin Tvrdya , Pavel, A. Frantsuzovc, ; Prashant, V. Kamat,Photoinduced electron transfer from semiconductor quantum dots to metal oxide nanoparticles *,PNAS*,**2011**,*108*,*1*, 29–34, .

8.AL-agealy, H. J. M.; Harbbi, K. H.; Hassooni, M. A.;Noori, R. I. Theoretical Study of Charge Transfer in Styryl Thiazilo Quinoxaline Dyes STQ-1, STQ-2, and STQ-3 in Organic Media System. *Baghdad Science Journal*,**2013**, *10*(*4*).

9. Maleki, E.; Ranjbar, M.; Kahani, S. A. The effect of antisolvent dropping delay time on the morphology and structure of the perovskite layer in the hole transport material free perovskite solar cells. *Progress in Color, Colorants and Coatings*,**2021**, *14*(*1*), 47-54.

10. Ellis, H.; Eriksson, S. K.; Feldt, S. M.; Gabrielsson, E.; Lohse, P. W.; Lindblad, R.; Hagfeldt, A. Linker unit modification of triphenylamine-based organic dyes for efficient cobalt mediated dye-sensitized solar cells. *The Journal of Physical Chemistry C*, **2013**,*117*(*41*), 21029-21036.

11. Tada, H.; Naya, S. I. Atomic level interface control of SnO2-TiO2 nanohybrids for the photocatalytic activity enhancement. *Catalysts*, **2021**, *11*(*2*), 205.

12. Xiong, L.; Guo, Y.; Wen, J.; Liu, H.; Yang, G.; Qin, P.; Fang, G. Review on the application of SnO2 in perovskite solar cells. *Advanced Functional Materials*,**2018**, *28*(*35*), 1802757.

13. Feng, Z.; Gaiardo, A.; Valt, M.; Fabbri, B.; Casotti, D.; Vanzetti, L.; Guidi, V. Investigation on Sensing Performance of Highly Doped Sb/SnO2. *Sensors*, **2022**, *22*(*3*), 1233.

14. Margan, P.; Haghighi, M. Hydrothermal-assisted sol–gel synthesis of Cd-doped TiO2 nanophotocatalyst for removal of acid orange from wastewater. *Journal of Sol-Gel Science and Technology*, **2017,***81*(*2*), 556-569.

15.Björklund, J., **2016**. *Electron transfer processes in a dye-TiO2/SnO2-acceptor assembly: Towards long lived charge separated states for solar fuels* (Master's thesis).

16.Hadi,J.M.Al-Agealy Rafah ,I.N.AL-Obaidi Charge transfer At Semiconductor / Liquid Interfaces,*Ibn Al -Hathim J. for Pure and Appl. SCI* .**2009**,*22* ,*2*.

17.Maadhde, T. S. A.; Jumali, M. H.; Al-Agealy, H. J.; Razak, F. B. A.;Yap, C. C. An Investigation of the Fill Factor and Efficiency of Molecular Semiconductor Solar Cells. In *Materials Science Forum*, Trans Tech Publications Ltd. **2021**,*1039*, 373-381.

18. Al-Obaidi, S. S.; Al-Agealy, H. J.; Abbas, S. R. Theoretical Evaluation of Flow Electronic Rate at Au/TFB Interface. In *Journal of Physics: Conference Series* , **2021**,*1879*,*3*,032096 IOP Publishing.

19.HadiJabbarAlagealy;Mohsin, A. Hassooni and Hind Mahdi Abdul Mageed,Theoretical Study of Electronic Transfer Current Rate at Dye-Sensitized Solar Cells,AIP Conference Proceedings 1968, 030055 (2018); doi: 10.1063/1.5039242View online:https://doi.org/10.1063/1.5039242

20.Hamann, T. W.; Gstrein, F.; Brunschwig, B. S.; Lewis, N. S. Measurement of the free-energy dependence of interfacial charge-transfer rate constants using ZnO/H2O semiconductor/liquid contacts. *Journal of the American Chemical Society*,**2005**, *127*(*21*), 7815-7824.

21.Al-Agealy, H. J.; Janeri, H. H. D. A. (2019, July). Investigation the flow charge rate at InAs/D149 and ZnO/D149 system using theoretical quantum model. In *AIP Conference Proceedings* ,**2019**, *2123*, *1*, 020055). AIP Publishing LLC.

22. Al-agealy, H. J. M.; Al-Hakany, J. S. H. Theoretical Calculations of Rate Constant of Electron Transfer Across N3/TiO2 Sensitized Dye Interface Solar Cell. *Ibn AL-Haitham Journal For Pure and Applied Science*,**2017**, *25*(*2*).

23. Saad, H. J. A. A. T.; Maudhady, A. Influence of The Polarity Function on the Probability of Transition Rate Constant (sec-1) At Metal/Molecule In Nano Scale Devices.**2014**.

24.Smallwood, I. (2012). *Handbook of organic solvent properties*. Butterworth-Heinemann.

25. Al-agealy, H. J.; Hassooni, M. A.; Sadoon, A. K.; Ashwiekh, A. M. Study and Invistagation of Electric Properties of Dye Sensitized Solar Cell. *Mesopotamia Environmental Journal*,**2016**. (Special Issue A).
26. Al-Agealy, H. J.; Al Maadhede, T. S.; Al Shafaay, B.; Mjeed, R. H.; Ashweik, A. M. Theoretical study of Charge Transfer simulation At Fe Metal with Ge and ZnO semiconductors Nano devices material. *Energy Procedia*, **2017**, *119*, 325-331.
27. Perevalov, T. V.;Gritsenko, V. A. Electronic structure of TiO2 rutile with oxygen vacancies: Ab initio simulations and comparison with the experiment. *Journal of Experimental and Theoretical Physics*,**2011**,*112*(*2*),310-316.
28.Gabrielsson, E.; Ellis, H.; Feldt, S.; Tian, H.; Boschloo, G.; Hagfeldt, A.;Sun, L. Convergent/Divergent Synthesis of a Linker-Varied Series of Dyes for Dye-Sensitized Solar Cells Based on the D35 Donor. *Advanced Energy Materials*,**2013,** *3*(*12*), 1647-1656.
29.Lewis, N. S. Progress in understanding electron-transfer reactions at semiconductor/liquid interfaces. *The Journal of Physical Chemistry B*,**1998**, *102*(*25*), 4843-4855.