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

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Article history: Received 3 April 2022, Accepted 17 May 2022, Published in July 2022.

Doi:10.30526/35.3.2839

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 in 1990s, 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 induction [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 induction [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].

$$K_{CTR} = \sum \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 \rho_d(E)$$  \hspace{1cm} (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 states. 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].

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

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

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

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

$$D_{ES} = \langle \hat{\rho}_j \rangle d_A^{-2/3} = \frac{e^{(\Delta + \Delta \rho)^2}}{\sqrt{(4\pi\Lambda\kappa B T)}} d_A^{-2/3}$$  \hspace{1cm} (4)

Where $d_A$ is the atomic density of a semiconductor.

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

$$K_{CTR} = \sum \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 e^{(\Delta + \Delta \rho)^2 \over 4\pi\Lambda\kappa B T} d_A^{-2/3} \frac{l_{el}}{(\pi e)^{1/3}}$$  \hspace{1cm} (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]:

$$f(E) = \frac{1}{e^{(E_C-E)/k_B T} + 1}$$  \hspace{1cm} (6)

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

$$K_{CTR} = \frac{4\pi^2}{h} |\langle C_{CTR}\rangle|^2 \frac{e^{(\Delta + \Delta \rho)^2 \over 4\pi\Lambda\kappa B T}}{\sqrt{(4\pi\Lambda\kappa B T)}} d_A^{-2/3} \frac{l_{el}}{(\pi e)^{1/3}} \int_0^{E_C} \frac{dE}{e^{(E_C-E)/k_B T} + 1}$$  \hspace{1cm} (7)

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

$$\Delta F^0 = E_C - \phi$$  \hspace{1cm} (8)

Inserting Eq.(8) in Eq.(7) to result:
\[ K_{CTR} = \frac{4\pi^2}{h} \left( \frac{(\Delta+E_C-\phi)^2}{4\pi^2k_BT} \right)^{2/3} \frac{d_A}{\sqrt{4\pi\alpha k_BT}} \int_0^{E_C} \frac{dE}{e^{k_BT} + 1} \] (9)

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

\[ \int_0^{E_C} \frac{dE}{e^{k_BT} + 1} \ln 2 - \ln \left( 1 + e^{k_BT} \right) \] (10)

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

\[ U(\Lambda, \phi) = \frac{(E_C - \phi + \Lambda)^2}{4A} \] (11)

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

\[ K_{CTR} = \frac{4\pi^2}{h} \left( \frac{(\Delta+E_C-\phi)^2}{4\pi^2k_BT} \right)^{2/3} \frac{d_A}{\sqrt{4\pi\alpha k_BT}} \frac{\epsilon}{\epsilon + \epsilon_d} k_BT \ln 2 - \ln \left( 1 + e^{k_BT} \right) \] (12)

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

\[ \Lambda(eV) = \frac{e^2}{8\pi\epsilon_c} \left[ \frac{1}{R^2} - \frac{1}{n^2} - \frac{1}{2D} \left( \frac{n^2 - n^2}{n^2 + n^2} \right) \left( \frac{1}{n^2} - \frac{\epsilon^2 - \epsilon_e^2}{\epsilon^2 + n^2 \epsilon_e^2} \right) \right] \] (13)

Where \( e \) and \( \epsilon_e \) are charge and permittivity, \( n \) and \( n_e \) are the refractive index of solvent and semiconductor, \( \epsilon \) and \( \epsilon_c \) are the dielectric constant of solvent and semiconductor, \( R \) 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 \( \rho_m \) due to the spherical approach formula [23].

\[ R(A^0) = \left( \frac{3}{4\pi} \right)^{\frac{1}{3}} \left( \frac{MW}{NA\rho_m} \right)^{\frac{1}{3}} \] (14)

Where \( NA \) 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 (cP) | Dielectric constant (ε) | 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              |
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], $150.71$ g/mol [25] and $79.866$ g/mol [27] for D35CPDT molecule, $SnO_2$ and $TiO_2$ and taking the density $\rho_m=1.154$ 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, $2.0487$Å and $1.9563$ Å for D35CPDT, $SnO_2$ and $TiO_2$, 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 $D=9.33274$ Å between D35CPDT dye to $SnO_2$ and $D=9.24034$ Å from D35CPDT dye to $TiO_2$. Results are listed in Table (3).

**Table 2.** Physical properties of $SnO_2$ and $TiO_2$ semiconductors.

| 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 $\times$ 10$^{19}$ | 1.163 $\times$ 10$^{25}$ |
| Refractive index                  | 1.45         | 2.609          |
| Lattice constant(Å)               | $a = b = 4.731$ Å and $c = 3.189$ Å | $a = 4.5936$, $c = 2.9587$ Å |
| Radius(Å)                         | 2.0487       | 1.9563         |
| Conduction band energy(eV)        | 3.2 eV       | 4.05           |
| Electron concentration (I/cm$^3$) | 5$\times$10$^{20}$ cm$^{-3}$ | 2$\times$10$^{20}$ cm$^{-3}$ |
| Electron affinity (eV)            | 4.5 eV       | 4.2            |

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

| Solvents      | Chemicals Formula | Dielectric constant $\epsilon$ | Refractive index (n) | Orientation energy for D35CPDT / $SnO_2$ | Orientation energy for 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                                  |
We can also calculate the driving energy for the charge transfer process using Eq.(8) as a function of the conduction band of $E_{cb} = 3.2 \text{ eV}$ for $SnO_2$, $E_{cb} = 4.05 \text{ eV}$ for $TiO_2$, and the electrochemical potential energy of D35PCDT are taken in the range $\phi = 3.1 \text{ eV}$ to $2.5 \text{ eV}$; results are listed in Table (4).

Table 4. Results of driving energy as a function of conduction $E_{cb} = 3.2 \text{ eV}$ for $SnO_2$ and $E_{cb} = 4.05 \text{ eV}$ for $TiO_2$ with electrochemical potential $\phi$ (eV) of dye.

| Electrochemical potential $\phi$ (eV) | The driving energy $\Delta F^0$(eV) |
|--------------------------------------|--------------------------------------|
|                                      | D3CPDT/ $SnO_2$                     |
|                                      | D3CPDT/ $TiO_2$                     |
| 3.1                                  | 0.1                                 |
| 3.0                                  | 0.2                                 |
| 2.9                                  | 0.3                                 |
| 2.8                                  | 0.4                                 |
| 2.7                                  | 0.5                                 |
| 2.6                                  | 0.6                                 |
| 2.5                                  | 0.7                                 |

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 D3CPDT / $SnO_2$ the system with the driving energy $\Delta F^0$(eV) = 0.6 eV and D3CPDT / $TiO_2$ system with the driving energy $\Delta F^0$(eV) = 1.25 eV, respectively.

Table 5. Data of potential energy $U(\Lambda, \phi)$ for D3CPDT/ $SnO_2$ and D3CPDT/ $TiO_2$ system.

| Solvent type         | Potential barrier $U(\Lambda, \phi)$ (eV) |
|----------------------|------------------------------------------|
|                      | D3CPDT/ $SnO_2$                         |
|                      | D3CPDT/ $TiO_2$                         |
| $\Lambda$(eV)        | $\Delta F^0 = 0.6 \text{ eV}$, $\phi$   |
|                      | $\Delta F^0 = 1.25 \text{ eV}$          |
| Pyridine             | 0.35762                                  |
| 2-Methoxyethanol     | 0.43648                                  |
| Methanol             | 0.50434                                  |
| Ethanol              | 0.47924                                  |
| Acetonitrile         | 0.50434                                  |

To understand the charge transfer properties, it has been pointed to calculate the charge transfer rate ($K_{CTR}$) associated with the transition energy $\Lambda$(eV) of D3CPDT/ $SnO_2$ and D3CPDT/ $TiO_2$. We calculate the charge transfer rate using Eq.(12) associated to the transition energy in table (3) for D3CPDT/ $SnO_2$ using the driving energy $\Delta F^0 = 0.6 \text{ eV}$ and D3CPDT/ $TiO_2$ using the driving energy $\Delta F^0 = 1.25 \text{ eV}$ and take the strong coupling $|\langle C_{CTR}\rangle|^2 = 1.25 \times 10^{-1}$, $2.25 \times 10^{-2}$, $3.25 \times 10^{-3}$, $4.25 \times 10^{-4}$ and $5.25 \times 10^{-5}$ (eV/ state) and take the atomic density $d_A = 6.95 (\text{ \text{1/cm}^3})$ [29] for $SnO_2$ and $d_A = 4.23 (\text{ \text{1/cm}^3})$ for $TiO_2$ [27-28] with the effective length $l_{el} = 3 \times 10^{-10} \text{m}$ [29]. Results are shown in Tables (6) and (7) for D3CPDT/ $SnO_2$ and D3CPDT/ $TiO_2$, respectively.
**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 SnO2 which has low dielectric constant 2.19 and a low refractive index 1.45 compared with TiO2 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/SnO2 and D35CPDT/TiO2 systems has large values with Methanol solvent but the D35CPDT/TiO2 system has smaller transition energy than D35CPDT/SnO2 that has large transition energy. Table (3) shows the transition energy for D35CPDT /SnO2 system is larger than the transition energy for D35CPDT /TiO2 by 0.1 eV with the same solvent; this is because of the effect of dielectric and refractive index of semiconductor. However, the transition energy can be noted to be large; it has about 0.40022eV for D35CPDT /TiO2 and

**Table 6.** Results of electrons transfer rate for D35CPDT/ SnO2 at ΔE^o = 0.6eV.

| Solvent       | A(eV)   | The charge transfer rate K_{CTR} 1/ Sec | [\left(C_{CTR}\right)^2](eV/ state)^2 |
|---------------|---------|----------------------------------------|---------------------------------------|
| Pyridine      | 0.35762 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| 2-Methoxyethanol | 0.43648 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| Ethanol       | 0.47924 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| Acetonitrile  | 0.50434 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| Methanol      | 0.51046 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |

Table 7. Results of electrons transfer rate for D35CPDT/TiO2 at ΔE^o = 1.25eV.

| Solvent       | A(eV)   | The charge transfer rate K_{CTR} 1/ Sec | [\left(C_{CTR}\right)^2](eV/ state)^2 |
|---------------|---------|----------------------------------------|---------------------------------------|
| Pyridine      | 0.27036 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| 2-Methoxyethanol | 0.33614 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| Ethanol       | 0.37318 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| Acetonitrile  | 0.39569 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
| Methanol      | 0.40022 | 1.25×10^{-1}                           | 2.25×10^{-2}                           | 3.25×10^{-3} | 4.25×10^{-4} | 5.25×10^{-5} |
0.51046 eV for D35CPDT/SnO2 with Methanol and about 0.39569 eV for D35CPDT/TiO2 and 0.50434 eV for D35CPDT/SnO2. Acetonitrile solvents comparing to the low transition energy around 0.27036 eV for D35CPDT/TiO2 and 0.35762 eV for D35CPDT/SnO2 with the Pyridine solvent. Table (6) shows the charge transfer rate in range 1.6692E-47 to 4.3922E-26 with the strength $|\langle C_{CTR} \rangle|^2 = 1.25 \times 10^{-1}$ (eV/state)$^2$ associated with the transition energy in the range 0.35762 -0.51046 eV for D35CPDT/SnO2 system. Table (7) shows the charge transfer rate in the range 1.2631E-52 to 3.9436E-45 with strength $|\langle C_{CTR} \rangle|^2 = 1.25 \times 10^{-1}$ (eV/state)$^2$ associated with the transition energy in the range 0.27036-0.40022 eV for D35CPDT/TiO2 system. A large charge transition rate of the D35CPDT/SnO2 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/TiO2 is to be large 3.9436E-45 associated with the transition energy 0.40022 eV 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 $\phi$ (1.2-2.5eV) 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/TiO2 in scale (0.95 to 1.55eV) compared to D35CPDT/SnO2 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 $\Delta F^0 \approx 0.6$ eV for D35CPDT/SnO2 compared to $\Delta F^0 = 1.25$ eV for D35CPDT/TiO2. Table (6) shows the charge transfer rate in the range from 1.1877E-26 to 1.8447E-29 for D35CPDT/SnO2 while the charge transfer rate in the table (7) for D35CPDT/TiO2 in the range from 1.2631E-52 to 3.9436E-45. That means the charge transfer rate for D35CPDT/SnO2 is larger than the charge transfer rate for D35CPDT/TiO2. The charge transfer rate was substantially less from 1.1877E-26 at strength coupling $1.25 \times 10^{-1}$ (eV/state)$^2$ and reach 4.9883E-30 at coupling $1.25 \times 10^{-5}$ (eV/state)$^2$ in the case of D35CPDT/SnO2 at $\Delta F^0 = 0.6$ eV with Pyridine solvents. Also, we note, that the charge transfer rate is large from 4.3922E-26 at coupling $1.25 \times 10^{-1}$ (eV/state)$^2$ to reach 1.8447E-29 at coupling $1.25 \times 10^{-5}$ (eV/state)$^2$ for D35CPDT/SnO2 with Methanol solvents. However, the charge transfer rate has become minimum at coupling 11.25 $\times 10^{-5}$ (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 $1.25 \times 10^{-5}$ (eV/state)$^2$ for D35CPDT/TiO2 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/TiO2 and D35CPDT/SnO2 with Pyridine solvents while reaching to minimum 1.7011eV and 0.6039 eV for D35CPDT/TiO2 and D35CPDT/SnO2 with Methanol solvents, respectively. The greater transfer rate increases for both systems with the coupling $1.25 \times 10^{-1}$ (eV/state)$^2$ and
decreases in the charge transfer rate with decreasing of the coupling. It reaches the minimum with the strength coupling $5.25 \times 10^{-5} \text{ (eV/ state)}^2$ and reduces to decrease the charge transfer process. The charge transfer rate becomes low with the Pyridine solvent in both systems. It has in range $1.877 \times 10^{-26} - 4.9883 \times 10^{-30}$ for D35CPDT/SnO$_2$ and reaches $1.2631 \times 10^{-52} - 5.3049 \times 10^{-56}$ for D35CPDT/TiO$_2$. The D35CPDT/SnO$_2$ and D35CPDT/TiO$_2$ systems with Methanol have a charge transfer rate large in range $4.3922 \times 10^{-26} - 1.8447 \times 10^{-29}$ for D35CPDT/SnO$_2$ and reaches $3.9436 \times 10^{-45} - .6563 \times 10^{-48}$ 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.

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