Determining of Efficiency for the N749 Dye Contact with TiO$_2$ in Dye Sensitized Solar Cell

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Abstract

In this research, we investigate and evaluate the efficiency of a hetero junction N749-TiO$_2$ device based on a simple donor-acceptor model for electron transfer. Electron transfer from a photo-excited N749 sensitized into a wide-band gap TiO$_2$ is the basic charge separation in dye-sensitized solar cells, or "DSSCs". Due to the understanding of the current of the DSSCs functioning mechanism, the energy levels of the hetero junction N749-TiO$_2$ device surrounded by DCM solvent as polar media must be continuum levels. The current-voltage (J-V) characteristics of the N749-TiO$_2$ device are calculated in two concentrations at room temperature (T=300 k) and $100\frac{mW}{Cm^2}$ irradiation. The fill factor and efficiency of the device are found to be 0.134 and 6.990 for concentration $3.5 \times 10^{18} \left(\frac{1}{cm^3}\right)$ compared to 0.146 and 9.974 for concentration $4.5 \times 10^{18}(\frac{1}{cm^3})$. The efficiency of the N749-TiO$_2$ device is in agreement with experimental results. It also offers a rational for the suggestion to use the application of N749-TiO$_2$ high-performance solar cells.

Keywords: Efficiency, N749 Dye , TiO$_2$, Dye Sensitized Solar Cell

1. Introduction

Energy use continues to increase, increasing the depletion of fossil resources and increasing greenhouse gas emissions, which has driven tremendous efforts to provide more clean and renewable energy [1]. The dye-sensitized solar cells DSSC photovoltaic solar cell technology has drawn wide attention due to its simple fabrication process, low cost, and higher photovoltaic efficiency [2]. The DSSCs convert the sunlight into electric energy when excited the dye by absorbing the light to trigger a charge transition from the sensitized dye into the conduction band of the TiO$_2$, and regenerating oxidized dye molecules by the electron donation from the redox couple in the system. Finally, the electron transfer through the load completed the circuit [3]. The donor-acceptor model is one of the simplest models used to discuss the electron transfer, which neither forms nor breaks any chemical bond in the system [4]. The electronic transfer reaction

process with the molecule-semiconductor plays a main role in the DSSCs operation systems. Quantum transfer theory indicates a greater challenge to the attention of interface contact between the two materials required for electron transfer in the donor-acceptor system [5–6]. Hadi et al. indicate that alignment energy levels and reorganization energy are the main parameters for electron transfer reactions in various devices [7]. Charge transfer in hetero junction materials occurs when electrons are transferred from the donor level to the acceptor level in the system of solar cell devices [8]. Furthermore, the contact region of a molecule in a semiconductor system has received more attention in different technological applications because the electron transfer reaction occurred at the cross-interface [9]. The DSSC is a photovoltaic device cell from the third generation; it contains a sensitized molecular dye and a photoactive electrode consisting of metal oxide semiconductors [10]. The N719 dye is categorized as a ruthenium metal-based organic dye, which includes the sensitizers for DSSCs due to their broad optical absorption spectrum [11]. The N749 dye is the organic attractive sensitized dye used in the DSSC solar cells; it has the chemical formula [(C4H9)4N]. 3[Ru(Htcterpy)(NCS)3] C69H117 N9O6RuS3, Tris [N,N,N-tributyl-1-butanaminium] {[2,2″6′,2″-terpyridine] -4,4′,4″-tricarboxylato (3-)-N1,N1′,N1″}tris (thiocyanato-N)hydrogen ruthenated [12]. The N749 ruthenium dye is the main sensitizer because of its advantages of thermal and chemical stability, good absorption of light, and more interested optoelectronic and electronic properties [13]. Its structure is shown in Figure 1 [14]. Currently, the TiO_2 semiconductor is extensively used as a donor electrode in solar cells due to its high chemical stability and wide bandgap [15]. The mobility of electrons in electrodes relates to the strength of the coupling coefficient, and electrons will travel a distance from the donor to reach conduction oxide before the charge recombination [16].
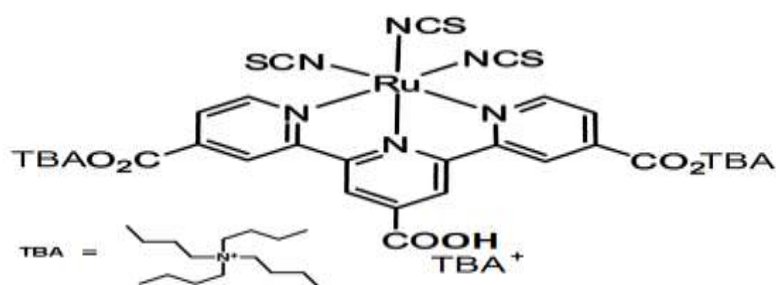

Figure 1. Structure of N749 sensitised dye [14].

Recently, the improvement of the performance of the solar cell by efficiency of DSSCs has increased to be reached more than 15%, it achieves with more extensive and low-cost ,it makes a crucial case for energy applications [17]. In this work, we extend a quantum donor-acceptor model based on the electron transfer theory with density-dependent transfer and strength coupling constants to calculate the current density and efficiency of N749 contact with titanium dioxide TiO_2 semiconductors in heterojunction solar cell devices.

2. Theory

The efficiency of DSSCs is defined as the ratio of output power to its incident light power density, as written by [18].

$$\eta = \frac{J_{Sc}V_{oc}.FF}{J_o} \times 100\% \qquad (1)$$

where J_o is incident light intensity($100\frac{mW}{Cm^2}$)and FF is the fill factor and gives ratio [19].

$$FF = \frac{J_m V_m}{J_{Sc}V_{oc}} \qquad (2)$$

Where J_m is the average of current density in open-circuit, V_m is the voltage in open-circuit, J_{Sc} is short-circuit current density, and V_{oc} is open circuit voltages. The current density in solar cell devices is given by [20].

$$I = eT(E) \sum[F(E_D) - F(E_A)] \qquad (3)$$

Where e is electronic charge, $F(E_D)$ and $F(E_A)$ are the Fermi distribution in donor and acceptor, $T(E)$ is the probability transmission coefficient. It is given by

$$T(E) = \frac{2\pi}{\hbar} |\langle C_{SCET}\rangle|^2 \rho_{eff}(E) \qquad (4)$$

Where, C_{SCET} is the strength coupling of electron transfer and $\rho_{eff}(E)$ is the effective density in the system written as [21].

$$\rho_{eff}(E) = \rho_S l_{eff} / \left(\frac{6}{\pi}\right)^{1/3} \qquad (5)$$

Where ρ_S is electronic density in semiconductors and l_{eff} is effective length .The electronic density in semiconductor is given by [22].

$$\rho_S = \rho_B(E)\langle\hat{\rho}\rangle d_S^{-2/3} \qquad (6)$$

Where $\rho_B(E)$ is the density of state of the Black dye system, d_s is the atomic density of semiconductors and $\langle\hat{\rho}\rangle$ is the density of state in system and given by:

$$\langle\hat{\rho}\rangle = \frac{e^{-\frac{(\lambda_S^B + \Delta u^0)^2}{4\lambda_S^B k_B T}}}{\sqrt{4\pi\lambda_S^B k_B T}} \qquad (7)$$

Here, λ_S^B and Δu^0 are transition energy and the driving free energy as functions of conduction band energy E_c and optical bandgaps Eg of N749($\Delta u^0 = E_c - E_g$). The transition energy λ_S^B (eV) in equilibrium is [23].

$$\lambda_S^B(eV) = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{D}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] - \frac{1}{2R}\left[\frac{n_{Sem}^2 - n^2}{n_{Sem}^2 + n^2}\frac{1}{n^2} - \frac{\varepsilon_{Sem}^2 - \varepsilon^2}{\varepsilon_{Sem}^2 + \varepsilon^2}\frac{1}{\varepsilon^2}\right]\right] \qquad (8)$$

Where, $\varepsilon_\circ$ is permittivity, D and $R = D_{N749} + D_{TiO_2}$ are the radius of the molecule and the distance between the molecule and semiconductor, n and ε are the refractive index and dielectric constant of the solvent, n_{Se} is the refractive index of semiconductor and ε_{Se} is the dielectric constant of semiconductor. The radius is [24].

$$D = \left(\frac{3}{4\pi}\frac{M}{N\rho}\right)^{\frac{1}{3}} \tag{9}$$

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

Inserting Eqs. (7), (6) and (5) in Eq.(4) to give

$$T(E) = \frac{2\pi}{\hbar}\frac{\rho_B(E)}{\sqrt{4\pi\lambda_S^B k_B T}}|\langle C_{SCET}\rangle|^2 e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}}\frac{l_{eff}}{\left(\frac{6}{\pi}\right)^{1/3}}d_S^{-2/3} \tag{10}$$

Inserting the Eq. (10) in Eq. (3) with $F(E) = [F(E_D) - F(E_A)]$ to result

$$I(E) = \frac{2\pi e}{\hbar}\frac{1)}{\sqrt{4\pi\lambda_S^B k_B T}}|\langle C_{CET}\rangle|^2 e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}}\frac{l_{eff}}{\left(\frac{6}{\pi}\right)^{1/3}}d_S^{-2/3}\int_0^E \rho_B(E)F(E)\,dE \tag{11}$$

The solution integral in Eq. (11) is given [25].

$$\int_0^E F(E)\rho_B(E)\,dE = n_s \tag{12}$$

Where n_s is the electronic concentration at the surface semiconductor's in unit (states cm-3). The Eq. (12) substituting in Eq. (11) to yield:

$$I(E) = \frac{2\pi e}{\hbar}\frac{1}{\sqrt{4\pi\lambda_S^B k_B T}}|\langle C_{SCET}\rangle|^2 e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}}\frac{l_{eff}}{\left(\frac{6}{\pi}\right)^{1/3}}d_S^{-2/3}n_s \tag{13}$$

The atomic density d_S calculates due to relation [25].

$$d_S = \frac{D_S}{D_n} \tag{14}$$

Where D_n is the number of states per atom per eV in the semiconductor and D_S is the density of states for the semiconductor as a function of carrier concentration N_e, at the Fermi level and the Fermi energy, E_F, and given by [25] .

$$D_S = \frac{3}{2}\left(\frac{N_e}{E_F}\right) \tag{15}$$

3. Results

A combination of the quantum picture of the donor-acceptor model and electron transfer theory was applied to scrutinize and calculate the current density cross-interface of N749 contact with TiO2 based DSSCs. Due to calculate the current density produces in N749-TiO$_2$ solar cell, it can be calculated the transition energy as a function of radius of N749 and TiO$_2$, dielectric and refractive index of solvent and TiO2 by using Eq. (8). The radii of N749 dye and TiO2 estimate using Eq.(9) by inserting molecular weight M=1364.98 g/mol [26] and M=79.866 g/mol [27] and density $\rho = 1.28\ \frac{g}{cm3}$ [26]) and $\rho = 4.23\ \frac{g}{cm3}$ [27] for N749 and TiO$_2$, respectively, results are 7.472 A^0 and 1.956 A^0 for N749 and TiO$_2$.

The transition energy was calculated onto the N749-TiO2 system with pure Dichloromethane solvent used in DSSCs by inserting refractive 2.609 and dielectric constant 55 of TiO_2 semiconductor [27] and refractive 1.4241 with dielectric constant of Dichloromethane (DCM) solvent 8.93 [28] in Eq.(8) with results $\lambda_S^B = 0.27 \ eV$ Next, the atomic density is calculated using Eq.(14) and (15) by taking The carrier concentration $N_e = 1.4 \times 10^{14} 1/cm^3$[29], Fermi energy $E_F = 4.52 eV$ [30], and take effective density of states $D_n = 8$ (states /eV) of TiO_2 [31] to result $d_{TiO2} = 5.80 \times 10^{12} \frac{1}{Cm^3}$. The electronic current produces from N749-TiO_2 with DCM solvent calculates using Eq. (13) with inserting the strength coupling $|\langle C_{CET} \rangle|^2$=0.1.0.2,0.3,0.4,0.5,0.6,0.7, 0.8, 0.9, 1,1.1and $1.5 \ x10-2$ |eV|^2, $\lambda_S^B = 0.27 \ eV$, effective length $l_{eff} = 3 \times 10^{-10} m$[32], atomic density $d_{TiO_2} = 5.80 \times 10^{12} \frac{1}{Cm^3}$ and concentration $n_s = (3.5,4.5) \times 10^{18} \frac{1}{Cm^3}$ [31] and $\Delta u^0 = 3.4 - 3.52 = -0.12 eV$ using MATLAP program, results show in the **Table (1).**

Table 1. Results of electronic current for N749-TiO_2 with (DCM) solvent.

Strength coupling $|\langle C_{CET} \rangle|^2 x10^{-2}$ (eV/ state)^2	The electronic current in (A)	
	The electronic concentration n_s ($\frac{1}{Cm^3}$)	
	3.5×10^{18}	4.5×10^{18}
0.1	6.0412E-04	7.7673E-04
0.2	1.2082E-03	1.5535E-03
0.3	1.8124E-03	2.3302E-03
0.4	2.4165E-03	3.1069E-03
0.5	3.0206E-03	3.8837E-03
0.6	3.6247E-03	4.6604E-03
0.7	4.2289E-03	5.4371E-03
0.8	4.8330E-03	6.2138E-03
0.9	5.4371E-03	6.9906E-03
1	6.0412E-03	7.7673E-03
1.1	6.6454E-03	8.5440E-03
1.2	7.2495E-03	9.3208E-03
1.3	7.8536E-03	1.0097E-02
1.4	8.4577E-03	1.0874E-02
1.5	9.0619E-03	1.1651E-02

The probed current density $J_m = \frac{I}{A}$ was calculated by the current relative to the area A of the cell (0.158 cm^2) [34] ,results list in **Table (2).**

Table 2. The current density calculated for N749-TiO$_2$ with DCM solvent.

Strength coupling $\|\langle C_{CET}\rangle\|^2 x10^{-2}$ (eV/ state)^2	Current density (A.cm^{-2})	
	The electronic concentration(cm^{-3})	
	3.5×10^{18}	4.5×10^{18}
0.1	3.8236E-03	4.9160E-03
0.2	7.6471E-03	9.8320E-03
0.3	1.1471E-02	1.4748E-02
0.4	1.5294E-02	1.9664E-02
0.5	1.9118E-02	2.4580E-02
0.6	2.2941E-02	2.9496E-02
0.7	2.6765E-02	3.4412E-02
0.8	3.0589E-02	3.9328E-02
0.9	3.4412E-02	4.4244E-02
1	3.8236E-02	4.9160E-02
1.1	4.2059E-02	5.4076E-02
1.2	4.5883E-02	5.8992E-02
1.3	4.9706E-02	6.3908E-02
1.4	5.3530E-02	6.8824E-02
1.5	5.7354E-02	7.3740E-02

The characteristic of current density J(mAcm2) verses voltage in Volt is shown in **Table (3)**

Table 3. The J -V characteristic of N749-TiO$_2$ devices

The electronic concentration			
3.5×10^{18}(1/cm^3)		4.5×10^{18}(1/cm^3)	
V(Volt)	Current(A/cm^2)	V(Volt)	Current(A/cm^2)
0.834	0	0.857	0
0.8	3.8236E-03	0.8	4.9160E-03
0.75	7.6471E-03	0.75	9.8320E-03
0.7	1.1471E-02	0.7	1.4748E-02
0.65	1.5294E-02	0.65	1.9664E-02
0.6	1.9118E-02	0.6	2.4580E-02
0.55	2.2941E-02	0.55	2.9496E-02
0.5	2.6765E-02	0.5	3.4412E-02
0.45	3.0589E-02	0.45	3.9328E-02
0.4	3.4412E-02	0.4	4.4244E-02
0.35	3.8236E-02	0.35	4.9160E-02
0.3	4.2059E-02	0.3	5.4076E-02
0.25	4.5883E-02	0.25	5.8992E-02
0.2	4.9706E-02	0.2	6.3908E-02
0.15	5.3530E-02	0.15	6.8824E-02
0.1	5.7354E-02	0.1	7.3740E-02
0	6.054 E-02	0	7.878 E-02

The characteristic of J−V curves of N749 dye-contact with TiO$_2$ solar cell devices using two concentrations 3.5×10^{18} (1/Cm^3)and 4.5×10^{18} (1/Cm^3) are shown in **Figure 2**.

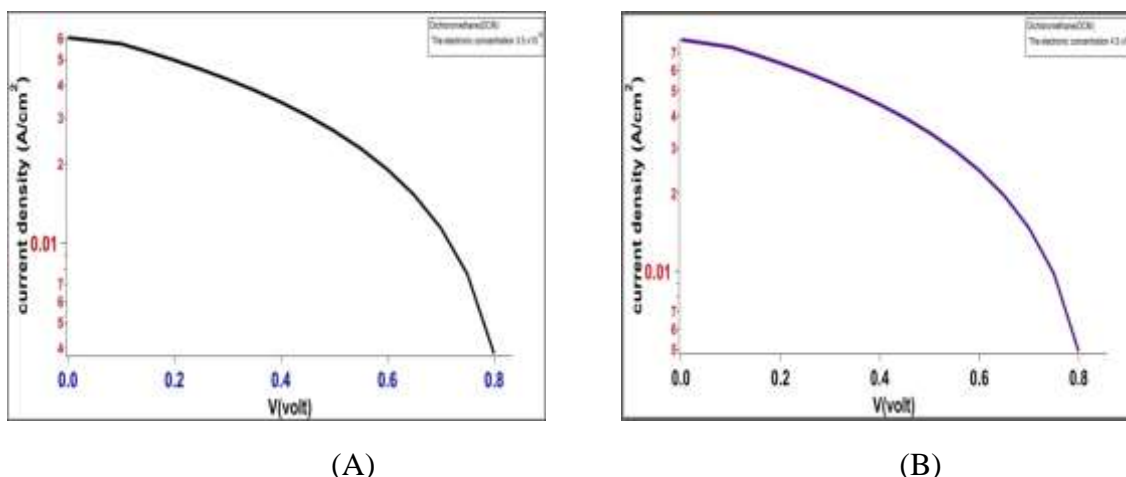(A)   (B)

Figure 2. The current density versus voltage under concentration $3.5 \times 10^{18}(1/cm^3)$ and 4.5×10^{18} ($1/cm^3$) of the same devices.

The fill factor and efficiency evaluate by using Eq. (2) and Eq. (1), respectively, with the data in **Table (3)** and **Figure 2**, and the results are shown in **Table (4)** for N749- TiO_2 devices

Table 4. The photovoltaic parameters calculated for the N749-TiO_2DSSCs sensitized

Variables	The electronic concentration	
	$3.5 \times 10^{18}1/cm^3$	$4.5 \times 10^{18}1/cm^3$
$J_{Sc}(mA/cm^2)$	60.54	78.78
V_{oc} Volt	0.864	0.867
$J_m(mA/cm^2)$	9.545	13.57
V_m Volt	0.7324	0.735
F.F	0.134	0.146
efficiency	6.990	9.974

4.Discussion

We looked at how well N749 black dye-in solar cells work with a dichloromethane (DCM) solvent and a TiO_2 photoanode. We used two different electron concentrations in the system because we thought that the concentration would have a great effect on how well the cells worked with the same solvent. Table 1 indicates that electronic current is influenced by the strength of the electronic coupling and carrier concentration of the N749-TiO_2 solar cell. We can find that the current increases upon increasing the strength of the electronic coupling from 0.1 to 1.5 eV. The concentration change of the electron-transfer cross-interface is related to the current density of N749- TiO_2 devices and is equal to the product of how well they work and how many electrons they transfer. As seen in **Table 2**, the current increased alternatively with an increased concentration of carrier in Table 2. In contrast, the reorganization energy (eV) provided the system with the required energy of about 0.27 eV to yield charge injection quantum, which means the system needs less energy than the reconfiguration system to start the electron transfer process from excited levels of N749 dye to the conduction band in TiO_2 semiconductor. A simple donor-acceptor model has been established that allows for the description of the kinetics of electronic current through system devices. In fact, the electronic transfer behavior is limited by the potential at the interface, but the effective transition energy supplied by the energy to transfer due to polar media is a function of the dielectric constant and refractive index. The current density J increased

when the concentration increased for all strength couplings in **Table 2**. A larger efficiency of solar cells is indeed expected when the carrier concentration of the system increases. The current-voltage characteristic, in turn, was what determined the efficiency. Also, the current density is affected by the transition energy and the strength of the coupling of electrons; as the strength of the coupling increases, so does the current density in devices that use solvent media. The decreases in transition energy indicated decreased potential at the interface and increases in electron transfer for large photocurrents. Upon excitation of the N749 dye, the current density of N749- TiO_2 is large at 4.5 compared with 3.5, which indicates an increase in electrons through the interface of the N749-TiO_2 device with DCM solvents.

Another important parameter affecting the performance of solar cells is the strength of the coupling. Furthermore, the significant role of the increased current density as a result of increasing the strength of the coupling of charge transfer and recombination was assessed by reorganization energy with both concentrations of N749/TiO_2 working in a DCM solvent medium, where the oxidation-reduction reaction between N749dye- and TiO_2 is used as an index to explain the charge transfer effect of the solar cell system. As can be seen, the currents were calculated in units (mA/cm^2) in Table (4) to estimate the efficiency, the current versus voltage is listed in **Table 3 and Figure 2**. From the data in Table 4, the average open-circuit photovoltage V_m(Volt) and current $J_m(\frac{mA}{cm^2})$ are estimated from **Figure 2** and formulated in **Table 4.** The performance of solar cells affects the strength of electronic coupling, and increasing the strength of electronic coupling plays a significant role in the increased current density. The recombination process is assessed by transition energy, strength of electronic coupling, and the carrier concentration of N749/ TiO_2 operation in the DCM media. Data results reported in Figures 2A and 2B show that in pure DCM solvent, the average open-circuit photovoltage V_m(Volt) and current J_m $(\frac{mA}{cm^2})$ estimated from **Figure 2** are listed in Table 4. The efficiency of the N749-TiO_2 calculated increased with carrier concentration increases, and the two curves closely matched the behaviour observed. To study the influence of carrier concentration during the optimization process, we take two values of carrier concentration in the cells $3.5 \times 10^{18} \ 1/cm^3$ and $4.5 \times 10^{18} \ 1/cm^3$, respectively, keep the distance between the N749 and TiO2 constant with the DCM solvent. It is clear that Eq. (1) indicates that efficiency is proportional to current density, and efficiency increases with an increase in current density and vice versa. As can be seen, the efficiency increased from 6.990 to 9.974 for the N749-TiO2 sensitised DSSCs. The increase in the concentration of electrons leads to an increase in current and efficiency. Table 4 shows the increases in efficiency with increasing concentration from $3.5 \times 10^{18} \ 1/Cm^3$ to $4.5 \times 10^{18} \ 1/Cm^3$ with transition energy for the N749/TiO2 system. The influence of electronic current is limited to the fill factor, efficiency and characteristic of the cell. Moreover, the concentration and strength of electronic coupling were influenced by V_{oc}, J_{sc}, FF, and efficiency, as summarized in Table 4. The peak of both the current density and voltage difference of the solar cell indicates of the electronic recombination at a given concentration value. As shown in table 4, in the solar cell of concentration $3.5 \times 10^{18} 1/Cm^3$, the peak-to-peak voltage and current density differences in the solar cell of concentration $4.5 \times 10^{18} 1/Cm^3$ are 0.003 V and 18.24 $\frac{mA}{cm^2}$, respectively.

From the data in **Table 3**, the average current and open-circuit photo voltage (V_{oc}) are estimated and formulated in Table 4. However, the fact that the voltage difference and peak current density both rise as the carrier concentration does suggests that there is more charge recombination, which makes the solar cell more efficient. The parameters of photovoltaic in Table 4 show that Voc, Jsc,

and efficiency increase with increasing the concentration of electrons, and decreasing the F.F further results in an increase in overall solar cell performance. These results are in agreement with the experimental results of I-V characteristic behavior in ref. [34].

5. Conclusion

 In summary, a simple donor-acceptor model has been used to study and evaluate the current density, fill factor, and efficiency of a heterojunction N749-TiO$_2$ device with DCM solvent for its potential in photovoltaic solar cell applications. The current density and efficiency in N749-TiO$_2$ devices are largely influenced by the carrier concentration and strength of the electronic coupling at limited transition energy. The efficiency was significantly enhanced from 6.990 to 9.974. The corresponding enhancement in efficiency can be attributed to the increased electron concentration in a system with limited transition energy, leading to an increase in electron transfer cross in N749-TiO$_2$ heterojunction devices, which in turn enhanced the I-V characteristic, fill factor, and efficiency of the solar cell.

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