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Theoretical Calculation of The Fill Factor of N749/TiO_2 Solar Cells

Naeem Nahi Abd ALI *
Department of Physics, Collage of Education for Pure Science Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq.

Hadi J. M. Al – Agealy
Department of Physics, Collage of Education for Pure Science Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq.

Hossain Milani Moghaddam
Department of Solid-State Physics, Faculty of Basic Sciences, University of Mazandaran, Babolsar, Iran.

***Corresponding Author:** Naeem.Nahi1104a@ihcoedu.uobaghdad.edu.iq

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Abstract

In this paper, the fill factor of the N749/$\mathbf{TiO_2}$ solar cell is studied and calculated using the analysis method at standard conditions; i.e., at room temperature T=300k and 100 $\frac{mW}{cm^2}$ irradiation. The current density was derived and calculated using the donor-acceptor model according to the quantum transfer theory in DSSC solar cells. We estimate the influence parameters in the dye-sensitized solar cells DSSC that's an equivalent circuit to the I-V curves for three solvents. The fill factor parameters of the N749/$\mathbf{TiO_2}$ device are found to be 0.137,0.146 and 0.127 with Butanol, Ethanol and Acetonitrile for carrier concentration $1.5 \times 10^{18} \frac{1}{cm^3}$ respectively. The photovoltaic characteristics I_{Sc} , V_{oc} , $I_m$and V_m are calculated depending on the current-voltage (J-V) characteristics of the device at room temperature. As a result of the fill factor analysis, N749/$\mathbf{TiO_2}$ cells showed different fill factors dependent on solvents type for the I_{Sc} and V_{oc} .

Keywords: The Fill Factor , N749/TiO_2 Solar Cells.

1. Introduction

The increased energy crisis and environmental problems will be necessary for the substantial exploration of renewable and clean energy materials[1]. The technology of renewable energy is vital part to reduce green-house gases and reduce all risks posed by global warm. Transition to renewable energies sources of electric was a vital solution to risks problems posed by global warm[2]. The electric generates from solar cells is the best option for the sustainable energy

requirement of the world [3]. Solar cells are an essential diverse entirety to be solved the increasing energy crisis that will eventually replace energy sources like fossil fuels in increasing resources [4]. Now, the dye-sensitized solar cells DSSC become a more significant great interest in technological of solar energy conversion as a result of low costs, optical properties and ease of production [5] . However, the DSSCs are promised devices consisting of a light-sensitive and another electrode together with an electrolyte can convert the light energy into electrical[6]. As such, the electron transfer process occurs from the donor to the acceptor level states[7], it requires to the alignment of both energy levels states and it is close to each other donor and acceptor.In addition to fundamental and important reactions, Hadi et al indicate that reorganization energy is the main parameter to understanding of mechanism electron transfer processes in variety electronic devices [8]. In heterostructure interfaces, the theory for electron transfer with molecules essentially occurred between molecule donor energy levels and solid acceptor under concept of donor-acceptor model for electron transfer potential [9]. The fill factor (FF) is an important parameter because it determines the power that a solar cell can generate. It's well known that it is influenced by the recombination current[10].The calculation of the fill factor in the current generation of DSSCs is the main key for further enhancement efficiency improvement[11].The calculation of current density and the fill factor role are used to calculate the efficiency of the solar cell [12]. Fill factor analysis of solar cells is the best and most efficient method to diagnose the thermal stability problem accurately[10]. In this work ,we study and calculate the fill factor of N749 contacted with TiO_2semiconductor depending on estimated the photovoltaic characteristics I_{Sc} , V_{oc} , $I_m$and V_m using the current-voltage (J-V) curves.

2.Theory

The fill factor defines as the ratio of actual max power for the production of short-circuit current (I_{sc}) and pen-circuit voltage (V_{oc}) . It calculates by using [13].

$$FF = \frac{V_{mp} I_{mp}}{V_{oc} I_{sc}} \qquad (1)$$

Where V_{mp} and I_{mp} are the maximum power voltage and current, V_{oc} and I_{sc} denote the open circuit voltage and the short circuit current are evaluated from current $I(E)$ – voltage $V(volt)$ curves . The electronic current $I(E)$ is given by [14].

$$I(E) = e \sum T(E) F(E) \qquad (2)$$

where $F(E)$ is the Fermi distribution of system , $T(E)$ is transmission coefficient and given by .

$$T(E) = \frac{2\pi}{\hbar} \, |\langle C_C \rangle|^2 \rho_e \, (E) \qquad (3)$$

Where C_C is strength of electronic coupling and $\rho_e(E)$ is effective density in system ,its written as [15].

$$\rho_e \, (E) = \rho_S l_e / \, (\frac{6}{\pi})^{1/3} \qquad (4)$$

where l_e is effective length and ρ_S is electronic density in semiconductor is [16].

$$\rho_S = \rho_B(E) d_S^{-2/3} \langle \hat{\boldsymbol{\rho}} \rangle \qquad (5)$$

Where $\rho_B(E)$ is the density of state in dye system , d_s is the atomic density of TiO_2 and $\langle\widehat{\boldsymbol{\rho}}\rangle$ is the density of state in system and writes as . $\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B T}$

$$\langle\widehat{\boldsymbol{\rho}}\rangle = \frac{1}{\sqrt{4\pi\lambda_S^B k_B T}} e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}} \qquad (6)$$

Where Δu^0 is the driving energy , k_B is the Boltzmann constant and T is room temperature .The reorganization energy λ_S^B (eV) is [17].

$$\lambda_S^B(eV) = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{D}\left[\frac{1}{n^2}-\frac{1}{\varepsilon}\right]-\frac{1}{2R}\left[\frac{n_{Sem}^2-n^2}{n_{Sem}^2+n^2}\frac{1}{n^2}-\frac{\varepsilon_{Sem}^2-\varepsilon^2}{\varepsilon_{Sem}^2+\varepsilon^2}\frac{1}{\varepsilon^2}\right]\right] \quad (7)$$

where e is electronic charge , $\varepsilon_\circ$ is permittivity. The D and R are the radius of the molecule and the distance between molecule and semiconductor, n and ε are refractive index and dielectric constant of solvent, n_{Se} is the refractive index of semiconductor and ε_{Se} is the dielectric constant of semiconductor. The radius is [18].

$$D = \left(\frac{3}{4\pi}\frac{M}{N\rho}\right)^{\frac{1}{3}} \qquad (8)$$

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

Furthermore, the fill factor is ratio relative to J-V curve's maximum power is unitless Inserting Eqs.(4) ,(5) and (6) in Eq.(3) to give

$$T(E) = \frac{2\pi}{\hbar}\frac{\rho_B(E)}{\sqrt{4\pi\lambda_S^B k_B T}}|\langle C_C\rangle|^2 e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}}\frac{l_e}{\left(\frac{6}{\pi}\right)^{1/3}} d_S^{-2/3} \qquad (9)$$

here λ_S^B is the useful transition energy, Δu^0 is the driving free energy and T is the temperature, inserting the Eq. (9) in Eq. (2) an assume continuum media for donor and acceptor and integrated to results .

$$I(E) = \frac{2\pi e}{\hbar}\frac{|\langle C_C\rangle|^2}{\sqrt{4\pi\lambda_S^B k_B T}} e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}}\frac{l_e}{\left(\frac{6}{\pi}\right)^{1/3}} d_S^{-2/3}\int_0^E \rho_B(E)F(E)\,dE \quad (10)$$

The solution integral in Eq.(10) is given [19].

$$\int_0^E \rho_B(E)F(E)\,dE = n_s \ldots\ldots (11)$$

Where n_s is electronic concentration at the semiconductor's ,the Eq. (10) becomes .

$$I(E) = \frac{2\pi e}{\hbar}\frac{|\langle C_C\rangle|^2}{\sqrt{4\pi\lambda_S^B k_B T}} e^{-\frac{(\lambda_S^B+\Delta u^0)^2}{4\lambda_S^B k_B T}}\frac{l_e}{\left(\frac{6}{\pi}\right)^{1/3}} d_S^{-2/3} n_s \qquad (12)$$

The atomic density d_S is [19].

$$d_S = \frac{3}{2D_n}\left(\frac{N_e}{E_F}\right) \qquad (13)$$

Where D_n is the number of states per atom per eV in the semiconductor , N_e is carrier concentration and E_F is the Fermi energy.

2. Results

The generic of N749/TiO_2 the solar cells may be described by a fill factor parameter according to the current density model consisting of a donor-acceptor ideal junction. The scenario calculates the current density parameters, which can fit the calculate and plot I-V curve and is estimated from the I-V curves all parameters to calculate the fill factor. The reorganization energy $\lambda_S^B(eV)$ can be calculated according to Eq. (7) and (8). The radii of N749 and TiO_2 are calculated due to Eq.(8) with inserting molecular weight and mass density M= 1364.98 g/mol and $\rho = 1.28\ \frac{g}{cm3}$ [20]) for N749 dye [20] and M=79.866g/mol and $\rho = 4.23\ \frac{g}{cm3}$ [21] for TiO_2 to results radii are 7.47 A^0 and 1.96 $A^0$for both N749 and TiO_2 respectively . The reorganization energy is deduced using Eq.(7) as follows ;we insert both dielectric constant 55 and refractive index 2.609 of TiO_2 semiconductor [21] and refractive index 1.3993**,** 1.359 22 and 1.3441with dielectric constant 17.51 **,** 24.55 and 37.5 of 1-Butanol , Ethanol(EtOH) and Acetonitrile(MeCN) solvents [22] the results are tabulated in **Table(1).**

Table 1. Results of calculated the reorganization energy $\lambda_S^B(eV)$ of N749 /$TiO2$ devices.

Type of solvents	Refractive index(n)[22]	Dielectric constant(ε)[22]	$\lambda_S^B(eV)$
1-Butanol	1.399	17.51	0.329
Ethanol(EtOH)	1.359	24.55	0.363
Acetonitrile(MeCN)	1.344	37.5	0.383

Atomic constant d_S calculates via Eq.(13) with taking concentration of carrier $N_e = 1.4 \times 10^{14} cm^{-3}$[23] and Fermi energy $E_F = 4.52eV$ [24] and density of states $D_n = 8$ (state /eV) of TiO2 [25] ,result is $5.80 \times 10^{18}\ \frac{1}{m^3}$.Taking into account the electronic concentration $n_s = 1.5 \times 10^{24}\ \frac{1}{m^3}$ [26], we determined the electronic current using Eq.(12) with appropriate electronic 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 $1.2\times 10^{-2}\ |eV|^2$, effective length $l_{eff} = 3A^0$[27] and $\lambda_S^B\ (eV)$ from **Table(1)** in accordance with the improved MATLAB program method, the results are list in **Table (2)** for N749/TiO_2 devices .

Table (2). The electronic current of N749 /TiO_2 devices with three solvents at carrier concentration $1.5 \times 10^{18}\ 1/cm^3$.

Strength coupling $\|\langle C_{CET}\rangle\|^2 x10^{-2}$ $\|eV\|^2$	The electronic current I(Amper)		
	1-Butanol	Ethanol	Acetonitrile
0.1	1.4166E-04	1.0010E-04	8.0888E-05
0.2	2.8331E-04	2.0019E-04	1.6178E-04
0.3	4.2497E-04	3.0029E-04	2.4266E-04
0.4	5.6663E-04	4.0038E-04	3.2355E-04

0.5	7.0828E-04	5.0048E-04	4.0444E-04
0.6	8.4994E-04	6.0057E-04	4.8533E-04
0.7	9.9160E-04	7.0067E-04	5.6622E-04
0.8	1.1333E-03	8.0076E-04	6.4710E-04
0.9	1.2749E-03	9.0086E-04	7.2799E-04
1	1.4166E-03	1.0010E-03	8.0888E-04
1.1	1.5582E-03	1.1010E-03	8.8977E-04
1.2	1.6999E-03	1.2011E-03	9.7066E-04
1.3	1.8415E-03	1.3012E-03	1.0515E-03
1.4	1.9832E-03	1.4013E-03	1.1324E-03
1.5	2.1249E-03	1.5014E-03	1.2133E-03

The current density of three sample devices would be obtained by dividing the results of the current on the area of the solar cell 0.158 cm^2 [28] results of current density for N749/TiO_2 with 1-Butanol , EtOH and MeCN solvents are shown in **Table (3).**

Table 3. Results of current density of N749 / TiO_2devices with three solvents at carrier concentration $1.5 \times 10^{18}\ 1/cm^3$.

Strength coupling $\|\langle C_{CET}\rangle\|^2 x10^{-2}$ $\|eV\|^2$	The current density A/cm^2		
	1-Butanol	Ethanol	Acetonitrile
0.1	8.9656E-04	6.3351E-04	5.1195E-04
0.2	1.7931E-03	1.2670E-03	1.0239E-03
0.3	2.6897E-03	1.9005E-03	1.5359E-03
0.4	3.5862E-03	2.5341E-03	2.0478E-03
0.5	4.4828E-03	3.1676E-03	2.5598E-03
0.6	5.3794E-03	3.8011E-03	3.0717E-03
0.7	6.2759E-03	4.4346E-03	3.5837E-03
0.8	7.1725E-03	5.0681E-03	4.0956E-03
0.9	8.0691E-03	5.7016E-03	4.6076E-03
1	8.9656E-03	6.3351E-03	5.1195E-03

1.1	9.8622E-03	6.9687E-03	5.6315E-03
1.2	1.0759E-02	7.6022E-03	6.1434E-03
1.3	1.1655E-02	8.2357E-03	6.6554E-03
1.4	1.2552E-02	8.8692E-03	7.1673E-03
1.5	1.3448E-02	9.5027E-03	7.6793E-03

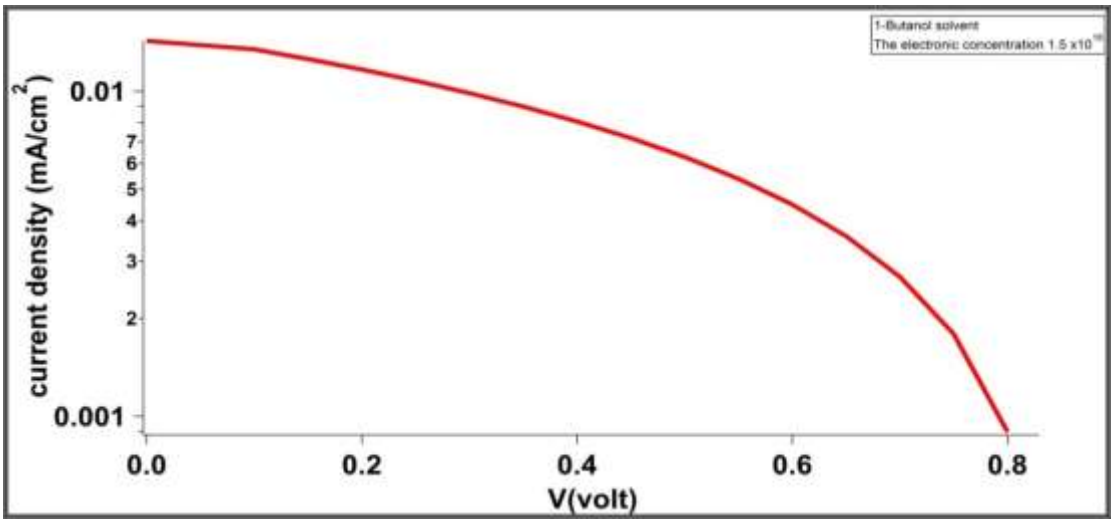
However, the I -V characteristic of current density I(mAcm2) and voltage in Volt at carrier concentration $1.5 \times 10^{18} \frac{1}{cm^3}$is shown in table (4) for 1-Butanol , Ethanol (EtOH) and Acetonitrile (MeCN) solvents devices .

Table 4. Results of I-V characteristic of N749 TiO_2devices with three solvents at carrier concentration $1.5 \times 10^{18}\ 1/cm^3$.

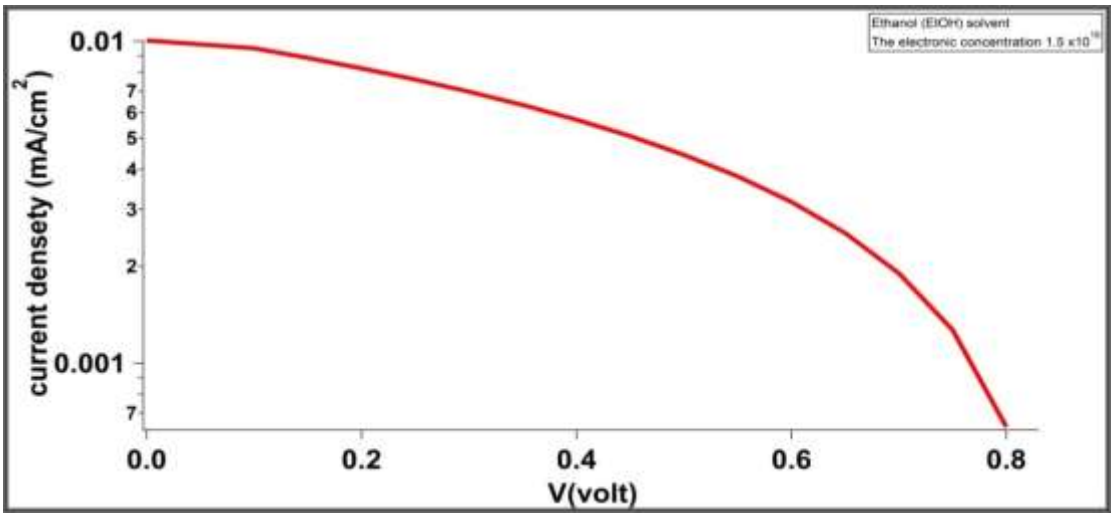
Butanol		Ethanol		Acetonitrile	
V(Volt)	$I(A)$	V(Volt)	$I(A)$	V(Volt)	$I(A)$
0.829	0	0.8423	0	0.8423	0
0.8	8.9656E-04	0.8	6.3351E-04	0.8	5.1195E-04
0.75	1.7931E-03	0.75	1.2670E-03	0.75	1.0239E-03
0.7	2.6897E-03	0.7	1.9005E-03	0.7	1.5359E-03
0.65	3.5862E-03	0.65	2.5341E-03	0.65	2.0478E-03
0.6	4.4828E-03	0.6	3.1676E-03	0.6	2.5598E-03
0.55	5.3794E-03	0.55	3.8011E-03	0.55	3.0717E-03
0.5	6.2759E-03	0.5	4.4346E-03	0.5	3.5837E-03
0.45	7.1725E-03	0.45	5.0681E-03	0.45	4.0956E-03
0.4	8.0691E-03	0.4	5.7016E-03	0.4	4.6076E-03
0.35	8.9656E-03	0.35	6.3351E-03	0.35	5.1195E-03
0.3	9.8622E-03	0.3	6.9687E-03	0.3	5.6315E-03
0.25	1.0759E-02	0.25	7.6022E-03	0.25	6.1434E-03
0.2	1.1655E-02	0.2	8.2357E-03	0.2	6.6554E-03
0.15	1.2552E-02	0.15	8.8692E-03	0.15	7.1673E-03
0.1	1.3448E-02	0.1	9.5027E-03	0.1	7.6793E-03

0	1.4278E-02	0	10.0507E-3	0	10.0507E-3

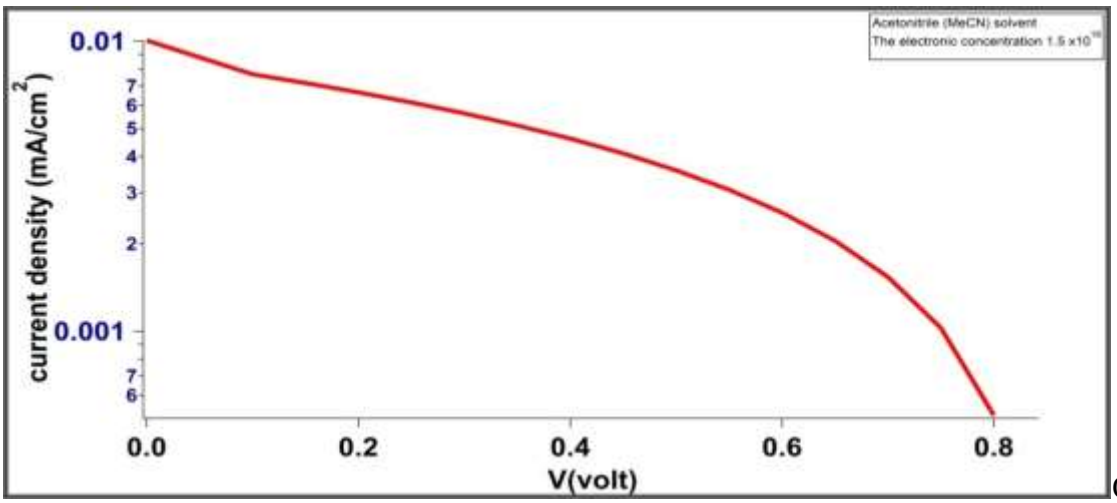
The values of I-V parameters are obtained according to the plot of the calculated I-V data, as shown in **Figure 1.**



A



B



C

Figure 1. Shows the I-V graph of N749/TiO_2 device with A-1-Butanol , B-Ethanol(EtOH) and C-Acetonitrile(MeCN) solvents.

The $I_{Sc}(mA/cm^2)$, V_{oc} Volt , $I_m(mA/cm^2)$ and V_m Volt can be obtained from the I-V curve in figure(1) ,the values of these parameters with three solvents at carrier concentration $1.5 \times 10^{18}\ 1/cm^3$ are listed in table (5) below.

Table 5. Results of illuminated I-V calculated and fill factor of N749 /TiO_2 devices with three solvents at carrier concentration $1.5 \times 10^{18}\ 1/cm^3$.

Variables	The electronic concentration $1/cm^3$		
	Butanol	Ethanol	Acetonitrile
$I_{Sc}(mA/cm^2)$	1.428 E-02	1.0057E-2	1.005E-02
V_{oc} Volt	0.829	0.8301	0.842
$I_m(mA/cm^2)$	2.193E-03	1.676E-03	1.479E-03
V_m Volt	0.738	0.728	0.728
F.F	0.137	0.146	0.127

The fill factor is calculated for three sample devices using Eq.(1) by inserting the values of current and voltage from the **Table(5)** to results0.137 , 0.146 and 0.127 for N749 /TiO_2 devices with 1-Butanol , Ethanol(EtOH) and Acetonitrile(MeCN) solvents

4. Discussion

For the heterojunction N749/TiO_2 photovoltaic, the current density (I) is calculates as a function of reorganization energy and strength coupling with same values of concentration and atomic mass results of the reorganization energy of the N749/TiO_2 are shown in **Table(1),** these results reveal slightly increasing with increasing the dielectric constant and with decreasing the refractive index of solvents. The results of reorganization energy indicated the ability of system with solvents to start electron transfer process more efficiently .The results of reorganization energy is more effect on the quantity of current and current density and finally effected the characteristic of solar cell through effecting the fill factor and efficiency of cells. The results in **Table(1)** are obtained by stepwise changing the value of polarity parameter of solvents in reorganization energy expression .The N749/TiO_2 photovoltaic has low reorganization energy 0.329 eV with 1-Butanol solvent comparing with large reorganization energy 0.383 eV with Acetonitrile solvents .

To investigate the photovoltaic performance of N749/TiO_2 device, we must estimate the quantitative values of fill factor (FF) according to calculate current density and graph I-V in **Figure (1)**.**Table (2)** shows the currents are different with varied reorganization energy and the strong coupling values of the N749/TiO_2 solar cell. The current decreases upon increasing the reorganization energy but current increases with increasing the strength coupling , as seen in the current increased alternatively with increasing strength coupling from $0.1 \times 10^{-2}|eV|^2$ to reach maximum current at $1.5 \times 10^{-2}|eV|^2$. The increased value of current and current density is ascribed to the transfer of more electron-hole pairs in the absorber N749/TiO_2 system which separates into electrons and holes at the interface of N749/TiO_2 heterojunction, it leads to an excess of photocurrent. In fact, the current and current density in **Tables (2) and (3)** decrease with increasing the reorganization energy and reach to higher current density with 1-Butanol solvent comparing with lower current density with Acetonitrile solvents . Furthermore, the maximum current density was 1.3448E-02 with 1-Butanol comparing with minimum current density was 7.6793E-03 with Acetonitrile and it increased with increasing strength coupling . Three curves of current density I(mA/Cm^2) vs. Voltage (volt) of heterojunction N749 black dye-TiO_2 in solar cell devices at concentrations $1.5 \times 10^{18}\ 1/Cm^3$ plotted and instead as shown in **Figure 1** which are calculated at STC, i.e. 100 mW/ Cm^2 and 25 0C. The curves are the calculated I-V curves, which are obtained by theoretical donor-acceptor model for electron transfer. Depending on the I-V curves, the values of parameters I_{Sc} , V_{oc} , $I_m$and V_m can be fixed and gained respectively ,there are limited in **Table(5).** The electron transfer significantly influences the I_{Sc} of the I-V curve, which is moved through interface from donor to acceptor in variety devices of solar cells. That Isc could be improved slightly by increasing the electron transfer from donor to acceptor .Also ,the V_{oc} increases slightly when I_{Sc} increased, while obvious change in both I_m and V_m are observed .The influence of the I_m and V_m parameters on the estimation of fill factor from the I-V curve, therefore ,it is quantificational revealed as seen in **Table(5).** In turn and based on the parameters that's gotten above, the values of the fill factor of each curve is obtained .The difference in fill factor was obvious, this difference indicated the difference in efficiency of solar cell.The fill factor of system devices is higher with Ethanol and reach to 0.146 ,while the fill factor was minimum and determined to equal 0.127 with Acetonitrile solvent for N749/TiO_2 devices .The fill factor was not uniform with reorganization energy and I-V characteristic .However, the non-uniformity indicated to the different solvents type that used in N749/TiO_2solar cells devices, which might be due to the uneven and effect of electron transfer rate of N749/TiO_2 during the charge transfer process. The I_{Sc}significantly effected the V_{oc} of the I-V curve, which is co-directionally moved following the variety of I_{Sc}. When I_m increases, no obvious change was observed Fill Factor and the shape of I-V curve in **Figure (1). Figure (1)** shows three I-V curves and become more declining between the maximum I_{Sc} point and the maximum point voltage .No obvious change was observed in V_{oc} and I_{Sc} and the shape of I-V curve when fill factor varies, so that FF is varied when I_m decreases .In fact , the fill factor was influenced by I_m and V_m .

5. Conclusions

In conclusion, the fill factor increases with increasing both I_m and V_m and dependence of the I_{Sc} and V_{oc} of N749/TiO_2 cells based on the donor-acceptor model. It was confirmed that reorganization energy effected the current density . However, the I_m and V_m are the main parameters that dominantly contribute to fill factor ,the fill factor different depending on the Im

of the devices .For N749/TiO_2 devices , the I_{Sc} and V_{oc} were the main parameters of fill factor decreases . However, the contribution of the fill factor decreased as the $I_{Sc}$to rose with increasing I_m .It can be estimated that the N749/TiO2 cell has potential improved fill factor by optimizing I_m and V_m or decreasing I_{Sc} and V_{oc}On the other hand N749/$TiO_2$with Ethanol has a higher fill factor ratio 0.146 than other solvents, but the ratio of fill factor reduced to 0.127 with Acetonitrile due to the rapid decrease in the I_m and V_m. Therefore, we suggest that optimize the fill factor led to reduce the I_{Sc} for the N749/TiO_2cell by optimizing the N749/TiO_2 contacts and electron transfer .

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