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Article

Theoretical Studies on the Effect of Sensitizing Dyes on yhe Performance of Ruthenium Dye-Sensitized Solar Cells DSSCs Based on Quantum Electronic Transition

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Abstract: In this work, the efficiency and characteristic of ruthenium sensitized based on TiO2 semiconductor in dye sensitized solar cells DSSCs are calculated and studied using electron transfer theory .The electron transfer raction occurred from the donor state in excited ruthenium dye N3 and N719 dyes to the acceptor state in the semiconductor TiO2 has been elucidated. The current density was calculated using the quantum charge transport theory, based on the donor-receiver model. In this model, the current density as results of electron transfer from the excited N3 and N719 dyes into the TiO2 is subjected to the effects of reorganization energy, the atomic density, and the charge concentration and coupling.The reorganization energy a N3/TiO2 and N719/TiO2 cells depends greatly on polarity of the acetonitrile solvent medium, the physic strength, al structure of N3 ,N719 and TiO2 materials the distance between the N3 and N719 dyes and TiO2.A high reorganization energy for N3/TiO2 decreases the probability of electron transfer and increase reocobination charge , while a low reorganization energy for N719/TiO2 increases the rate of electon transfer and decreases the rate of reocobination charge. A discussion of the reorganization energy reveals that N3,N719 , TiO2 and acetonitrile solvent properties play a crucial role in modifying electron transfer between N3 and N719 dyes and TiO2 surfaces under different coupling strength, and room temperatures. The current density increases significantly with decreasing the reorganization energy and increasing coupling overcoming, as a result of the increased alignment energy level of the materials system.The high current density occurred mainly as a result of the strong bond between the N719 dye and TiO2 comparing with low at N3 with TiO2 , which led to increased wavefunction overlap at the interface, thus enhancing the electron transport of the N719/TiO2 device. Based on the results, the overall performance of the N719/TiO2 device can be improved by increased charge transport and reach to 5.337% larger than 3.783% for N3/TiO2 , where reorganization energy affects controls, and coupling controls the electron transport.

Keywords: Sensitizing Dyes , Ruthenium, Quantum, Electronic Transition,N3,N719,TiO2.

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Introduction

Over the past few decades, the depletion of fossil fuel resources, as a result of the world's unprecedented economic growth, increased energy consumption, and greenhouse gas emissions, has been one of the most important environmental

challenges that has prompted intensive efforts to promote renewable and clean energy sources [1]. Receltaly, organic dye sensitized solar cells (photovoltaic cells) have received increasing attention due to their flexibility, low cost, and light weight.To date, the efficiency of these organic cells has reached more than 13%, thanks to large studies on the integrated innovation of materials and the architecture of electronic devices[2]. The renewable energy sector is moving towards low-cost renewable energy sources, such as solar, wind, and hydroelectric power, with the aim of reducing emissions and achieving climate goals. In light of these developments, the sun is considered a primary energy source, providing a clean and convenient source of power, and can play a pivotal role in future energy solutions [3]. One of the many types of solar cells, dye-sensitized solar cells (DSSCs) are gaining increasing attention and are considered a practical option due to their low cost and high efficiency in converting sunlight into electricity [4]. Dye-sensitive solar cells (DSSCs), known for the pioneering work of Gratzel and Brian O'Regan, are an important research topic in solar energy conversion technology due to their ease of manufacture, low cost, environmental friendliness, and high efficiency [5].Today, solar cells come in different generations. The first generation relies on semiconductors made of silicon, which are more expensive than fossil fuel energy sources.The second generation consists of thin films (cadmium telluride (CdTe) and cadmium sulfide (CdS), amorphous silicon, and microcrystalline silicon. The third generation includes technologies such as organic materials, perovskites, DSSC (dye-sensitized solar cells), quantum dots, and multi-junction cells[6]. DSSC cells are considered an efficient and promising technology in the field of photovoltaic cells. They are clean-energy photovoltaic devices that are relatively low-cost and easy to manufacture in electronic applications [7]. The TiO2 used in dye-sensitized solar cells (DSSCs). It is a wide-bandgap semiconductor with an adsorbed dye that is regenerated by an electrolyte solution containing an oxidation-reduction intermediate [8]. In organic solar cells, the active medium is an integral part of them, and usually consists of donor and acceptor materials [9]. DSSC cells consist of an electrode attached to a titanium dioxide (TiO2)-sensitive dye, a counter electrode, and an electrolyte solution containing a redox medium. These cells function when the dye is excited by incident photon light and electrons are injected into the conduction band of the titanium dioxide. The injected electrons transfer to the counter electrode, and the redox medium is reduced to the counter electrode. Finally, the excited dye returns to its ground state by electrons accepted from the redox medium [10]. In DSSC cells, electron transfer from dye to a semiconductor can occur across the interfaces. Therefore, the compatibility of energy levels at these interfaces is a key criterion for understanding these cells [11]. Depending on the composition and properties of the photosensitive organic ruthenium dye , both optically and electrochemically, it can be used in solar cells [12]. The electron transport reaction is a fundamental process for discussing the understanding of how solar cells and a variety of electronic devices operate [13]. Electron transfer is a fundamental process in solar cells, and it depends on the transfer of photoexcited electrons from the excited molecular dye contact point to semiconductor-based DSSC solar cells [14]. Based on a simplified model of Marcus theory, the process of electron transfer from the excited state in dye to conduction band in semiconductors is a fundamental process in optoelectronic devices in particular [15].In DSSC cells, the N719 and N3 ruthenium complex dyes are among the most studied and used photosensitive materials due to their high stability, exceptional oxidation-reduction properties, high absorption , and higher ability to inject electrons into titanium dioxide [16]. Ruthenium N3 has superior light absorption and electron transfer capabilities to the conduction band, thus improving overall device efficiency. This compound shows great potential in improving the solar energy collection efficiency

of dye-sensitized solar cells (DSSCs) [17]. The ruthenium N719 dye is an organic dye has main sensitization, higher absorption, good stablility with interesting electronic and optoelectronic properties and is main sensitizer for DSSCs based on its broading absorption [18]. This work aims to highlight the potential impact of ruthenium dyes N3 and N719 on the performance of titanium dioxide (TiO2)-based dye-sensitized solar cells (DSSCs), using quantum electron transport theory to improve sustainable energy solutions. N3 and N719 dyes were used as contact sensitizers for titanium dioxide in acetonitrile solvents within the DSSCs. The rearrangement energy was calculated assuming continuous energy levels, while the fill factor and efficiency were calculated based on current density.

Theory

The quantum electron transfer probability is a fundamental parameters used to determine the current density in solar cells ,it is written by [19].

$$|T_R| = \frac{4\pi^2}{h}\int_0^E |\langle K_E\rangle|^2 \rho_E(E_D - E_A)dE \qquad (1)$$

Where h is the Planck constant, $\langle K_E\rangle$ is expectation values of strength coupling and $\rho_E(E_D - E_A)$ is the density of state and E_D and dye E_A are energies in dye and acceptor in conduction band in semiconductor.The density of state $\rho_E(E_D - E_A)$ in dye- semiconductor is [20].

$$\rho_E(E_D - E_A) = \langle \hat{\boldsymbol{\rho}}_{\boldsymbol{p}}\rangle \rho_A^{-2/3} \frac{l_s}{(\frac{6}{\pi})^{1/3}} \rho_D(E) \qquad (2)$$

Where $\langle \hat{\boldsymbol{\rho}}_{\mathbf{p}}\rangle$ is activation electronic density, ρ_A is the atomic density ,l_s is the path length in semiconductor and $\rho_D(E)$ is the electronic density of the semiconductor. The activation electronic density, $\langle \hat{\boldsymbol{\rho}}_{\mathbf{p}}\rangle$ for charge transfer from donor dye to conduction band of semiconductor acceptor is [21].

$$\langle \hat{\boldsymbol{\rho}}_{\mathbf{p}}\rangle = \frac{e^{-\frac{\left(\Lambda_C^R + \Delta U^0\right)^2}{4\Lambda_C^R k_B T}}}{\sqrt{4\pi\Lambda_C^R k_B T}} \qquad (3)$$

Where Λ_C^R(eV) is transition energy , ΔU^0 is driving energy , k_B is the Boltzmann constant and T is temperature. The driving energy is function as band energy E_b and chemical potential q^o for dye [22].

$$\Delta U^0 = E_b - q^o \qquad (4)$$

Subtititing the Eq. (4) and Eq. (3) in Eq. (2) to results.

$$\rho_E(E_D - E_A) = \frac{e^{-\frac{\left(\Lambda_C^R + \Delta U^0\right)^2}{4\Lambda_C^R k_B T}}}{\sqrt{4\pi\Lambda_C^R k_B T}} \rho_A^{-2/3} \frac{l_s}{(\frac{6}{\pi})^{1/3}} \rho_D(E) \qquad (5)$$

Substituting Eq.(5) in Eq.(1) to obtain.

$$|T_R| = \frac{4\pi^2}{h}\int_0^E |\langle K_E\rangle|^2 \frac{e^{-\frac{\left(\Lambda_C^R + \Delta U^0\right)^2}{4\Lambda_C^R k_B T}}}{\sqrt{4\pi\Lambda_C^R k_B T}} \rho_A^{-2/3} \frac{l_s}{(\frac{6}{\pi})^{1/3}} \rho_D(E)dE \qquad (6)$$

The reorganization energy Λ_C^R(eV) of dye-semiconductor system is [23].

$$\Lambda_C^R(\text{eV}) = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{r}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] + \frac{1}{2D_D}\left[\left(\frac{\varepsilon_{Sem}^2 - \varepsilon^2}{\varepsilon_{Sem}^2 + \varepsilon^2}\right)\frac{1}{\varepsilon^2} - \frac{n_{Sem}^2 - n^2}{n_{Sem}^2 + n^2}\right)\left(\frac{1}{n^2}\right)\right]\right] \qquad (7)$$

where e , ε_0 , r and D_D are charge, permittivity , radius of RuN3 or CdSe and distance between dye and semiconductor, S_{sem} are s, $n_{sem}$and n are the dielectric constant and refractive index of the semiconductor and solvents. The radius of the dye molecule is [24].

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

Where M is the molecular weight, N_A is Avogadro's number, and ρ is the mass density.The current insolar cell, J_E that produced fro electron transfer from dye to semiconductor is given by [25]:

$$\mathbf{J_E} = \mathbf{q}|\mathbf{T_R}| \qquad (9)$$

where $\boldsymbol{q}$ is charg of electron , substitute Eq. (6) into Eq. (9) with Fermi distribution will result:

$$\mathbf{J_E} = \frac{\mathbf{4q\pi^2}}{\mathbf{h}} \int_0^{\mathbf{E}} |\langle \mathbf{K_E} \rangle|^2 \frac{e^{-\frac{\left(\Lambda_C^R + \Delta U^0\right)^2}{4\Lambda_C^R k_B T}}}{\sqrt{4\pi\Lambda_C^R k_B T}} \boldsymbol{\rho}_\mathbf{A}^{-2/3} \frac{\mathbf{l_s}}{(\frac{6}{\pi})^{1/3}} \boldsymbol{\rho}_\mathbf{D}(\mathbf{E}) \mathbf{f_{(k)}} \mathbf{dE} \qquad (10)$$

The current density estimate by divides Eq.(10) on area of cell A and simply to produce.

$$\mathbf{J_{EC}} = \frac{\mathbf{4q\pi^2}}{\mathbf{hA}} |\langle \mathbf{K_E} \rangle|^2 \frac{e^{-\frac{\left(\Lambda_C^R + \Delta U^0\right)^2}{4\Lambda_C^R k_B T}}}{\sqrt{4\pi\Lambda_C^R k_B T}} \boldsymbol{\rho}_\mathbf{A}^{-2/3} \frac{\mathbf{l_s}}{(\frac{6}{\pi})^{1/3}} \int_0^{\mathbf{E}} \boldsymbol{\rho}_\mathbf{D}(\mathbf{E}) \mathbf{f_{(k)}} \mathbf{dE} \qquad (11)$$

The **solved** integral in Eq.(**11**) results to concentration [A] **by**[26].

$$\int_0^{\mathbf{E}} \boldsymbol{\rho}_\mathbf{D}(\mathbf{E}) \mathbf{f_{(k)}} \mathbf{dE} = [\mathbf{A}] \qquad (12)$$

Insert Eq. (12) in Eq.(11) to results.

$$\mathbf{J_{EC}} = \frac{\mathbf{4q\pi^2}}{\mathbf{hA}} |\langle \mathbf{K_E} \rangle|^2 \frac{e^{-\frac{\left(\Lambda_C^R + \Delta U^0\right)^2}{4\Lambda_C^R k_B T}}}{\sqrt{4\pi\Lambda_C^R k_B T}} \boldsymbol{\rho}_\mathbf{A}^{-2/3} \frac{\mathbf{l_s}}{(\frac{6}{\pi})^{1/3}} [\mathbf{A}] \qquad (13)$$

The efficiency of solar cells can calculate as function a fill factor FF using [27].

$$\boldsymbol{\eta} = \frac{\boldsymbol{FFJ_{Sc}.V_{oc}}}{\boldsymbol{P_{in}}} \times \mathbf{100}\% \qquad (14)$$

where$\boldsymbol{V_{oc}}$ (V) and $\boldsymbol{J_{sc}}$ ($\boldsymbol{mA/cm^2}$) and $\boldsymbol{P_{in}}$ are short-circuit ,current density and voltage input power.FF is calculated for the solar cells using [28].

$$\mathbf{FF} = \frac{\boldsymbol{Jm \times Vm}}{\boldsymbol{J_{sc} \times V_{oc}}} \qquad (15)$$

Results

Due to transition theory, the current density $\mathbf{J_{EC}}(\frac{mA}{cm^2})$ calculation in the ruthenium N3 and N719 contact with TiO_2 based DSSCs solar cells may acceptable method to evaluation the efficiency and studies of characteristics of the DSSC.The reorganization energy in Eq.(7) is active parameters affected on current density in Eq.(13). However , the reorganization energy of the both N3/TiO2 and N719 / TiO2 solar cells is a function of the refractive index and dielectric constant of acetonitrile solavent and TiO2 semiconductor and radii of N3,N719 and TiO2 ,respectively . The radii of N3 ,N719 dyes and TiO_2 calculate using Eq.(8) taken the molecular weight M(705.64$\frac{\text{g}}{\text{mol}}$[29],1188.55g/mol[30] and79.866g/mol [30]) and density (1.36$\frac{\text{g}}{cm^3[24]}$[31], 1.52 $\frac{\text{g}}{\text{cm3}}$[30] and 4.23$\frac{\text{g}}{\text{cm3}}$[30])for of N3 ,N719 dyes and TiO_2 results are5.93 A^0, 6.769 $A°$ and 1.956 $A^0$for N3,N719 and $Ti0_2$. The reorganization energy $\boldsymbol{\Lambda_C^R}$ (eV) of electron transfer process from N3 or N719 to TiO2 can calculate using Eq.(7) with MATLAP software and taken refractive index 2.609 and dielectric constant 55 of TiO2 [32], refractive index 1.3441and dielectric constant 37.5of Acetonitrile (MeCN) [21] to results $\boldsymbol{\Lambda_C^R}$ (0.435 and 0.427)eV for N3/ TiO2 or N719/ TiO2 solar cells. In essence, the J-V characteristics can investigate to calculate the efficiency of DSSC , it depends on the current density . The current density given in Equation (13) for N3/ TiO2 or N719/ TiO2 solar cells affected by the reorganization energy because it is provided a suitable energy levels for initiating the electron transfer process. The current density $\mathbf{J_{EC}}$ of N3/TiO2 and N719/TiO2 solar cells with acetonitrile solvent calculates using Eq. (13) taken account $\boldsymbol{\Lambda_C^R}$ (0.435 and 0.427)eV , the cell area A (0.490cm²)[32],$\boldsymbol{\rho_A} = 5.81 \times 10^{12} \frac{1}{cm^3}$[33], the strength coupling $\langle \mathbf{K_E} \rangle$ [0.035,0.050,0.060,0.067,0.075,0.080,0.085,0.090,0.095,0.105,0.115,0.125,0.135,0.145 and 0.155]eV, $l_s = 3A^0$[33], and concentration(3×10^{18} $\frac{1}{\text{cm}^3}$) [34], , results show in table(1).

Table 1. Results of current density $\mathbf{J_{EC}}(\frac{\mathbf{mA}}{\mathbf{cm^2}})$ calculation for N3/$Ti0_2$ and N719/$Ti0_2$with Acetonitrile solvent.

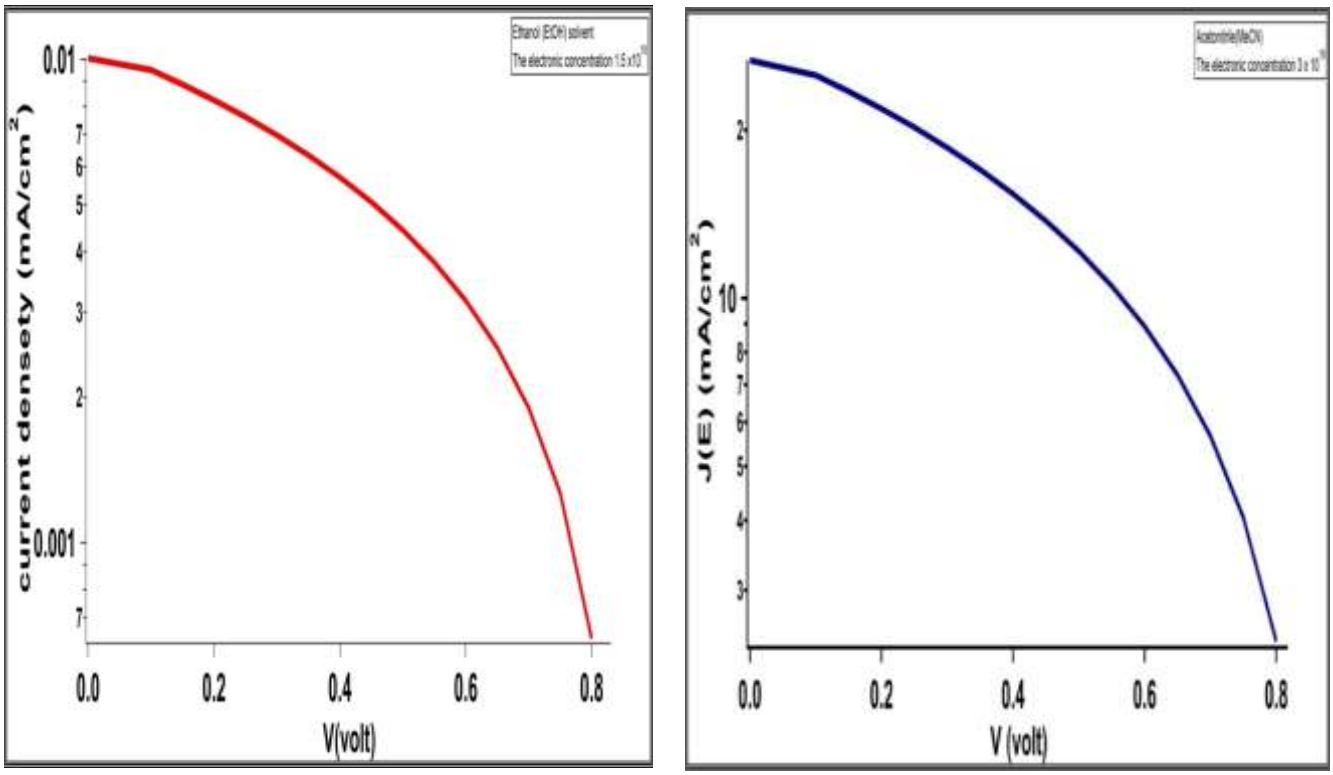
Strength coupling $\langle \mathbf{K_E} \rangle$ eV	The electronic concentration	
	N3/$Ti0_2$	N719/$Ti0_2$
0.035	1.195	2.430
0.050	2.376	4.347
0.060	3.594	6.666
0.067	4.783	7.510
0.075	5.973	8. 038
0.080	6.168	9. 225
0.085	7.373	10.143
0.090	7.667	11.061
0.095	8.231	12.376
0.105	8.987	13.836
0.115	9.146	14.724
0.125	9.476	15. 612
0.135	9.289	17.551
0.145	9.629	19.477
0.155	9.979	21.094

.The characteristic of $\mathbf{J_{EC}}$-V for N3/TiO2 and N719/TiO2 solar cells using the simulation MAT:LAB software using theoretical approach of current density $\mathbf{J_{EC}}$ (mAcm2) and voltage in Volt as can be shown in Table(2).

Table 2. Results of voltage V(Volt) verse current density $\mathbf{J_{EC}}\left(\frac{\mathbf{mA}}{\mathbf{cm^2}}\right)$for N3/TiO2 and N719-$Ti0_2$ with Acetontrile solvent.

The electronic concentration			
N3/TiO2		N719-TiO2	
V(Volt)	$J(\frac{mA}{cm^2})$	V(Volt)	$J(\frac{mA}{cm^2})$
0.805	0	0.811	0
0.8	1.195	0.8	2.430
0.75	2.376	0.75	4.347
0.7	3.594	0.7	6.666
0.65	4.783	0.65	7.510
0.6	5.973	0.6	8. 038
0.55	6.168	0.55	9. 225
0.5	7.373	0.5	10.143
0.45	7.667	0.45	11.061
0.4	8.231	0.4	12.376
0.35	8.987	0.35	13.836
0.3	9.146	0.3	14.724
0.25	9.476	0.25	15. 612
0.2	9.289	0.2	17.551
0.15	9.629	0.15	19.477
0.1	9.979	0.1	21.094
0	10.108	0	22.234

In fact, the fill factor and efficiency can be calculated when ploted the curve between current denxity and voltage $\mathbf{J_{EC}}$-V for N3/TiO2 and N719/TiO2 .cells,it can be shown in Figure 1



(A) (B)

Figure 2. The characteristic $\mathbf{J_{EC}}$-V of A)the N3/$Ti0_2$devices and B) N719/$Ti0_2$ with MeCN solvents.

However, the fill factor and efficiency calculate using Eq. (15) and Eq. (14) respectively using the results in Table (2) and curves in Figure 1 to determining the average open circuit current $J_{Sc}$and voltage V_{oc}, the results are shown in Table 3 under simulated AM 1.5 global sunlight (1 Sun, 100 mWcm−2) .

Table 3. The fill factor and efficiency of N3/TiO2 and N719/$Ti0_2$ DSSCs with Acetontrile solvent.

Variables	The electronic concentration $1/cm^3$	
	N3/TiO2	N719-TiO2
$J_{Sc}(mA/cm^2)$	10.108	22.234
V_{oc} Volt	0.805	0.811
$J_m(mA/cm^2)$	7.417	10.237
V_m Volt	0.511	0.523
FF	0.465	0.296
Efficiency	3.783	5.337

Discussion

The current density $\mathbf{J_{EC}}\left(\frac{\mathbf{mA}}{\mathbf{cm^2}}\right)$in Eq. (13) and results in Table (1) shows the current density increases with increases the reorganization energy and as increases strength coupling constant $\langle \mathbf{K_E} \rangle$ in the solar cell system.The values of $\mathbf{J_{EC}}(\frac{\mathbf{mA}}{\mathbf{cm^2}})$ increases from 1.195 to 9.979 for N3/$Ti0_2$ while from 2.430 to 21.094 for N719/$Ti0_2$ when strength coupling increases from 0.035eV t0.035 to 0.155eV ,that's indicated

the current for N719/TiO_2 cell is larger than N3/TiO_2 cell by 56% approximately . Furthermore ,results in Table 1 shows the current density influenced by increasing coupling constant as well as reorganization energy of N3/TiO2 and N719/TiO2 -based solar cell.Study and calculate the efficiency of N3 or N719 based on TiO2 photoanode solar cells with acetonitrile solvent fulfillment with concentrations3×10^{18} cm^{-3} of charge in two solar cells system with the expectation that the concentration would have a greater influences on efficiency with reorganization energy and strength bond .As mentioned above, the current density $\mathbf{J_{EC}}\left(\frac{\mathbf{mA}}{\mathbf{cm^2}}\right)$ will be increased upon increased coupling bond and decreases reorganization energy.The reorganization energy can play an important effect in improved the efficiency of N3/ TiO2 and N719/TiO2 by increasing the energy of electron transfer from N3 or N719 dyes to the TiO2 metal oxides. However, the reorganization energy energy is about 0.427 eV indicates that N719/ TiO2 solar cell system needs less energy to reorientation system comparing to N3/ TiO2 system has more energy $0.435\ eV$ to reconfiguration energy levels to start electron transition reaction from excited dye N3 or N719 to the conduction band in the TiO2, therefore the oxide–reduced reaction in N3/TiO2 and N719-TiO2 heterojunction used to understand electron transfer influenced of solar cell systems. Current density can show in Tables (1) indicated increasing upon increase coupling bond from 0.035 eV/ state to 0.155 eV/ state by immobilizing N3 and N719 dye through the interaction between the ligand of N3 and N719 dye and oxygen on TiO2 for system . In contrast, the current density determined by the reorganization energy increases as the carrier increases with acetonitrile solvent in N3/ TiO2 or N719/ TiO2 solar cells DSSC and affects the filling factor, efficiency and electronic properties. In turn, current density increases with decreases the reorganization energy from $0.435eV$ to $0.427\ eV$ for N3/ TiO2 or N719/ TiO2 solar cells indicates that current density increases by 2.33 for increased bonding ,its indicated that increases bonding leads to more electrons will transfer fromN3 or N719 dye to conduction band of TiO2 in solar cell . The electronic characteristics $\mathbf{J_{EC}} - V$ of N3/ TiO2 or N719/ TiO2 solar cells are limited by the reorganization energy and coupling constant ,and increase with increased coupling constant for both N3/ TiO2 or N719/ TiO2 solar cells. . In contrast, to calculate the fill factor and efficiency, the $\mathbf{J_{EC}} - V$ values can plott in two curves for two c for N3/ TiO2 or N719/ TiO2 solar cells in Figure (1). Eq. (14) can also indicated that efficiency directly proportional to current density, and it can note that efficiency increases with increasing current density and vice versa. The $\mathbf{J_{EC}} - V$characteristic can obtain from two curves of N3/ TiO2 or N719/ TiO2DSSC using concentration $3 \times 10^{18} cm^{-3}$. Table(3) indicated to maximum current density $J_m$is 7.417 (mA/cm^2) and voltage V_m is 0.511V in open-circuit for concentration $3 \times 10^{18} cm^{-3}$ with current density J_{Sc} is 10.108 (mA/cm^2) and voltages V_{oc} is 0.805V in open circuit and that N3/TiO2 cell achieved a FF = 0.465 and efficiency3.783% . While the maximum current density $J_m$is 10.237 (mA/cm^2) and voltage V_m is 0.523V in open-circuit for concentration $3 \times 10^{18} cm^{-3}$ with current density J_{Sc} is 22.234 (mA/cm^2) and voltages V_{oc} is 0.811V in open circuit and that N719/TiO2 cell achieved a FF = 0.296 and efficiency5.337% . The efficiency of N719/ TiO2 solar cells is highest than N3/ TiO2 ,it indicates the charge transport in N719/ TiO2 solar cells faster than N3/ TiO2 or N719/ TiO2 solar cells and the recompination injected of electrons in N719/ TiO2 was lower than N3/ TiO2 . This indicated to produces decreased current density and efficiency with low charge transfer rate of electrons in N3/ TiO2 device. The efficiency DSSC increased from 3.783%for N3/TiO2 to 5.337% by 63% when the current density increased from 10.108 $mA/cm^2$to 22.234 mA/cm^2. The results of efficiency 5.337% was in good agreement with 6.54 %[32].

Conclusion

In the present work, the efficiency solar cell of the N3/ TiO2 or N719/ TiO2 solar cells was estimated and studied through a computation approach tool for estimating the performance efficiency of DSSCs. Two N3/ TiO2 or N719/ TiO2 solar cells had been used to explore the electronic by calculating the current density, fill factor as well as efficiency to understand the performance of N3/ TiO2 or N719/ TiO2 devices using different bonding coupling constants with Acetonitrile solvent at limited transition energy. Current density shows an increase with increases in the both reorganization energy and coupling constant . The fill factor and efficiency of the N719/TiO2 device larger than N3/ TiO2 ,it significantly affected by the reorganization energy and coupling. Increased strength coupling in both N3/ TiO2 or N719/ TiO2 solar cells leads to increased electron transfection reaction cross interface of the two materials in device and finally to effect on current density – voltage characteristic, fill factor and efficiency of DSSC. The photoelectric conversion efficiency for N719/ TiO2 solar cell gradually larger than N3/ TiO2,it increases from 3.783% to 5.337% and then increased due to the increase in the charge transport in the N719/TiO2 DSSC

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