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A theoretical calculation of the efficiency of indoline dyes-sensitized contact with ZnO in solar cell

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Original Research

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Abstract:

In this research, the efficiency of the D102-ZnO heterojunction device was evaluated using a quantum model based on electronic transport theory. The electron will move from the excited state D102 indoline-sensitive dye to the wide band gap ZnO. Given the current understanding of the working mechanism of DSSCs, the energy levels of the D102-ZnO heterojunction device must be continuously surrounded by an acetonitrile solvent electrode. The current-voltage (JV) characteristics of D102-ZnO are calculated at $T = 300$ k and 100 mW/cm^2 irradiation. The fill factor increases from 0.230 to 0.246 and the efficiency increases from 4.914 to 9.589 for the D102-ZnO device to increase the concentration from 1.65×10^{23} 1/m^3 to 4.65×10^{23} 1/m^3.

Keywords: Efficiency; D102 dye; ZnO; Dye sensitized solar

1. Introduction

Recently, the environmental impact of fossil fuels has increased as the demand for energy increases rapidly with the growing population, so the necessity of searching for alternative and sustainable energy resources has emerged [1, 2]. Sustainable energy is a reliable energy base for the global economy and a clean source and includes all types of renewable energy sources such as biomass, geothermal energy, tidal energy, wind energy, and solar energy [3, 4]. Renewable energy technology is a major exploration and a vital part of reducing greenhouse gases and reducing all risks resulting from global warming and environmental problems [5]. The main advantage of solar energy is that it is a good choice for sustainable and unlimited energy sources that are directly converted using small photovoltaic solar cells [6, 7]. Solar cells (SC) are often used to convert light into electricity and are considered one of the most important environmentally friendly energy sources. It can be divided into three categories; the first generation uses silicon (Si) and decreases efficiently with increasing temperature, the second generation has a thin filler and is cheaper than silicon, and the third generation is photovoltaic solar cells [8]. One of the main attractive types of photovoltaic solar cells is dye-sensitized solar cells (DSSCs). It has gained greater attention due to the expanding use of technology in various devices [9]. Dye-sensitized solar cells (DSSC) are receiving great attention and interest in solar energy conversion technology due to lower costs, optical properties, and ease of production [10, 11]. As such, the electronic transfer reaction process in dye semiconductor devices can occur under the movement of electrons from the donor state to the acceptor state across the interface of two materials [12–14]. The Hadi model shows that the current in heterostructure devices depends on energy redirection to form the solar cell device with energy level alignment. These are fundamental parameters that are important for electronic transport processes in solar cell devices [15, 16]. On the other hand, the fill factor (FF) plays an important factor in estimating efficiency, as it determines the power that can be generated from the solar cell [17]. The efficiency and fill factor FF of DSSCs depend on the current density, voltage and characteristics IV [18]. More attention has been paid to indoline dyes for use as sensitizers for dye-sensitized solar cells because they are the strongest sensitizers with good photoresponse in the visible region [19]. D102 dye is an organic indoline dye with a high extinction coefficient compared to ruthenium dye. It is a photosensitizer in low-cost electrochemical devices and dye-sensitized solar cells [20]. D102 is an attractive photosensitive organic dye used in DSSCs solar cells, and has the chemical formula

2-[(5Z)-5-[[4-[4-(2,2-diphenyl ethynyl)phenyl]-2,3,3a,8b-tetrahydro-1H-cyclopenta[b]indol-7-yl]methylidene]-4-oxo-2-sulfanylidene-1,3-thiazolidin-3-yl]acetic acid and has molecular formula $C_{37}H_{30}N_2O_3S_2$ [21]. Indoline dye D102 is the main sensitizer due to its advantages of thermal and chemical stability, good light absorption with more interesting electronic and optoelectronic properties [22] and the structure shown in Figure 1 [23].

Currently, ZnO is a widely interesting semiconductor, and it has been used as a donor electrode in solar cells due to its unique chemical and physical properties and wide range [24]. In recent years, the performance improvement of solar cells through the efficiency of DSSCs has increased and is achieved at a more comprehensive and lower cost, making a critical case for energy applications [25]. In this work, the main objective is the theoretical calculation of the contact efficiency of the indoline dye D102 with the semiconductor ZnO based on quantum electronic transport theory based on current density estimation using calculation of the reorganization energy, electronic density and force coupling of D102-ZnO heterojunction devices and solar cell devices.

2. Theory

The theoretical calculation was performed within the quantum theory of electronic transport and electron density in solar cell devices. The current I_s to transfer electrons from the dye to the semiconductor is [26].

$$I_s(E) = q\int_0^{\infty} T_s(E)F(E)dE \tag{1}$$

where q is the electronic charge, $T_s(E)$ is the transfer parameter and $F(E)$ is the Fermi density of electrons in solar cell devices. The transmission parameter is given by [27].

$$T_s(E) = \frac{4\pi^2}{h}|\langle\sigma_{EC}\rangle|^2\rho_E(E) \tag{2}$$

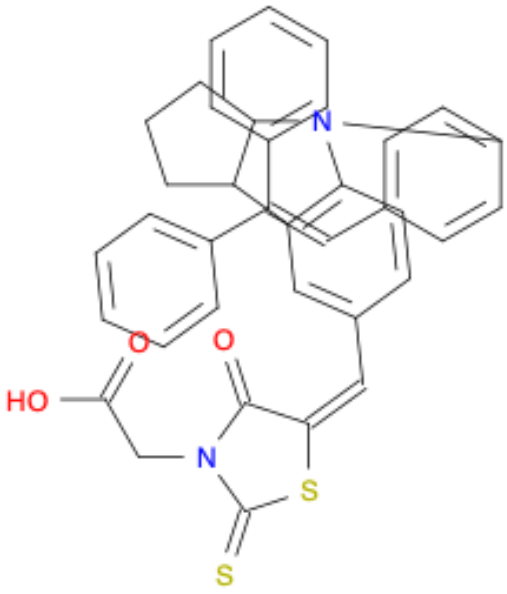

Figure 1. Structure of D102 sensitised dye [23]

where σ_{EC} is the electronic coupling constant and $\rho_E(E)$ is the electron density of activation in the device system, denoted by [28, 29].

$$\rho_E(E) = \rho_S\left(\frac{\pi}{6}\right)^{\frac{1}{3}} l_s \tag{3}$$

where l_s is the path length in the semiconductor and ρ_S is the electronic density in the semiconductor which is given by [30, 31].

$$\rho_S = \frac{\langle\hat{\rho}\rangle}{d_{\mathrm{ZnO}}^{2/3}}\rho_{EB}(E) \tag{4}$$

where $\rho_{EB}(E)$ is the electronic density of state in the dye, d_{ZnO} is the atomic density of ZnO and $\langle\hat{\rho}\rangle$ are the expected values of the density of state in the system, written as follows [27].

$$\langle\hat{\rho}\rangle = \frac{1}{\sqrt{4\pi\Lambda_{IZ}k_BT}}e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}} \tag{5}$$

where Λ_{IZ} (eV) is the reorganization energy, k_B is the Boltzmann equation, T is the temperature, and ΔU^0 is the driving force. Inserting Equations (5), (4) and (3) into Equation (2) to the results.

$$T_s(E) = \frac{4\pi^2}{h}|\langle\sigma_{EC}\rangle|^2\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{\mathrm{ZnO}}^{2/3}}\frac{1}{\sqrt{4\pi\Lambda_{IZ}k_BT}} \rho_{EB}(E)\left(\frac{\pi}{6}\right)^{\frac{1}{3}} l_s \tag{6}$$

Inserting Eq. (6) in Eq. (1) to obtain the current

$$I_s(E) = q\frac{4\pi^2}{h}\int_0^{\infty}|\langle\sigma_{EC}\rangle|^2\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{\mathrm{ZnO}}^{2/3}}\frac{1}{\sqrt{4\pi\Lambda_{IZ}k_BT}} \rho_{EB}(E)\left(\frac{\pi}{6}\right)^{\frac{1}{3}} l_sF(E)dE \tag{7}$$

The integral solution is given in Equation (7).

$$I_s(E) = q\frac{4\pi^2}{h}\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{\mathrm{ZnO}}^{2/3}}\frac{|\langle\sigma_{EC}\rangle|^2}{\sqrt{4\pi\Lambda_{IZ}k_BT}} \rho_{EB}(E)\left(\frac{\pi}{6}\right)^{\frac{1}{3}} l_s[C] \tag{8}$$

where $[C]$ is the carrier concentration, which is given by [32].

$$[C] = \int_0^{\infty}\rho_{EB}(E)F(E)dE \tag{9}$$

The current density $J_s(E)$ is given in form.

$$J_s(E) = \frac{I_s(E)}{A} \tag{10}$$

where A is an area of the solar cell. The fill factor is estimated relative to the ratio of the actual maximum power to produce short circuit current (I_{sc}) and pen circuit voltage (V_{OC}). The model used is calculated [33].

$$FF = \frac{V_pI_p}{V_{OC}I_{sc}} \tag{11}$$

where V_p and I_p are the maximum power voltage and current, V_{OC} and I_{sc} indicate the open circuit voltage and short circuit current respectively. The efficiency of DSSCs is the ratio of the output power to the incident light power density I_o which is [34].

$$\eta = \frac{J_{sc} V_{OC}.FF}{I_o} \times 100\% \tag{12}$$

The reorganization energy Λ_{IZ} (eV) is [35].

$$\Lambda_{IZ}(eV) = \frac{q^2}{8\pi\varepsilon_0 D}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] - \frac{e^2}{16\pi\varepsilon_0 R} \times \left[\frac{n_Z^2 - n^2}{n_Z^2 + n^2}\frac{1}{n^2} - \frac{\varepsilon_Z^2 - \varepsilon^2}{\varepsilon_Z^2 + \varepsilon^2}\frac{1}{\varepsilon^2}\right] \tag{13}$$

where ε_0 is the permittivity. D is the radius of the D102 molecule, R is the distance between the D102 molecule and the semiconductor ZnO, n and ε are the refractive index and dielectric constant of the solvent, n_Z is the refractive index of the semiconductor and ε_Z is the dielectric constant of ZnO. The radius is [36].

$$D = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \left(\frac{M}{N\rho}\right)^{\frac{1}{3}} \tag{14}$$

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

3. Results

In fact, the reorganization energy plays an important factor to account for the current resulting from electron transfer from excited D102 to the conduction band in ZnO semiconductor. Considering Equation (13), the reorganization energy can be calculated as a function of the radius of D102 and ZnO, the distance between them, and the dielectric and refractive index of the solvent and ZnO. The radii of ZnO and D102 based on Equation (14) with molecular weight $M = 81.38$ g/mol [37] and mass density 5.66 g/cm^3 [37] of ZnO and $M = 614.78$ g/mol [22] with density $\rho = 1.32$ g/cm^3 [22] for D102 dye, results are 3.8025 $\AA$ for ZnO and 5.694 $\AA$ for D102. The reorganization energy is calculated according to Equation (13) where taking the refractive index of 2.0033 and a dielectric constant of 8.5 for semiconductor ZnO [37] with solvent refractive index of 1.3441 and dielectric constant of 37.5 for solvent acetonitrile (MeCN) to results $\Lambda_{IZ} = 0.586$ eV for D102-ZnO with MeCN solvent. The current resulting from electron transfer between the excited state in D102 dye to the conduction band in ZnO with MeCN solvent is calculated using Equation (8) with the introduction of the square of the electronic coupling constant $|\langle\sigma_{EC}\rangle|^2 = 0.05$, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5, 0.55, 0.6, 0.65, 0.7 and $0.75 \times 10^{-1}|\text{eV}|^2$, $\Lambda_{IZ} = 0.586$ eV, path length $l_s = 3 \times 10^{-10}$ m [38], atomic density $d_{\text{ZnO}} = 8.6 \times 10^{22}$ 1/m^3 [39] and concentration $[C] = (1.65, 4.65) \times 10^{23}$ 1/m^3 [40] using MATLAP program, results show in the Table 1.

The current density can be calculated using Eq. (10) and taken as the area of the cell (0.25 cm^2); the results are listed in Table 2.

The $J_s - V$ characteristic of current density J_s (mAcm^2) versus voltage in Volt is shown in Table 3.

The characteristic of $J_s - V$ curves of D102 dye-contact with ZnO solar cell devices using two concentrations 1.65×10^{23}

Table 1. Results of current (A) for D102-ZnO with acetonitrile (MeCN) solvent.

Strength coupling	The electronic concentration 1/m^3	
$\lvert\langle\sigma_{EC}\rangle\rvert^2 \times 10^{-1}$ eV/state	1.65×10^{23}	4.65×10^{23}
0.05	2.5248E-07	7.1152E-07
0.1	5.0495E-07	1.4230E-06
0.15	7.5743E-07	2.1346E-06
0.2	1.0099E-06	2.8461E-06
0.25	1.2624E-06	3.5576E-06
0.3	1.5149E-06	4.2691E-06
0.35	1.7673E-06	4.9807E-06
0.4	2.0198E-06	5.6922E-06
0.45	2.2723E-06	6.4037E-06
0.5	2.5248E-06	7.1152E-06
0.55	2.7772E-06	7.8267E-06
0.6	3.0297E-06	8.5383E-06
0.65	3.2822E-06	9.2498E-06
0.7	3.5347E-06	9.9613E-06
0.75	3.7871E-06	1.0673E-05

Table 2. Results of current density (A.cm^{-2}) for D102-ZnO with acetonitrile (MeCN) solvent.

Strength coupling	The electronic concentration 1/m^3	
$\lvert\langle\sigma_{EC}\rangle\rvert^2 \times 10^{-1}$ eV/state	1.65×10^{23}	4.65×10^{23}
0.05	1.5979E-06	2.8461E-06
0.1	3.1959E-06	5.6922E-06
0.15	4.7938E-06	8.5383E-06
0.2	6.3918E-06	1.1384E-05
0.25	7.9897E-06	1.4230E-05
0.3	9.5877E-06	1.7077E-05
0.35	1.1186E-05	1.9923E-05
0.4	1.2784E-05	2.2769E-05
0.45	1.4382E-05	2.5615E-05
0.5	1.5979E-05	2.8461E-05
0.55	1.7577E-05	3.1307E-05
0.6	1.9175E-05	3.4153E-05
0.65	2.0773E-05	3.6999E-05
0.7	2.2371E-05	3.9845E-05
0.75	2.3969E-05	4.2691E-05

Table 3. The $J_s - V$ characteristic of D102-ZnO devices.

The electronic concentration			
1.65×10^{23} state		4.65×10^{23} state	
V (Volt)	Current (A/cm^2)	V (Volt)	Current (A/cm^2)
0.835	0	0.855	0
0.8	1.5979E-06	0.8	2.8461E-06
0.75	3.1959E-06	0.75	5.6922E-06
0.7	4.7938E-06	0.7	8.5383E-06
0.65	6.3918E-06	0.65	1.1384E-05
0.6	7.9897E-06	0.6	1.4230E-05
0.55	9.5877E-06	0.55	1.7077E-05
0.5	1.1186E-05	0.5	1.9923E-05
0.45	1.2784E-05	0.45	2.2769E-05
0.4	1.4382E-05	0.4	2.5615E-05
0.35	1.5979E-05	0.35	2.8461E-05
0.3	1.7577E-05	0.3	3.1307E-05
0.25	1.9175E-05	0.25	3.4153E-05
0.2	2.0773E-05	0.2	3.6999E-05
0.15	2.2371E-05	0.15	3.9845E-05
0.1	2.3969E-05	0.1	4.2691E-05
0	2.5567E-05	0	4.5537E-05

1/m^3 and 4.65×10^{23} 1/cm^{3}are shown in Figure 2.
The fill factor and efficiency evaluated using Eq. (11) and Eq. (12), respectively, with data in the Table 3 and Figure 2, results shown in Table 4 for D102-ZnO devices.

4. Discussion

To discuss and calculate the efficiency of D102 dye contacting ZnO photoanode in solar cells using acetonitrile solvent, two carrier concentrations of 1.65×10^{23} 1/m^3 and 4.65×10^{23} 1/m^3, respectively, were taken into the system. Table 1 shows the current effects by carrier concentration and electronic coupling for the D102-ZnO solar cell. The current was increased when the carrier concentration was increased by 2.8 times when the carrier increased from 1.65×10^{23} 1/m^3 to 4.65×10^{23} 1/m^3. This indicates a change in electronic transfer from the excited state of the D102 dye to the conduction band of the cross-linked ZnO interface with a proportional increase in the electron density of the devices and is also proportional to the increased packing factor and efficiency of the devices. As shown in the current data in Table 1, it increases alternately with the increase of electronic coupling $|\langle\sigma_{EC}\rangle|^2$ from (0.05 to 0.75) $\times 10^{-1}$ eV^2. In contrast, increasing the electronic coupling constant provides the wave function overlap of the D102 and ZnO energy levels in the system to produce more electrons and the cross-interface will be transferred in the D102-ZnO devices.
In addition, the movement of electrons is limited by the interface strength of the D102-ZnO heterojunction devices, but the interfering wave functions will provide the necessary energy for transport due to the polar media, which is a function of the dielectric constant. However, the current density in Table 2 increases by about 1.78 with increasing concentration and increasing electronic coupling, and it is expected that the efficiency will increase when the system carrier concentration increases. Furthermore, the important role played by increased current density due to increased electron transfer and electronic recombination through reorganization energy was evaluated as both the concentration of D102-ZnO in the acetonitrile solvent medium, where the redox reaction between D102 and ZnO for electron transfer occurs in solar cell devices. Table 4 shows the results of the filling factor and efficiency estimated using the $J_s - V$ curves shown in Table 3 and Figure 2. Table 4 shows the effect of carrier concentration on both fill factor and efficiency through the effect on the average open circuit image voltage V_m (Volt) and current J_m (mA/cm^2) estimated using Figure 2 and listed in Table 4. As we can see, the average open circuit voltage J_p (μA/cm^2) and the optical voltage V_p Volts increase with increasing concentration, and vice versa. Moreover, the filling factor will increase from 0.230 to 0.246 and the efficiency increases from 4.914 to 9.589 when the concentration increases from 1.65×10^{23} 1/m^3 to 4.65×10^{23} 1/m^3. However, increasing the concentration and electronic coupling has a strong effect on the V_{OC}, J_{sc}, FF, and efficiency, which are summarized in Table 4. Both the peak current density shift from 18.545 (μA/cm^2) to 34.87 (μA/cm^2) and the potential difference from 0.265 V to 0.275 V for the solar cell indicate that as the number of electrons increases they must recombine when the concentration increases from 1.65×10^{23} 1/m^3 to 4.65×10^{23} 1/m^3.

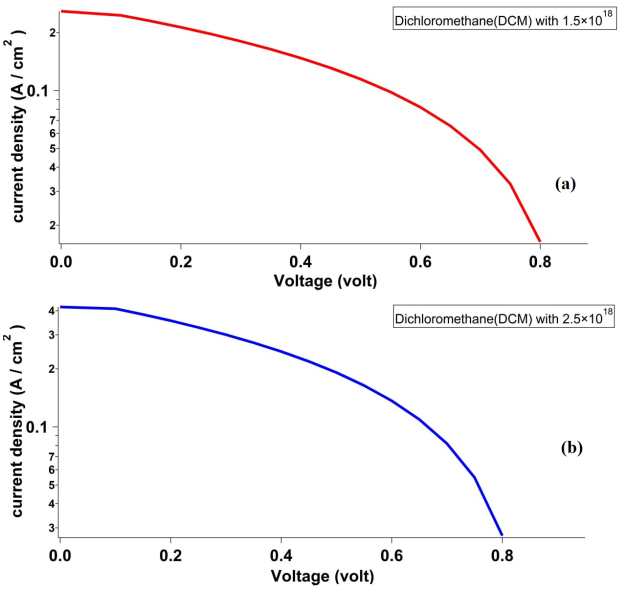

Figure 2. The current density versus voltage under concentration 11.65×10^{23} 1/m^3 and 4.65×10^{23} 1/m^3 of the same devices.

5. Conclusion

In conclusion, a quantitative model based on electronic transfer was presented to calculate and study the efficiency of the D102-ZnO heterojunction device with acetonitrile solvent based on calculating the current density and filling factor. The current strength, current density, fill factor, and efficiency in solar cells for D102-ZnO devices are affected by increasing carrier concentration and electronic coupling constant at limited reorganization energy.
The efficiency is significantly enhanced from 4.914 to 9.589 when the concentration is increased from 1.65×10^{23} 1/m^3 to 4.65×10^{23} 1/m^3. The corresponding improvement in efficiency can be attributed to the increased carrier concentration in D102-ZnO devices with limited reorganization energy which leads to increased cross-linking electron transfer in the D102-ZnO heterojunction system which in turn enhances the efficiency.

Authors Contributions
Authors have contributed equally in preparing and writing the manuscript.

Availability of data and materials
Data presented in the manuscript are available via request.

Conflict of Interests
The author declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Table 4. Results of current density ($A.cm^{-2}$) for D102-ZnO with acetonitrile (MeCN) solvent.

Variables	The electronic concentration $1/m^3$	
	1.65×10^{23}	4.65×10^{23}
J_{Sc} ($\mu A/cm^2$)	25.567	45.537
V_{OC} Volt	0.835	0.855
J_p ($\mu A/cm^2$)	18.545	34.87
V_p Volt	0.265	0.275
$F.F$	0. 230	0. 246
efficiency	4.914	9.589