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Study on the Efficiency of Zinc Oxide Solid-State Solar Cells Using Organic Dyes Based on Indolene D102 Dye

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Abstract

In this work, two carrier concentrations with dye D102 were used in a dye-sensitized solar cell to perform a comparative evaluation of the efficiency and influence on the study of key parameters affecting the device performance. To achieve this goal, the cell transfer power, current, current density and fill factor were calculated to estimate the power conversion efficiency (PCE) of DSSCs. Electrons move from the excited state of indolene D02 to the conduction band of ZnO to produce current for DSSCs through the assumed energy levels of donor indolene and acceptor ZnO in the hetero junction device to be continuous. The effect of carrier concentration and coupling strength on the improvement of the contact efficiency of D102 hetero junction dye with ZnO-based DSSCs is discussed using quantum charge transfer theory. D102-ZnO with ethanol-based DSSCs with PCEs up to (14.368%) were developed and the main J-V properties were investigated, the corresponding carrier concentration efficiency of $1.5 \times 10^{24}(1/m^3)$ is much lower (7.256%) compared to using a concentration of $3 \times 10^{24}(1/m^3)$ to reach (14.368%), mainly due to the lower charge transport.

Keywords: Efficiency, Indoline D102 Dye, Zinc Oxide, Solid-State Solar Cells.

1. Introduction

In recent years, countries have dealt with increasing demand for renewable energy due to increasing population growth and climate change, with the depletion of natural gas and the effects of warming (1). Over the past decade, energy supply production has focused on sustainability, including geothermal, wind, and solar energies (2).

Renewable energy is a major exploration to reduce greenhouse gases improve the efficiency of fossil fuels and reduce environmental problems (3).Research on the environmental performance evaluation of solar cell projects has indicated that solar energy is an acceptable option for sustainability (4). Solar energy technology has been growing in different applications which contribute significantly to solving energy problems (5).

A solar cell is a device that directly converts photons of light into electricity through the photoelectric effect. They are divided into 3rd generations: 1st generation uses silicon, 2nd generation thin film and 3rd generation uses photovoltaic solar cells (6).O 'Regan and Grätzel's s pioneered a novel type of solar cell, the dye-sensitised solar cell (DSSC), which is a photovoltaic cell low-cost and environmentally friendly (7). DSSCs are gaining significant attention and interest in solar energy conversion technology due to their ease of production and cheapness (8). Charge transport in dye-semiconductor devices occurs when electrons transfer from the donor-excited state of the dye to the acceptor state of the conduction band (9). Naeem and Al-Agealy presented a quantitative model of charge transport to show that the current in heterojunction interface devices depends on the reorganization energy (10).

The transfer of charge in DSSC is a fundamental process that occurs without the formation of any chemical bond (11).In a typical charge transfer, an electron from an excited state in the dye to a state in the semiconductor in DSSC (12). However, the current density is a basic parameter in estimating the fill factor and efficiency (13). Recently, more attention has been paid to indolene dyes for use as sensitizers for DSSC because they are the strongest sensitizers in the visible region (14). Indolene dyes in DSSCs, as a result, the photosensitizer in low-cost exhibits a higher extinction coefficient (15). Indoline D102 dye can be used as a sensitizing material for the fabrication of metal-free dye-sensitized solar cells (16).It has the chemical form C37H30N2O3S2 with the structure listed in **Figure 1** (17).

ZnO semiconductors are unique and have a wide band gap 3.3 eV. It's a widely attractive material for use in optoelectronics and as an electrode in DSCCs (18). At present, the performance of DSSCs has been improved, which has been achieved at a lower cost and more comprehensively (19). In the present work, the improved energy conversion efficiency of DSSC based on solid-state indoline dye D102 in contact with ZnO has been studied theoretically using quantum charge transfer theory. The characteristics and parameters that affect efficiency are discussed.

2. Materials and Methods

The transmission of charge transfer is (20).

$$T_s(E) = \frac{2\pi}{\hbar} |\langle \mathscr{O}_C \rangle|^2 \rho_e(E) \quad (1)$$

Where $\hbar$ is Planck's constant, $\mathscr{O}_C$ is a strong coupling constant and $\rho_e(E)$ is the density of charge transport in a heterojunction system, it's given by (21).

$$\rho_e(E) = \sqrt[3]{\left(\frac{\pi}{6}\right)}\, l_c \rho_S \quad (2)$$

Where l_c is the length path of the charge in the semiconductor and ρ_S is the charge density in a semiconductor and is given by (22).

$$\rho_S = \rho_D(E) d_S^{-2/3} \langle \hat{\rho} \rangle \quad (3)$$

Where $\rho_D(E)$ is the density of state in indoline dye, d_S is the atomic density of the semiconductor and $\langle \hat{\rho} \rangle$ is the expectation value of the density of state in the system. Inserting both Eq. (2) and Eq. (3) in Eq. (1) to result.

$$T_s(E) = \frac{2\pi}{\hbar} |\langle \mathscr{O}_C \rangle|^2 \sqrt[3]{\left(\frac{\pi}{6}\right)} l_c \rho_D(E) d_S^{-2/3} \langle \hat{\rho} \rangle \quad (4)$$

The expectation values of the density of state in the system is (20).

$$\langle \hat{\rho} \rangle = \frac{e^{-\frac{(\Lambda_Z + \Delta U^0)^2}{4\Lambda_Z k_B T}}}{2\sqrt{\pi\, \Lambda_Z k_B T}} \quad (5)$$

Where $\Lambda_Z(eV)$ is transferring energy, ΔU^0 is the driving force, k_B is the Boltzmann constant and T is temperature. Substituting Eq. (5) in Eq. (4) to give.

$$T_s(E) = \frac{2\pi}{\hbar} |\langle \sigma_C \rangle|^2 \sqrt[3]{(\frac{\pi}{6})} l_c \rho_D(E) d_S^{-2/3} \frac{e^{-\frac{(\Lambda_Z + \Delta U^0)^2}{4\Lambda_Z k_B T}}}{2\sqrt{\pi \Lambda_Z k_B T}} \quad (6)$$

The transfer energy Λ_Z (eV) can be written by (23).

$$\Lambda_Z(eV) = \frac{e^2}{8\pi\varepsilon_\circ{}_D}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] + \frac{e^2}{16\pi\varepsilon_\circ R}\left[\frac{\varepsilon_Z^2 - \varepsilon^2}{\varepsilon_Z^2 + \varepsilon^2}\frac{1}{\varepsilon^2} - \frac{n_Z^2 - n^2}{n_Z^2 + n^2}\frac{1}{n^2}\right] \quad (7)$$

Here $\varepsilon_\circ$ is permittivity, D and R are the radius and distance between the dye and the semiconductor electrode, ε and n are dielectric constant and refractive index of the solvent, ε_Z and n_Z are the dielectric and refractive index of ZnO. The radius is a function of molecular weight M and density ρ , it can be evaluated using (24).

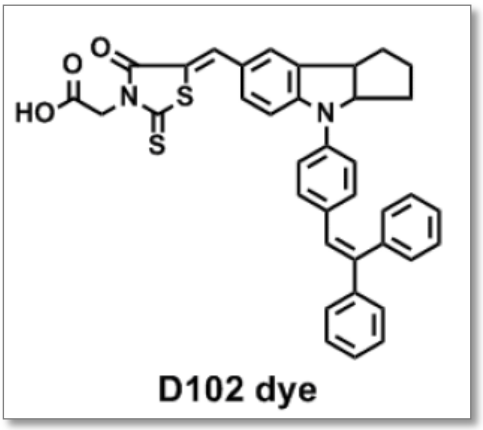

Figure 1.: Structure of D102 dye (17).

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

Where N is the Avogadro number N. The current I_s for electrons to move from the excited dye to the conduction band in a semiconductor is (25).

$$I_s(E) = e\int_0^\infty F(E)T_s(E)dE \quad (9)$$

Where $F(E)$ is the Fermi density function in cell devices. Substituting Eq. (6) in Eq. (9) to gets.

$$I_s(E) = \frac{2\pi e}{\hbar} |\langle \sigma_C \rangle|^2 \sqrt[3]{(\frac{\pi}{6})} l_c d_S^{-2/3} \frac{e^{-\frac{(\Lambda_Z + \Delta U^0)^2}{4\Lambda_Z k_B T}}}{2\sqrt{\pi \Lambda_Z k_B T}} \int_0^\infty F(E)\rho_D(E)dE \quad (10)$$

The current density $J_s(E)$ is the ratio of current $I_s(E)$ divides to cell area A and writes.

$$J_s(E) = \frac{I_s(E)}{A} \quad (11)$$

Insert Eq. (10) in Eq. (11) to give.

$$J_s(E) = \frac{2\pi e}{\hbar A} |\langle \sigma_C \rangle|^2 \sqrt[3]{(\frac{\pi}{6})} l_c d_S^{-2/3} \frac{e^{-\frac{(\Lambda_Z + \Delta U^0)^2}{4\Lambda_Z k_B T}}}{2\sqrt{\pi \Lambda_Z k_B T}} \int_0^\infty F(E)\rho_D(E)dE \quad (12)$$

The integral in the above expression can be solved to result (26).

$$\int_0^\infty F(E)\rho_D(E)dE = [A] \quad (13)$$

Where $[A]$ is the concentration of the carrier. Inserting Eq. (13) in Eq. (12) to obtain.

$$J_s(E) = \frac{2\pi e}{\hbar A} |\langle \sigma_C \rangle|^2 \sqrt[3]{(\frac{\pi}{6})} l_c d_S^{-2/3} \frac{e^{-\frac{(\Lambda_Z + \Delta U^0)^2}{4\Lambda_Z k_B T}}}{2\sqrt{\pi \Lambda_Z k_B T}} [A] \quad (14)$$

The efficiency $\eta(\%)$ of DSSCs is (27)

$$\eta(\%) = \frac{J_{Sc}V_{oc}.FF}{I_o} \quad (15)$$

Where J_{Sc} and V_{oc} They are short and open circuit of current and voltage, respectively. FF is the fill factor of the cell and I_o is incident light power density. The fill factor is the ratio of actual maximum power and the production power. It estimated using (28).

$$FF = \frac{V_m I_m}{V_{oc} J_{sc}} \quad (16)$$

Where V_m and J_m are the maximum power voltage and current density, respectively.

3. Results

The necessity of calculating the current density becomes apparent when estimating the efficiency of the organic dye Indoline D102-ZnO as a function of the fill factor using a theoretical approach based on charge transport theory. Within this framework, the reorganization energy can be calculated by assuming the continuum energy levels of charge transfer across the interface from the excited state of the D102 dye to the ZnO electrode. The transfer energy Λ_Z (eV) can be estimated for the D102-ZnO hetero junction in DSSCs, it is essential to evaluate the radii of D102 dye and ZnO in the device. The radii of D102 dye and ZnO calculate using Eq.(8) using M= 614.78g/mol with density $\rho = 1.32 \frac{\text{g}}{\text{cm3}}$ for D102 dye (29) and M=81.38 g/mol and density $5.66 \frac{\text{g}}{\text{cm3}}$ of ZnO (30), results are 35.694 $A^0$for D102 and 8025 Å for ZnO.The transfer energy Λ_Z (eV) may be calculated using Eq. (7) as a function of the radius of D102 5.694 A^0 and the distance between ZnO and D102 R 9.496$A^{0,}$ and taking into account the refractive index 1.3614 and 2.0033 (30) together dielectric constant of 24.5 and 8.5 (31) of Ethanol solvents and ZnO. The results of transfer energy Λ_Z (eV) is 0.486 eV for D_{102}-ZnO device with Ethanol solvent in DSSCs solar cell. The current produces in D102-ZnO with Ethanol solvent calculates using Eq.(10) by insert Λ_Z (eV)=0.486 eV and coupling constant $|\langle\sigma_C\rangle|^2$=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× 10^{-1} $|eV|^2$ The length path of electrons in ZnO $l_c = 3 \times 10^{-10} m$ (32), atomic density $d_{ZnO} = 8.6 \times 10^{22} \frac{1}{m^3}$ (33) and concentration $1.5 \times 10^{24} \frac{1}{m^3}$and $3 \times 10^{24} \frac{1}{m^3}$ (31) with MATLAP program. Results are listed in **Table (1)**.

Table 1. Current calculated for D102-ZnO DSSC with Ethanol at a concentration $1.5 \times 10^{24} \frac{1}{cm^3}$ and $3 \times 10^{24} \frac{1}{m^3}$.

$\|\langle\sigma_C\rangle\|^2 \times 10^{-1}$ $\|eV\|^2$	**The electronic current** **The electronic concentration**	
	$\mathbf{1.5 \times 10^{24}}$	$\mathbf{3 \times 10^{24}}$
0.15	0.731E-02	1.4621E-02
0.25	1.218E-02	2.4369E-02
0.35	1.705E-02	3.4116E-02
0.45	2.193E-02	4.3864E-02
0.55	2.680E-02	5.3612E-02
0.65	3.167E-02	6.3359E-02
0.75	3.655E-02	7.3107E-02
0.85	4.142E-02	8.2854E-02
0.95	4.630E-02	9.2602E-02
1.05	0.511E-01	1.0235E-01
1.15	0.512E-01	1.1210E-01
1.25	0.609E-01	1.2184E-01
1.35	0.652E-01	1.3159E-01
1.45	0.706E-01	1.4134E-01
1.55	0.756E-01	1.5109E-01

Current density is the most important aspect in calculating the filling factor and efficiency of a DSSC. It can be evaluated using Eq. (14) and taking the typical cell area $0.25\ \text{cm}^2$, the results are given in **Table (2**).

Table 2. Current density calculated for D102-ZnO DSSC with Ethanol at a concentration $1.5 \times 10^{24}\ \frac{1}{cm^3}$ and $3 \times 10^{24}\ \frac{1}{cm^3}$, respectuvelly.

$\|\langle\sigma_C\rangle\|^2 \times 10^{-1}\ \|eV\|^2$	**The current density The electronic concentration**	
	$\mathbf{1.5 \times 10^{24}}$	$\mathbf{3 \times 10^{24}}$
0.15	2.924E-02	5.8485E-03
0.25	4.873E-02	9.7476E-03
0.35	0.682E-01	1.3647E-02
0.45	0.872E-01	1.7546E-02
0.55	1.072E-01	2.1445E-02
0.65	1.267E-01	2.5344E-02
0.75	1.462E-01	2.9243E-02
0.85	1.657E-01	3.3142E-02
0.95	1.852E-01	3.7041E-02
1.05	2.042E-01	4.0940E-02
1.15	2.241E-01	4.4839E-02
1.25	2.436E-01	4.8738E-02
1.35	2.631E-01	5.2637E-02
1.45	2.826E-01	5.6536E-02
1.55	3.021E-01	6.0435E-02

The current density J_s(A/cm^2) vs voltage V(volt) J-V characteristic of D102-ZnO solar cell was shown in **Table (3)**.

Table 3. Theoretical J -V characteristic of D102 / ZnO DSSC with Ethanol solvent

V(Volt)	**The current density (A/cm^2)**	**V(Volt)**	**The current density (A/cm^2)**
	The electronic concentration		**The electronic concentration**
	$\mathbf{1.5 \times 10^{24}}$		$\mathbf{3 \times 10^{24}}$
0.848	0.0	0.867	0.0
0.8	2.924E-02	0.8	5.8485E-02
0.75	4.873E-02	0.75	9.7476E-02
0.7	0.682E-01	0.7	1.3647E-01
0.65	0.872E-01	0.65	1.7546E-01
0.6	1.072E-01	0.6	2.1445E-01
0.55	1.267E-01	0.55	2.5344E-01
0.5	1.462E-01	0.5	2.9243E-01
0.45	1.657E-01	0.45	3.3142E-01
0.4	1.852E-01	0.4	3.7041E-01
0.35	2.042E-01	0.35	4.0940E-01
0.3	2.241E-01	0.3	4.4839E-01
0.25	2.436E-01	0.25	4.8738E-01
0.2	2.631E-01	0.2	5.2637E-01
0.15	2.826E-01	0.15	5.6536E-01
0.1	3.021E-01	0.1	6.0435E-01
0.0	3.205E-01	0.0	6.8764E-01

One can mention that the data of photovoltaic characteristics of J−V curves for contacting the D102 dye with ZnO semiconductor based on DSSCs solar cell devices using Ethanol solvent at two concentrations 1.5×10^{24}(1/m^3) and 3×10^{24}(1/m^3) are shown in **Figure (2)**.

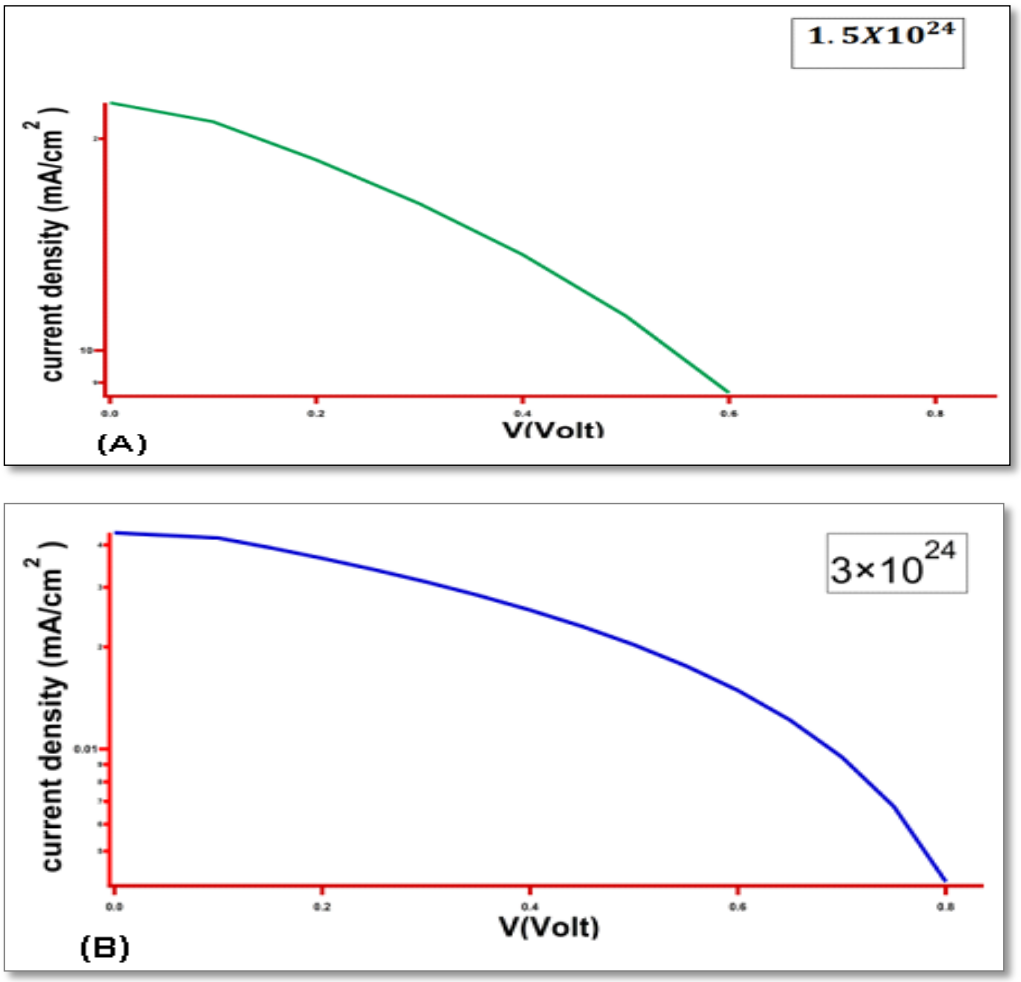

Figure 2. The $J_S - V$ characteristics for D102-ZnO DSSC with Ethanol at concentration (A) $1.5 \times 10^{24}(1/m^3)$ and (B) $3 \times 10^{24}(1/m^3)$.

Figure (2) shows the current density versus voltage V of the D102-ZnO hetero junction in DSSC with ethanol at concentrations of $1.5 \times 10^{24}(1/m^3)$ and $3 \times 10^{24}(1/m^3)$. The efficiency and fill factor were estimated using Eq. (15) and Eq. (16), respectively using results given in **Table (3)** and **Figure (2),** the filling factor was calculated by differentiating the capacity of the D102-ZnO heterojunction in solar cells for voltage and finding where it equals zero, the results are given in **Table (4)**. The conversion efficiency was limited to the current generated by the D102-ZnO solar cells based on DSSC. It was evaluated using Eq. (15) with the fill factor FF, $J_{Sc}(\frac{mA}{cm^2})$ and V_{oc}(Volt) data from **Table (4)** for the concentrations $1.5 \times 10^{24}(1/m3)$.and 3×10^{24} $(1/m3)$. with Ethanol solvent. The overall theoretical peak efficiency of D102-ZnO in DSSC was about (7.256%) with $1.5 \times 10^{24}(1/m^3)$ and (14.368%) with $3 \times 10^{24}(1/m^3)$.

Table 4. Photovoltaic parameters of the D102-ZnO in DSSCs with Ethanol solvent.

Variables	$\mathbf{1.5 \times 10^{24}(1/m^3)}$	$\mathbf{3 \times 10^{24}(1/m^3)}$
$\boldsymbol{J_{Sc}(mA/cm^2)}$	0.3205	0.68764
$\boldsymbol{V_{oc}}$ Volt	0.848	0.867
$\boldsymbol{J_m(mA/cm^2)}$	0.2106	0.4245
$\boldsymbol{V_m}$ Volt	0.335	0.3395
F.F	0.267	0.241
Efficiency	7.256 %	14.368 %

4. Discussion

The current and current density calculations are performed to characterize the effect of concentration on the estimated fill factor and efficiency of D102-ZnO DSSC, as shown in **Table (1)** and (**2**). **Table (1)** shows currents calculated versus combined strength coupling with two carrier concentrations $1.5 \times 10^{24}(1/m^3)$ and $3 \times 10^{24}(1/m^3)$, respectively, for Ethanol solvents. The current produced in D102-ZnO DSSC evaluated at multi strength coupling using the theoretical expression in Eq. (10) with transfer energy Λ_Z (eV) is 0.486 eV for D102 -ZnO device with Ethanol solvent in DSSCs solar cell.

Table (1) shows the contribution of current influences by the strong coupling of the D102-ZnO device. The current increases with increasing coupling strength and reaches the maximum observed current peaks of 3.021E-01, confirming the high-strength coupling of 1.55 for Ethanol solvent. The output current of D102–ZnO DSSC with carrier concentration 3 was increased by about 2 times when the coupling strength was increased at $3 \times 10^{24}(1/m^3)$ compared to $1.5 \times 10^{24}(1/m^3)$. This indicates a shift in the increase of charge transport from the excited D102 dye to the conduction band of the ZnO cross-linked interface with increasing relative concentration in the devices.

In contrast, as shown in the current density data in **Table (2)**, it increases alternately with the increase of strength coupling by approximately two times for D102-ZnO DSSC at carrier concentration $3 \times 10^{24}(1/m^3)$ compared to $1.5 \times 10^{24}(1/m^3)$ in Ethanol solvent. The current density is a function of the current and is inversely proportional to the area of the solar cell according to Eq. (13). Thus, the current density for D102-ZnO DSSC in Ethanol solvent is slightly larger with carrier concentration $3 \times 10^{24}(1/m^3)$ than $1.5 \times 10^{24}(1/m^3)$ in the same devices, it is proportional to increased conversion efficiency in devices with carrier concentration in Ethanol .Combining the increased coupling strength with the carrier concentration as well as transfer energy may improve the efficiency of DSSC, which can be reasonably explained by the fact that the current density of DSSC with $3 \times 10^{24}(1/m^3)$ is larger than that of DSSC with $1.5 \times 10^{24}(1/m^3)$ with the same Ethanol solvent.

In contrast, the increased carrier concentration together coupling strength increases indicate more overlapping wave functions of the energy levels of D102 dye and ZnO, it produces more electrons to be moved across the interface in D102-ZnO devices .**Tables (1**) together with **Table (2)** indicate that the current density and current increase are due to the increased electron transfer and electron recombination by increasing the concentration and coupling strength at which electron transfer occurs during the redox reaction between D102 and ZnO in solar cell devices. In addition, increasing the charge carrier results in more electrons in the excited state, which also enhances the calculated photocurrent. The result in **Table (4)** shows the contribution of J_{Sc}, V_{oc}, J_m, V_m in calculating both FF and efficiency in the dye producing high power and photocurrent. The filling factor and efficiency shown in **Table (4)** were calculated from the J-V curves shown in **Figure (2)** and **Table (3)**.

Table (4) indicates the effect of carrier concentration on the J-V, FF, and efficiency characteristics by influencing the average open circuit voltage V_m (volts) and current density Jm (mA/cm^2), estimated using **Figure (2**), and listed in **Table (4**). As shown in the data in **Table (4)**, the average voltage J_m increases from 0.2106 $(mA/cm^2)$with $1.5 \times 10^{24}(1/m^3)$ to 0.4245 (mA/cm^2) with $3 \times 10^{24}(1/m^3)$ and the photovoltage V_m increases from 0.335V to 0.3395 V, and the increase can be observed with the increase of the carrier concentration and strength coupling. Furthermore, the current increases from 0.3205 (mA/cm^2) with $1.5 \times 10^{24}(1/m^3)$ to 0.68764 (mA/cm^2) with $3 \times 10^{24}(1/m^3)$ in Ethanol and the efficiency increases from (7.256%) to (14.368%) when the strength coupling increases from 0.15 ×

10^{-1} (eV) to 1.55×10^{-1}(eV). In addition, the contact efficiency of D102 dye with ZnO showed an increase of two times with the increase in carrier concentration.

Moreover, the increase of carrier concentration as well as electronic coupling had a strong effect on V_{oc}, J_{Sc}, FF, and efficiency, as summarized in **Table (4)**. The efficiency spectrum showed an increase with increasing carrier concentration, and thus, the transport of electrons appears to be increasing. In particular, the use of Ethanol solvent with D102-ZnO DSSC can provide improved efficiency by increasing concentration. The computational efficiency results of D102-ZnO DSSC were (7.256%) with $1.5 \times 10^{24}(1/m^3)$ and (14.368%) with $3 \times 10^{24}(1/m^3)$, which are in agreement with the experimental values of (7 %) to (14.3%) (34).

5. Conclusion

In conclusion, the solid-state dye-sensitized solar cell SS-DSSCs based on the D102 -ZnO with Ethanol in solar cells demonstrated is more favorably suited for applications. The effect of the carrier concentration on the properties and efficiency of D102-ZnO DSSC is discussed based on the charge transfer from excited D102 dye to the conduction band of ZnO with Ethanol solvent in DSSCs.The current density, current, FF and efficiency of D102-ZnO DSSC are evaluated using two carrier concentrations $1.5 \times 10^{24}(1/m^3)$, $3 \times 10^{24}(1/m^3)$ and several force coupling constants. The use of suitable carrier concentration has led to the highest reported power conversion efficiency for ZnO-based D102 of (14.368%).

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Conflict of Interest:

The authors declare that they have no conflicts of interest.

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Ethical Clearance

The project was approved by the local ethical committee at the University of Baghdad.

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