Library Progress International *Print version ISSN 0970 1052*
Vol.44 No. 2s, Jul-Dec 2024: P.477-485 *Online version ISSN 2320 317X*

Original Article *Available online at www.bpasjournals.com*

Theoretical Calculation of Efficiency Solid-State Zinc Oxide Solar Cells Using Indoline-Based Organic Dyes

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How to cite this article: Firas Adel Shnain, Hadi J. M. Al –Agealy (2024) Theoretical Calculation of Efficiency Solid-State Zinc Oxide Solar Cells Using Indoline-Based Organic Dyes. *Library Progress International*, 44(2s), 477-485

ABSTRACT
In this research, the quantum transition theory of the electronic transfer process was applied to calculate and study the efficiency of sensitive contact of Indoline organic dye with zinc oxide in solar cells. Electrons move from the excited state of indoline of the dye to the conduction band state of Zinc oxide to produce the current density of Dye-sensitized solar cells "DSSCs", and the energy levels of indoline and ZnO in the heterojunction device surrounded by 1-butanol solvent media must be continuous.The current density, fill factor, and efficiency of D102-ZnO devices were calculated at two carrier concentrations from 1.65 ×10^23 1/m^3 to 4.65 ×10^23 1/m^3and strength coupling in range 〖[0.75×10^(-1)≥|⟨o_EC ⟩|〗^2≥0.05×10^(-1)] 〖 |eV|〗^2Increasing the characteristic carrier concentration led to an increase in the current density of the indoline dye with ZnO-based Dye-sensitized solar cells DSSC resulting in increases in the computational efficiency from 4.767% to 13.95% at a limited reorganization energy of 0.586 eV with a maximum current density from 30.2862 (mA/〖cm〗^2) to 85.354 (mA/〖cm〗^2).

Keywords: Efficiency, Indoline Dye, Zinc Oxide, Solar Cell.

INTRODUCTION

During recent decades, with the depletion of natural gas and coal as fuel and the negative effects of global warming, the need to equip ourselves with renewable energy sources instead of relying on traditional fossil fuel sources has become more apparent. [1].The biggest challenge to sustainability today is pollution due to greenhouse gas emissions and global climate change due to fossil fuels.Sustainable energy is the foundation of the global economy and a clean source and includes renewable energy sources such as geothermal energy, biomass, wind energy, tidal energy, and solar energy[2]. Renewable energy innovation is a major exploration to enhance the efficiency of existing fossil fuels and a vital part of reducing greenhouse gases and reducing all risks resulting from global warming and environmental problems[3]. The general advantage of solar energy is that it is the best option for sustainability, as it is an unlimited energy source that is converted directly using small photovoltaic solar cells[4]. Solar technologies include solar photovoltaics, solar heating, solar thermal, and solar electricity which can make significant contributions to solving the most pressing energy problems [5].The solar cell is often used to convert photons into electricity and is an important environmentally friendly primary energy source.It can be divided into generations: the first generation uses silicon (Si), which decreases efficiently with increasing temperature, the second generation makes a thin and cheaper silicon filler, and the third generation uses photovoltaic solar cells [6].Dye-sensitized solar cells (DSSCs) are the main attractive type of photovoltaic cells that have great interest in solar energy conversion technology due to their ease of production, low costs, and optical properties. [7].As such, the charge transfer process in dye-semiconductor contact in solar cell devices occurs under the movement of electrons between donor and acceptor states across the interface of two materials [8].

Quantum theory of charge transfer suggests that the biggest challenge is to pay attention to the heterogeneous interface that requires the transfer of charge from the donor state to the acceptor state [9]. The donor-acceptor model is the simplest model used to discuss charge transfer that does not break or form any chemical bond in the system [10]. Charge transfer in heterojunction devices occurs when charges are transferred from the donor state to the acceptor state in solar cell devices [11].Moreover, the contact interface in heterojunction devices between dye and semiconductor systems has received the most attention in various technological applications because the charge transfer process occurs across the interface [12].More attention was paid to organic dye including indoline dyes for use as sensitizers for dye-sensitized solar cells, and they were the strongest sensitizers and had good photoresponse in the visible region[13].Indoline-D102 dye is an attractive sensitive organic dye that has a high extinction coefficient, It has the formula 2-[(5Z)-5-[[4-[4-(2,2-diphenylethenyl)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 $C_{37}H_{30}N_2O_3S_2$ [14].and the chemical structure of Indoline D102 dye is listed in Fig.(1) [15].

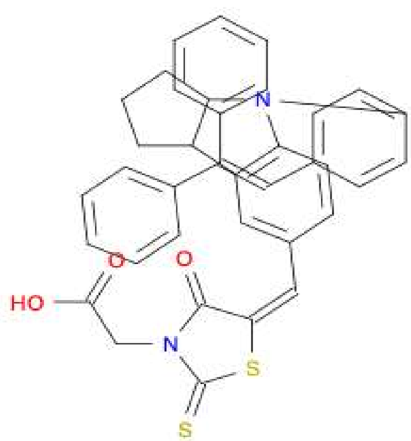


Figure (1): Structure of D102 sensitised dye [15].

Currently, ZnO is a widely interesting metal oxide semiconductor, which has been used as an electrode in DSCCs due to its unique chemical and physical properties compatibility and wide band gap[16].Recently, the performance of solar cells has been further improved by the efficiency of DSSCs, which has been achieved at a more comprehensive and low cost, making a critical case for energy applications[17].In this work, the theoretical calculation is used to calculate and examine the j-V characteristics and efficiency of the indoline dye D102 - ZnO heterojunction devices in DSSCs based on advanced charge transfer theory based on quantum theory .The MATLAB software tool was used to evaluation the solar cell efficiency with respect to current density, reorganization energy, electronic density, and coupling strength of D102-ZnO heterojunction devices.

Theory

Theoretical calculation of fill factors and efficiencies was performed based on the quantum theory of charge transfer as well as electron density in solar cell devices. Filling factor F.F is estimated relative to ratio of maximum power for producing of short-circuit current density (J_{sc}) and pen-circuit voltage (V_{oc}) . It estimates using form [18].

$$F.F = \frac{V_p J_p}{V_{oc} J_{sc}} \quad \text{……………………………(1)}$$

where V_p maximum voltage and J_p is maximum current density , V_{oc} and J_{sc} indicate to open circuit voltage and short circuit current density respectively .

The efficiency η of DSSCs is ratio of output power to its incident photons -light power density I_o and is [19].

$$\eta = \frac{J_{Sc} V_{oc} . F.F}{I_o} \times 100\% \quad \text{………………………………………..(2)}$$

The current density produces in DSSC can be given as

$$J_s = \frac{I_s}{A} \quad \text{…………………………………………..(3)}$$

where I_s is current produces in DSSC and A is area of solar cell.

The current I_s for electrons were transferred from D102 dye to ZnO electrode is [20].

$$I_s(E) = e\int_0^\infty F(E)T_s(E)dE\text{.....................} (4)$$

where e is charge of electrons , $F(E)$ is the Fermi density of electrons in devices and $T_s(E)$ is transmission parameter of electrons in solar cell devices . The transmission parameter is given by[21] .

$$T_s(E) = \frac{4\pi^2}{h}\,|\langle\sigma_{EC}\rangle|^2\rho_E\,(E)\text{.................}(5)$$

Where h is plank constant ,σ_{EC} is electronic strength coupling and $\rho_E\,(E)$ is activation density of electros in devices ,it's given as [22].

$$\rho_E\,(E) = \rho_S\,(\frac{\pi}{6})^{1/3}l_s\text{.....................}(6)$$

where ρ_S is electronic density of ZnO and l_s is path length of ZnO semiconductor . The electronic density ρ_S is [23].

$$\rho_S = \frac{\langle\hat{\rho}\rangle}{d_{ZnO}^{2/3}}\rho_{EB}(E)\text{.......................} (7)$$

where $\langle\hat{\rho}\rangle$ is expectation values of density of state in system, d_{ZnO} is atomic density of ZnO and $\rho_{EB}(E)$ is electronic density of state in dye, the $\langle\hat{\rho}\rangle$ is satisfied [21] .

$$\langle\hat{\rho}\rangle = \frac{1}{\sqrt{4\pi\,\Lambda_{IZ}k_BT}}e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}\text{...........} (8)$$

where $\Lambda_{IZ}(eV)$ is reorganization energy , k_B is Boltzmann coinstant , T is temperature ,and ΔU^0 is driving energy .Inserting both Eqs.(8), (7)and (6) in Eq.(5) to obtain.

$$T_s(E) = \frac{4\pi^2}{h}\,|\langle\sigma_{EC}\rangle|^2\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{ZnO}^{2/3}}\frac{\rho_{EB}(E)}{\sqrt{4\pi\,\Lambda_{IZ}k_BT}}\,(\frac{\pi}{6})^{1/3}l_s\text{.........} (9)$$

Substituting Eq.(9) in eq.(4) to obtain .

$$I_s(E) = e\frac{4\pi^2}{h}\int_0^\infty F(E)|\langle\sigma_{EC}\rangle|^2\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{ZnO}^{2/3}}\frac{\rho_{EB}(E)}{\sqrt{4\pi\,\Lambda_{IZ}k_BT}}\,(\frac{\pi}{6})^{1/3}l_sdE\text{......} (10)$$

The solution integral term in Eq.(10) to give.

$$I_s(E) = e\frac{4\pi^2}{h}\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{ZnO}^{2/3}}\frac{|\langle\sigma_{EC}\rangle|^2}{\sqrt{4\pi\,\Lambda_{IZ}k_BT}}\left(\frac{\pi}{6}\right)^{1/3}l_s[C]\text{......} (11)$$

where $[C]$ is carrier concentration ,it's written by [24].

$$[C] = \int_0^\infty F(E)\,\rho_{EB}(E)dE\text{.................}(12)$$

Inserting current Eq.(11) in Eq.(3) to obtain the current density $J_s(E)$ in form.

$$J_s(E) = \frac{e}{A}\frac{4\pi^2}{h}\frac{e^{-\frac{(\Lambda_{IZ}+\Delta U^0)^2}{4\Lambda_{IZ}k_BT}}}{d_{ZnO}^{2/3}}\frac{|\langle\sigma_{EC}\rangle|^2}{\sqrt{4\pi\,\Lambda_{IZ}k_BT}}\left(\frac{\pi}{6}\right)^{1/3}l_s[C]\text{......}(13)$$

The reorganization energy Λ_{IZ} (eV) is [25].

$$\Lambda_{IZ}(eV) = \frac{q^2}{8\pi\varepsilon_\circ D}\left[\frac{1}{n^2}-\frac{1}{\varepsilon}\right] - \frac{e^2}{16\pi\varepsilon_\circ R}\left[\frac{n_Z^2-n^2}{n_Z^2+n^2}\frac{1}{n^2}-\frac{\varepsilon_Z^2-\varepsilon^2}{\varepsilon_Z^2+\varepsilon^2}\frac{1}{\varepsilon^2}\right]\text{..........} (14)$$

where $\varepsilon_\circ$ is permittivity., D and R are radius of D102 dye and distance between D102 molecule and ZnO semiconductor, n and ε are refractive index and dielectric of solvent, n_Z is refractive index of ZnO and ε_Z is dielectric constant of ZnO. The radius is [26].

$$D = (\frac{3}{4\pi})^{\frac{1}{3}}(\frac{M}{N_A\rho})^{\frac{1}{3}}\text{..} (15)$$

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

THE RESULTS

The current density for the D102-ZnO heterojunction plays important to calculate the characteristic of DSSC, it is essential to calculate the reorganization energy of the device. However, the reorganization energy must be calculated to identify the main important factors that affect motivational efficiency .It can be calculated using the expression in equation (14) as a function of the radius D102 and the zinc oxide and the distance between them, and the dielectric and refractive index of the 1-Butanol solvent and zinc oxide.The radii of ZnO together D102 dye based on Eq.(15) with molecular weight M = 81.38 g/mol[27] and density 5 .66 $\frac{g}{cm^3}$ [27] of ZnO and M= 614.78g/mol[28] with density $\rho = 1.32 \frac{g}{cm^3}$ [28] for D102 dye ,results are 3.8025 Å for ZnO and 5.694 $A^0$for D102 .Reorganization energy can be calculated using Eq.(14) by inserted the dielectric constant 8.5 and refractive index 2.0033 of ZnO semiconductor [27] and refractive index 1.399 as well as dielectric constant 17.51 of 1-Butanol solvent to results $\Lambda_{IZ}(eV) = 0.442\ eV$.

By quantum transition theory calculations, the current produces from electrons will be moving from excited state of D102 dye to conduction band in ZnO with 1-Butanol solvent evaluates using Eq.(13) , insert reorganization energy $\Lambda_{IZ}(eV) = 0.586\ eV$,electronic strength 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$\times 10^{-1}$ $|eV|^2$, active path length $l_s = 3 \times 10^{-10} m$[29], atomic density $d_{ZnO} = 8.6 \times 10^{22} \frac{1}{m^3}$[30] and carrier concentration $[C] = (1.65, 4.65) \times 10^{23} \frac{1}{m^3}$ [31] with MATLAB program. Results are shown in the Table (1).

Table (1): Current in unit (A) calculated for D102-$ZnO$with 1-Butanol solvent.

Strength coupling $|\langle\sigma_{EC}\rangle|^2 x10-1\ |eV|^2$	The electronic concentration	
	1.65×10^{23} 1 /m3	4.65×10^{23}1 /m3
0.15	0.6883E-03	1.9398E-03
0.25	1.1471E-03	3.2330E-03
0.35	1.6061E-03	4.5263E-03
0.45	2.0649E-03	5.8194E-03
0.55	2.5238E-03	7.1125E-03
0.65	2.9827E-03	8.4058E-03
0.75	3.4416E-03	9.6992E-03
0.85	3.9005E-03	10.9926E-03
0.95	4.3594E-03	12.2853E-03
1.05	4.8182E-03	13.5786E-03
1.15	5.2771E-03	14.8720E-03
1.25	5.7359E-03	16.1653E-03
1.35	6.1952E-03	17.4587E-03
1.45	6.6539E-03	18.751E-03
1.55	7.1126E-03	20.044E-03

The current density can be calculated by the charge transfer reaction mechanism described in Eq.(13) and divided by the area of the cell (0.25 cm^2) performed throughout Eq.(3), results are listed in Table (2).

Table (2): Current density ($\frac{A}{cm^2}$) calculated for device D102-$ZnO$with 1-Butanol solvent.

Strength coupling $|\langle\sigma_{EC}\rangle|^2 x10-1\ |eV|^2$	The electronic concentration $\frac{1}{m^3}$	
	1.65×10^{23}	4.65×10^{23}
0.15	2.7533E-03	0.7759E-02
0.25	4.5888E-03	1.2932E-02
0.35	6.4245E-03	1.8105E-02
0.45	8.2599E-03	2.3277E-02
0.55	10.0952E-03	2.8450E-02
0.65	11.9311E-03	3.3624E-02

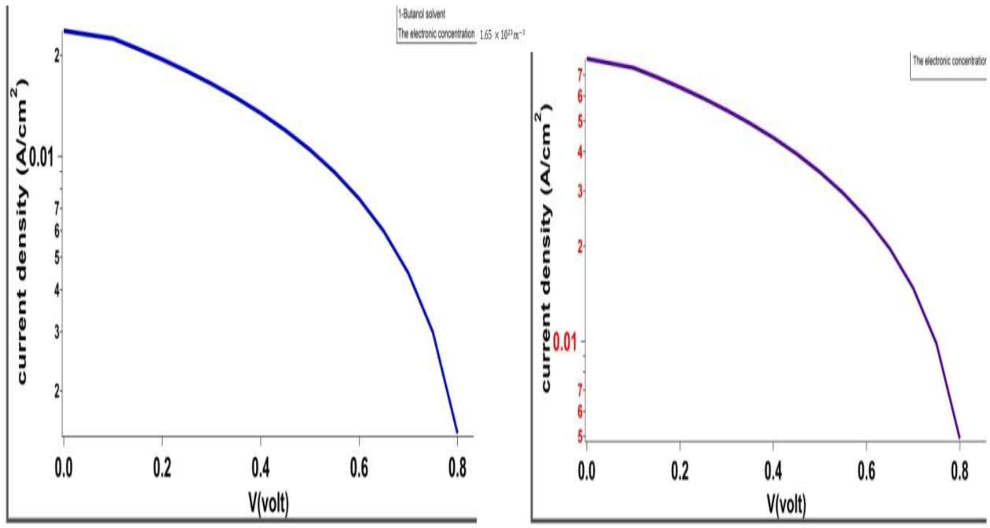
0.75	13.7665E-03	3.8796E-02
0.85	15.6018E-03	4.3969E-02
0.95	17.4377E-03	4.9142E-02
1.05	19.2731E-03	5.4315E-02
1.15	21.109E-03	5.9488E-02
1.25	22.9443E-03	6.4660E-02
1.35	24.7797E-03	6.9836E-02
1.45	26.6156E-03	7.5004E-02
1.55	28.4509E-03	8.0179E-02

Photovoltaic data of device D102-ZnO DSSC is demonstrated by the (current-voltage,$J_s - V$) characteristic of current density J_s (mAcm2) verses voltage V in Volt was shown in table (3)

Table (3): The J_s-V **characteristic of D102-ZnO devices.**

The electronic concentration			
$1.65 \times 10^{23} \frac{1}{m^3}$		$4.65 \times 10^{23} \frac{1}{m^3}$	
V(Volt)	Current(mA/cm^2)	V(Volt)	Current(mA/cm^2)
0.8198	0.000	o.8105	0.000
0.8	2.7533	0.8	7.759
0.75	4.5888	0.75	12.932
0.7	6.4245	0.7	18.105
0.65	8.2599	0.65	23.277
0.6	10.0952	0.6	28.450
0.55	11.9311	0.55	33.624
0.5	13.7665	0.5	38.796
0.45	15.6018	0.45	43.969
0.4	17.4377	0.4	49.142
0.35	19.2731	0.35	54.315
0.3	21.109	0.3	59.488
0.25	22.9443	0.25	64.660
0.2	24.7797	0.2	69.836
0.15	26.6156	0.15	75.004
0.1	28.4509	0.1	80.179
0	30.2862	0	85.354

The characteristic of J_s−V curves of devices D102 dye-contact with ZnO solar cell using two concentrations 1.65×10^{23} (1/m^3) and 4.65×10^{23} (1/cm^3) were displayed in Figure 2.



(A) (B)

Figure 2. Current density versus voltage under concentration $1.65\ \times 10^{23}$(1/m^3)and $4.65\ \times 10^{23}$ (1/ m^3) of D102-ZnO devices.

The theoretical value of the fill factor FF of the solar cell can be determined using the expression in equation (1) by differentiating the power of D102-ZnO heterojunction in solar cell concerning the voltage and finding where it equals zero, results listed in table(4).The conversion efficiency factor was limited to the current generated by a D102-ZnO DSSC, it was calculated using E.(2) using data of FF, $J_{Sc}(mA/cm^2$ and V_{oc} Volt from Table (4) for two concentration($1.65\ \times 10^{23} 1/m^3$ and $4.65\ \times 10^{23} 1/m^3$) . Overall peak theoretical efficiency for current D102-ZnO in DSSCs are about 4.767 with concentration $1.65\ \times 10^{23} 1/m^3$ and 13.95 with concentration $4.65\ \times 10^{23} 1/m^3$.

Table (4): Photovoltaic parameters estimated of the D102-ZnO DSSCs sensitized solar cell.

Variables	**The electronic concentration**	
	$1.65\ \times 10^{23} 1/m^3$	$4.65\ \times 10^{23} 1/m^3$
$J_{Sc}(mA/cm^2)$	30.2862	85.354
V_{oc} Volt	0.8198	0.8298
$J_p(mA/cm^2)$	25.146	69.836
V_p Volt	0.190	0.2
F.F	0.192	0.197
efficiency	4.767%	13.95%

DISCUSSION

Collected in Table 1 are the current and strength coupling of D102-Zno solar cell parameters with an 1-Butanol solvent for two carrier concentrations$1.65\ \times 10^{23} 1/m^3$ and $4.65\ \times 10^{23} 1/m^3$,respectively in this study. For clarity, the current increases for D102-ZnO solar cells with strength electronic coupling to the energy levels state and carrier concentration of the D102 dye and ZnO used are shown in Table 1.As is clear in Table 1, the current increases alternately with the increase of strength electronic coupling $|\langle\sigma_{EC}\rangle|^2$from (0.05 to 0.75) $\times 10^{-1} eV^2$. The current increases when the concentration increases from $1.65\ \times 10^{23} 1/m^3$ to $4.65\ \times 10^{23} 1/m^3$by 2.8 times, due to the electron transfer reaction from the excited state of D102 dye to the conduction band of zinc oxide, and the efficiency is expected to increase when the carrier concentration in the system increases.It is interesting to note that the coupling strength increases under the condition that the wave function of the energy levels of D102 and ZnO in the system overlap to produce more electrons to be transferred across the interface in D102-ZnO devices. Additionally , the transfer of electrons was limited by strength coupling 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.As known from results in both table(1) and table(2) , increasing electronic transition as a consequence of increasing current or current density and recombination electronic coupling through reorganization energy was evaluated as both D102-ZnO concentration in a 1-Butanol solvent medium, where the redox reaction between D102 and ZnO to occur electron transfer in solar cell devices. The reason was that electrons in an excited state also increased to enhance the measured photocurrent.This result in table (4) shows the contribution of J_{Sc} , V_{oc} , J_p, V_p , F.F and efficiency to the dye yielded high energy and photocurrent. Moreover, the average open circuit J_p increases from 25.146 (mA/cm^2) to 69.836 (mA/cm^2) and the photovoltage V_p increases from 0.190 V to 0.2 V, and an increase can be observed with increasing concentration. As can be seen, current density increases from 30.2862 (mA/cm^2) to 85.354 (mA/cm^2) and efficiency increases from 4.767% to 13.95% when increases concentration from $1.65\times10^{23} 1/m^3$ to $4.65\times10^{23} 1/m^3$.Efficiency in Table 4 shows that the efficiency value of D102 dye contact with ZnO increased by 2.92 with increased concentration from to.The filling factor and efficiency are estimated according to the $J_{Sc}-V$ curves shown in Fig.(2) shown in Table (3) and Fig.(2). Table (4) shows the effect of carrier concentration on both fill factor and efficiency through the effect on the average open circuit and voltage V_p (Volt) and current J_p (mA/cm^2), estimated using Fig.(2) and listed in Table (4).Moreover, the increased concentration and electronic coupling are strongly influenced on V_{oc}, J_{Sc}, FF, and efficiency, as summarized in Table (4). The efficiency spectrum showed an increase with increased concentration, thus the absorption of photons appears to be increasing.

CONCLUSION

A theoretical calculation of the efficiency of indoline dye contact with a zinc oxide device with a 1-butanol solvent in DSSCs has been introduced based on the electronic transfer theory. Current density, filling factor and efficiency in D102-ZnO solar cell devices had been calculated using carrier concentration in a range from $1.65\times10^{23} 1/m^3$ to $4.65\times10^{23} 1/m^3$and electronic coupling constant at limited reorganization energy.

Increased concentration resulted in increased computational efficiency from 4.767% to 13.95% and increased maximum current density from 30.2862 (mA/cm^2) to 85.354 (mA/cm^2) with increased contribution of maximum current density Jp from 25.146 (mA/cm^2) to 69.836(mA/cm^2) at limited reorganization energy 0.586 eV and strength coupling in the range of $[\,0.75\times10^{-1}\geq|\langle\sigma_{EC}\rangle|^2\geq0.05\times10^{-1}\,]\,|\mathrm{eV}|^2$. The corresponding improvement in efficiency can be attributed to the increased electronic transport in the D102-ZnO heterojunction which in turn enhances the efficiency.

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