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Theoretical Study of the Influence of Donor Sensitize Dye on Performance of Dye-sensitized D149/ ZnO and Alq3/ZnO Solar Cells DSSCs

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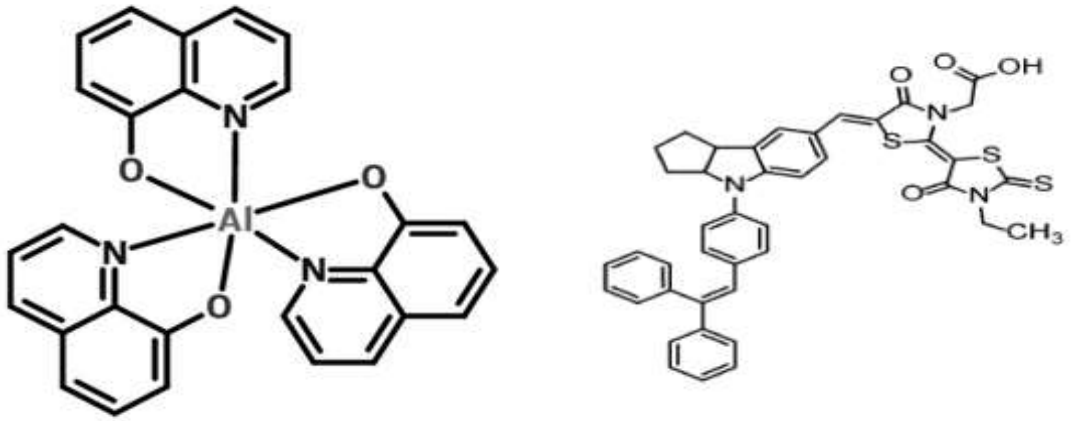
Abstract

In this paper, a theoretical study was introduced to discussion the Influence of donor sensitizer on efficiency of solar cell with clear focusing on dye sensitized solar cell DSSCs applications was presented. Use of donor as -sensitizer dye in solar cells was a viable contender in photovoltaic due to their spectrum of excited state to transfer more electrons to conduction band of semiconductor .In this study, two systems Alq3/ZnO and D149/ZnO devices taken with same two solvents .Transition energy ,coupling strength and transition parameters are used to calculate the electron current density , it uses to calculate the photovoltaic characteristic I-V ,fill factor and the efficiency of the solar cell .Especially, the largest performance was for the both D149/ ZnO and Alq3/ZnO solar cells based on Acetonitrile as a solvent with electron current density of (430 and 13.8) mA/cm^2 between (0.1 to 0.6) V and produced the highest efficiency calculated 2.593 and 0.938for the both solar cell was corresponds to the lowest efficiency about 0.536 for Alq3/ZnO with Ethanol solvent.

Keyword: Donor Sensitize Dye **,** Alq3/ZnO **,** D149/ZnO

1.Introduction

Today, with the increasing population, the humanity is embarking upon the path of dependency to demanded for sustainable and continuous energy supply because fossil fuels represent finite resources and most estimates suggest that proven oil reserves will not be sufficient to meet global demand by at least the mid-21st century [1]. The main of strategies to meet this demand is alternative energy sources or renewable energy sources ,its clean energy and safe, from the surround such as solar, wind, hydropower, geothermal energy, hydropower and biomass[2].The solar technological has been constituting a sizable chunk to give the abundance of approximated to one hour of solar irradiation amounted for annual global energies that's needed from solar energy [3]. The photovoltaic (PV) solar cell is devices woks to convert the sun light directly into electricity . It is well-suited for a variety of outdoor applications, indoor and at various application [4]. To fulfill this goal of low cost and clean energy produced using renewable resources, it has been necessary to fabrication higher efficient photovoltaic with lower cost[5].Dye-sensitized solar cells (DSSCs) are becoming a promised because higher efficiency, cost-effectiveness, ease of fabrication, and environmentally friendly[6]. Several experimental techniques and variety theoretical were adopted to improvement the works performance of DSSCs and understand the mechanism to enhancement their efficienc[7].Operation of DSSCs are depended on the charge transfer process from excited dye molecules to conduction band semiconductor material [8]. Hadi et al studied charge transfer interaction process in different heterostructure devices depending on the investigation of the orientation energy with the alignment of energy levels of materials in electronic devices. The electron' moves from one state to another were required to close energy levels in both materials [9]. The charge transfer in variety of heterostructure devices depends on the transition of the energy state in both donor and acceptor states of contact in heterostructure devices [10].Recently, the searches develop device structures, sensitizers and redox mediators that's improvement the performance of DSSCs [11]. It's very interesting to utilize dye molecules, that have a broad absorption spectrum, to absorb photons to increase the electric conversion efficiency of cells [12]. Alq3 is one of sensitizer dye uses in many application named Tris (8-hydroxyquinolinato) Aluminium (Alq3),it has the molecular weight 459.43(g/mol),density 1.31(g/cm3),ionization energy5.8 eV, chemical formula $C_{27}H_{18}AlN_3O_3$ and structure is illustrated in figure (1-A) [13]. On the other hand ,the D149 sensitized dye named(5-[[4-[4) -2,2- Diphenylethenyl)phenyl]-1,2,3-3a,4,8b-hexahydrocyclopent[b]indol-7-yl]methylene]-2-(3-ethyl-4-oxo-2-thioxo-5-thiazolidinylidene)-4-oxo-3-thiazolidineacetic acid, Indoline) and have ,molecular weight 741.94,2.141 g.cm-3 ,chemical structure $C_{42}H_{35}N_3O_4S_3$ and structure is given in figure (1-B) [14]. The chemical structure of organic Alq3 and D149 dyes are shown in Figures 2(A) and 2(B), respectively.



A **B**

Figure 1. Chemical structure of sensitized dyes (A) (Alq3)dye and (B) D149 [13,14].

Furthermore, Alq3 and D149 are attractive organic dyes are already using in DSSCs solar cells. The schematic of energy levels is depicted in Figure 2[15].

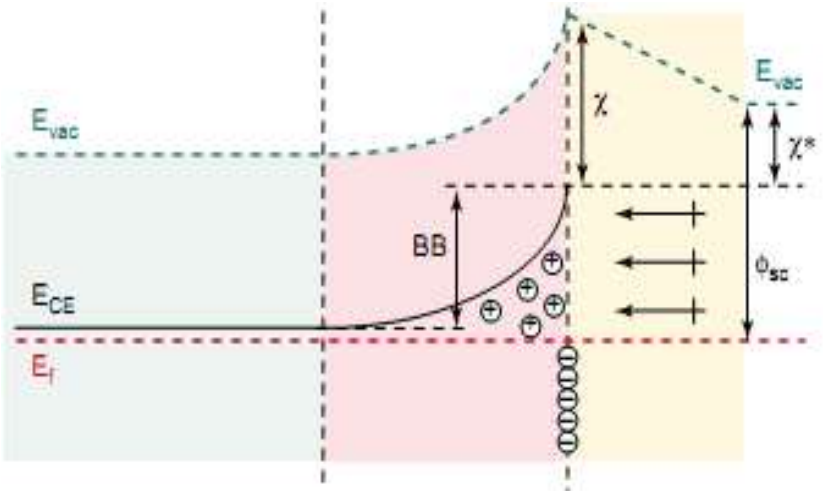


Figure2. Illustrated of charge transfer at molecules-semiconductor interfaces [15].

Both ZnO and TiO2 semiconductors are wide band gap (3.73eV and 3.2eV) of the II-VI semiconductor group ,there are promising in materials science and have crystal structure (tetragonal rutile and Wurzite) , molecular weight 81.38 g/mol and 79.866 g/mol , mass density 5.66 g/cm3 and 4.23 g/cm3, dielectric constant 8.5 and 55 with refractive index2.0033 and 2.5688 and electrons concentration $N(E) = 2.2 \times\times 10^{24}(1/\text{cm}^3)$ and $1.163\times 10^{25}(1/\text{cm3})$ [16]. In this paper, theoretical study based on quantum theory approach introduced to discussion the influence of donor sensitizer dyes Alq3 and D149 on performance of DSSCs devices .

2. Theory

The current of electrons transfer from the one state to the other state (I) s given by [17]:

$$I_n = e\sum_{n=1}^{\infty} F(E_n)\ T_D^A(E) \qquad (1)$$

where e is the electronic charge, $F(E_n)$ is Fermi-Dirac probability of charge transfer from donor to acceptor states and $T_D^A(E)$ is transmission probability.Transmission probability has been given as [18]:

$$T_D^A(E) = \frac{2\pi}{\hbar}\langle \mathbb{M}_D^A\rangle^2\ \delta(E_n) \qquad (2)$$

where $\hbar$ is Dirac constant , $\mathbb{M}_D^A$ is the strength coupling constant between the donor and the acceptor $\delta(E_n)$. Substituting Eq.(2) into Eq. (1) and introduced the current density $\hat{\mathcal{P}}(E_n)$ into

get .

$$I_n = \frac{2\pi e}{\hbar}\sum_{n=1}^{\infty} F(E_n)\,\langle \mathbb{M}_D^A\rangle^2 \hat{\mathscr{p}}(E_n)\delta(E_n) \qquad (3)$$

The current density of states $\hat{\mathscr{p}}(E_n)$ is given as [19]:

$$\langle \hat{\mathscr{p}}(\in_i)\rangle = \sqrt{\frac{1}{4\pi\Lambda_{AD}\mathrm{k_B T}}}e^{\frac{-(\Lambda_{AD}+\Delta E^0)^2}{4\Lambda_{AD}k_BT}} \qquad (4)$$

where ΔE^0 is the driving force energy as function of conduction band energy E_{CB} and chemical potential qE^0 for molecule dye . Substituting Eq. (4) in Eq. (3) and integrate to results .

$$I_n = \frac{2\pi e}{\hbar}\int_{-\infty}^{\infty} F(E_n)\langle \mathbb{M}_D^A\rangle^2 \sqrt{\frac{1}{4\pi\Lambda_{AD}\mathrm{k_B T}}}e^{\frac{-(\Lambda_{AD}+\Delta E^0)^2}{4\Lambda_{AD}k_BT}}\delta(E_n)\ \mathrm{dE} \qquad (5)$$

The density of state for semiconductor ($\rho_{e(Se)}$(E)) in the system which given by [20].

$$\rho_{e(Se)}(E) = \delta(E_n) = D_s\frac{l_S}{(\frac{6}{\pi})^{1/3}}d_S^{-2/3} \qquad (6)$$

where D_s is the electronic density of states in semiconductor, l_S is effective length, and d_s is atomic density of the semiconductor.Substituting Eq. (6) into Eq. (5), the result is :

$$I = \frac{2\pi e}{\hbar}\sqrt{\frac{1}{4\pi\Lambda_{AD}\mathrm{k_B T}}}\int_{-\infty}^{\infty} F(E)\,\langle \mathbb{M}_D^A\rangle^2 e^{\frac{-(\Lambda_{AD}+\Delta E^0)^2}{4\Lambda_{AD}k_BT}}D_s\frac{l_S}{(\frac{6}{\pi})^{1/3}}d_S^{-2/3}dE \qquad (7)$$

However, the potential barrier ($\mathbb{U}$) at interface of donor and the acceptor is [21]:

$$\mathbb{U} = \frac{[\Lambda_{AD}+(E_{cb}-qE^0))]^2}{4\Lambda_{AD}} \qquad (8)$$

Substituting Eq.(8) into Eq. (7) to give:

$$I = \frac{2\pi e}{\hbar}\sqrt{\frac{1}{4\pi\Lambda_{AD}\mathrm{k_B T}}}\langle \mathbb{M}_D^A\rangle^2 e^{-\frac{[\Lambda_{AD}+(E_{cb}-qE^0)]^2}{4\Lambda_{AD}k_BT}}\frac{l_S}{(\frac{6}{\pi})^{1/3}}d_S^{-2/3}\int_{-\infty}^{\infty} F(E)\,D_s dE \qquad (9)$$

The solving of the integral is given electron concentration $N_S\,(E)$ at the surface of semiconductor [22] :

$$\int_{-\infty}^{\infty} F(E)\,D_s dE = N_S\,(E) \qquad (10)$$

The Eq. (9) together Eq.(10) reduced to:

$$I = \frac{2\pi e}{\hbar}\sqrt{\frac{1}{4\pi\Lambda_{AD}\mathrm{k_B T}}}\langle \mathbb{M}_D^A\rangle^2 e^{-\frac{[\Lambda_{AD}+(E_{cb}-qE^0)]^2}{4\Lambda_{AD}k_BT}}\frac{l_S}{(\frac{6}{\pi})^{1/3}}d_S^{-2/3}N_S(E) \qquad (11)$$

The transition energy Λ_{AD} is energy has taken for reorientation the system , it is given by [23]:

$$\Lambda_{AD} = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{D}\left[\frac{1}{n^2}-\frac{1}{\varepsilon}\right]-\frac{1}{2R}\left[\frac{n_{Se}^2-n^2}{n_{Se}^2+n^2}\frac{1}{n^2}-\frac{\varepsilon_{Se}^2-\varepsilon^2}{\varepsilon_{Se}^2+\varepsilon^2}\frac{1}{\varepsilon^2}\right]\right] \qquad (12)$$

where ε° is the permittivity, D is radius of the Alq3 molecule, n is refractive index of solvent, ε is dielectric constant, R is the distance between the molecule and the semiconductor, n_{Se} is the refractive index of semiconductor and ε_{Se} is the dielectric constant of the semiconductor. Furthermore, radii can be calculated using spherical approach [24]:

$$D(m) = \left(\frac{3}{4\pi}\frac{m}{N\rho}\right)^{\frac{1}{3}} \qquad (13)$$

where m is the molecular weight, N is Avogadro's number and ρ is the density of the material. The fill factor value (FF) is a ratio of maximum power to the short circuit power based on I-V curves and given by [25]:

$$FF = \frac{I_m V_m}{I_{sc} V_{oc}} \quad (14)$$

where I_m is maximum current, V_m is maximum voltage, I_{sc} is the short-circuit current and V_{oc} is the open-circuit voltage. The efficiency of solar cells is indicated the amount of power converted by the cell compared to the absorbed power ,it's a ratio of the maximum electrical power output (Pm) to the incident power (Pin) [26]:

$$\eta = \frac{P_m}{P_{in}} = \frac{I_{Sc} V_{oc} FF}{P_{in}} \quad (15)$$

3. Results and Discussion

According to current expression in Eq.(11) based quantum transition model ,the current in both Alq3/ZnO and D149/ZnO devices was strongly affected by transition energy, coupling strength, driving force energy and potential between the dye and semiconductor . Two D149 and Alq3 dyes sensitized contact with ZnO-based solar cells containing 2,2,2-Trifluoroethanol and 1-propanol solvents, respectively were designed. The current I, current density J, fill factor FF, and efficiency η of the two designed DSSCs are evaluated . To calculate the current density depend on several constants such as transition energy ,diving energy atomic density effective length ,coupling constant and potential energy . Firstly ,the transition energy depends on radii of molecules dye and atomic of ZnO ,that's depend on weight M, and mass density ρ for Alq3 ,D149and ZnO from tables(1) and (2) are needed. The radii of Alq3 ,D149 and ZnO were calculated using the Eq.(13) to give 5.181×10^{-8} cm , 5.16×10^{-8} cm and 3.8025×10^{-8} for Alq3 , D149 and ZnO respectively.

Table 1. Several properties of Dyes.

Properties	D149[27-28]	Alq3[29]
Molecular weight(g.mol^{-1})	71.94	459.43
Chemical formula	$C_{42}H_{35}N_3O_4S_3$	$C_{27}H_{18}AlN_3O_3$
Mass Density (g.cm^{-3})	1.47	1.31
LUMO(eV)	-5.13	2.85
HOMO(eV)	-2.55	5.62
Radius (Å)	5.16	5.181
Ionization energy(eV)	5.2	5.8
Melting Point(°C)	284-289	415.4

Table 2. Essential properties of ZnO.

Properties	ZnO[30]
Molecular weight (g.mol^{-1})	81.38
Dielectric Constant	8.5
Mass Density (g.cm^{-3})	5.66
Density of state (N$_s$.cm^{-3})	2.22×10^{24}
Refractive index	2.0033
Radius (Å)	3.8025
Valance band	7.8
Conduction band energy (eV)	4.5
Refractive index	2.0041
Electron concentration (cm^{-3})	2×10^{20}
Electron affinity (eV)	4.3

Transition energy of both Alq3/ZnO and *D149 – ZnO* devices can be calculated using Eq.(12) with the properties of the two solvents from table (3) and properties of ZnO from table(2).Firstly, inserting the radii of Alq3 dye (5.181×10^{-8}) , D149 dye(5.16×10^{-8}) and ZnO(3.8025×10^{-8}), refractive index and dielectric constant of two solvents and ZnO with Eq. (12) using MATLAB program to calculate the values of Λ_{AD} . The resulted values are listed in Table (3) .

Table 3. Results of transition energy of D149/ZnO and Alq3/ZnO solar cell devices .

Solvent	Chemical formula	Refractive index[31]	Static dielectric constant[31]	Transition energy (eV)	
				D149/ZnO	Alq3/ZnO
Ethanol	C_2H_6O	1.3614	24.5	0.61559	0.589
Acetonitrile	C_2H_3N	1.3441	37.5	0.65059	0.623

Table(3) shows that Λ_{AD} was influenced by the dielectric constant and refractive index of the solvents.

It can be seen the Λ_{AD} increased as the refractive index decreased and decreased as the dielectric constant decreased as results of polarity influence of the solvents. Transition energy $\Lambda_{AD}(eV)$ for both D149/ZnO and Alq3/ZnO systems reach to 0.65059 eV and 0.623eV with Acetonitrile solvents compare with 0.61559 eV and 0.589 eV with using Ethanol solvents .It indicates that both system with Acetonitrile solvents have bit lower energies to alignment. The current I(A) in D149/ZnO and Alq3/ZnO devices has been calculated using Eq.(11) based on the values of Λ_{AD} in Table (3), the coupling overlap ($|\mathbb{M}_D^A(eV)|^2$) takes 0.35, 0.45, 0.55, 0.65, 0.75 and 0.85 $\times10^{-11}$ in unit (eV)^2,the ionization energy 5.2 eV and 5.8 eV for D149 and Alq3 dyes, $l_s = 3A^o$ [32] .The results of the current listed in Table (4) for D149/ZnO and Alq3/ZnO devices.

Table 4. Results of current I of charge transfer for Alq3/ZnO and *D149 – ZnO* devices .

Coupling strength $\lvert\mathbb{M}_D^A(eV)\rvert^2\times10^{-11}$ |eV|^2	Ethanol Solvent		Acetonitrile Solvent	
	D149/ ZnO	Alq3/ZnO	D149/ ZnO	Alq3/ZnO
0.35	3.758E-02	0.149E-03	2.668E-02	0.812 E-03
0.45	4.832E-02	0.191E-03	3.430E-02	1.044E-03

0.55	5.906E-02	0.234E-03	4.192E-02	1.276 E-03
0.65	6.980E-02	0.277E-03	4.954E-02	1.508 E-03
0.75	8.054E-02	0.319E-03	5.717E-02	1.740 E-03
0.85	9.128E-02	0.362E-03	6.479E-02	1.972 E-03

The current density (J) in both devices D149/ZnO and Alq3/ZnO devices calculated by dividing the current in table(4) on the area (0.4cm×0.4cm). The results of the current density list in Table (5) for D149/ZnO and Alq3/ZnO devices.

Table 5. Results of current density for *D149 – ZnO* and Alq3/ZnO solar cell devices .

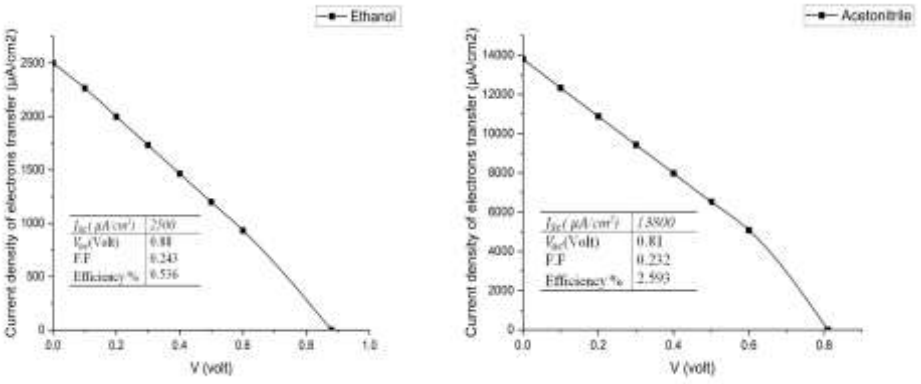
Coupling strength $\lvert\mathbb{M}_D^A(eV)\rvert^2\times 10^{-11}$ |eV|^2	Ethanol Solvent		Acetonitrile Solvent	
	D149/ ZnO	Alq3/ZnO	D149/ ZnO	Alq3/ZnO
0.35	2.349E-01	0.932E-03	1.667E-01	5.07 E-03
0.45	3.020E-01	1.199 E-03	2.143E-01	6.525 E-03
0.55	3.691E-01	1.465 E-03	2.620E-01	7.981 E-03
0.65	4.362E-01	1.732 E-03	3.096E-01	9.43 E-03
0.75	5.033E-01	1.998E-03	3.573E-01	10.881E-03
0.85	5.705E-01	2.265E-03	4.049E-01	12.331E-03

Tables (4) and (5) show that the current and current density related to the solvent media , which increases with decreases of Λ_{AD} in Table (3) , while reach to large with small transition energy belongs to the device.This means the current and current density in the solar cells influence by polarity through the refractive index and the dielectric constant of the solvent . Polarity was inversely related to the Λ_{AD},its clearly shown in Eq. (12) .Current density increases when Λ_{AD}decreases for system and transition become more probable .The current and current density of electron in D149 /TiO_2 is larger than Alq3 /TiO_2 and increases with decreases the potential at interface .However ,the current and current density in both Tables (4) and (5) are increased with increased the strength coupling and large for D149/ ZnO with solvent and electrons are transition from donor to the conduction band in acceptor semiconductor.Furthermore ,the open circuit photo-voltage can be estimated from the *I-V* curves and using to calculate the efficiency and fill factor ,the current density with voltage is tabulated in table(6) for both systems . The J–V characteristics of two system are shown in the Figure (3).

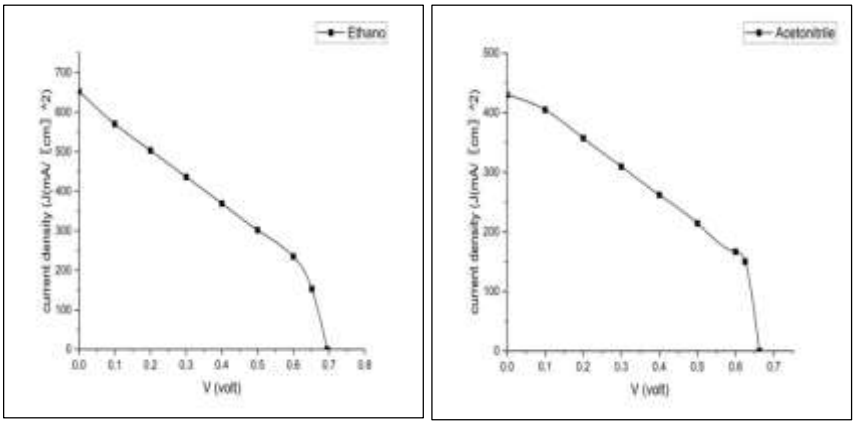
Table 6 . The I-V characteristic with voltage (V) of *D149 – ZnO and* ALq3/ZnO.

Current density ($mA.cm^{-2}$) of D149 - ZnO		Current density(μA/cm^2) of ALq3/ZnO		Voltage (V)
Ethanol	Acetonitrile	Ethanol	Acetonitrile	
570.516	404.974	2265.60	12331.00	0.1
503.397	357.330	1998.70	10881.00	0.2
436.277	309.686	1732.50	9431.00	0.3
369.157	262.042	1465.60	7981.00	0.4
302.038	214.398	1199.30	6525.00	0.5

234.918	166.754	932.50	5078.70	0.6



A For ALq3/ZnO



B For D149/ZnO

Figure (3): The J–V graph of A) Alq3/ZnO **and B)** D149/ZnO solar cell device.

Table(7)Solvent dependent current, voltage, FF and efficiency.

System	Photovoltaic parameters of the DSSCs sensitized			
	V_{oc}(Volt)	J_{Sc}(mA/cm^2)	F.F	efficiency
D149/ ZnO- Ethanol	0.695	652	0.210	0.997
Alq3/ZnO- Ethanol	0.88	2.5	0.243	0.536
D149/ ZnO- Acetonitrile	0.663	430	0.329	0.938
Alq3/ZnO- Acetonitrile	0.81	13.8	0.232	2.593

The photo-voltage V_{oc} and the current density J_{Sc} in Table (7) use to calculate the fill factor and efficiency using Eq. (14) and (15) ,results listed in table(7). Table(7) indicates the efficiency an increased with acetonitrile comparing with Ethanol is used. As a result, Alq3/ZnO- Acetonitrile has high efficiency comparing with Alq3/ZnO- Ethanol ,while the D149/ ZnO- Ethanol has large efficiency comparing with D149/ ZnO- Acetonitrile ,this refers the Acetonitrile solvent best media strongly with ZnO surface .On the other hand, the lowest efficiency values for Alq3/ZnO-Ethanol because Ethanol has the lowest dielectric constant comparing to the Acetonitrile solvent .According to work by Burak Y. Kadem et al in 2015[33] show efficiency form 1.81 and 3.92

supply. Interestingly, the efficiency estimates in this paper are in good agreement with the acetonitrile solvent [33].

4. Conclusions

A simple model for current density based on quantum transfer theory introduced to the estimated the efficiency for solar cell devices according to density of state, transition energy ,strength coupling ,driving energy and concentration .The short-circuit current estimates depended on the current density and the other electronic coefficient. In general, the higher efficiency of solar cells produced with using Acetonitrile solvent has large transition energy.

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