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Article

A Study of Effect of Concentration on Efficiency of dye-Sensitized Solar cells (DSSC) Based on ZnS

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Abstract: In this work, the effect of concentration on efficiency can be studied based on theoretical approach for N3 dye contact ZnS semiconductor based on dye sensitized solar cells DSSCs . The impact current density based on transition energy, , atomic density, length of charge, concentration as well as polarity of both N3 -ZnS system on the electronic transport process. The chemical Ethanol solvents using a polar media with N3 dye –ZnS semiconductor system. The current density component is evaluated relative to transition energy, driving energy, potential and coupling parameters. The strength coupling and concentration on the current density behavior can be discussion in N3-ZnS devices, that's reflected in the electronic transport results.The current density results reveal the behaviour of current density has been strongly affected by the concentration, it determine the efficiency of N3-ZnS devices. The electron transfer ability has been limited current density due to transition energy, driving force and potential. The efficiency, influenced by the carrier concentration increases of N3-ZnS devices ,it plays a significantly in the increases current density as well as limited the electrical properties of N3-ZnS devices. Specifically, the overlapping coupling between N3 dye and ZnS was influenced on the electronic current density.In general, the increases in concentration from $3 \times 10^{18} cm^{-3}$ to $5 \times 10^{18} cm^{-3}$ is favorable and increases efficiency from 4.09 % to 4.448 %% ,it suggests that N3 dye a suitable contact for ZnS -based DSSCs devices.

Keywords: Concentration , Efficiency , N3-Ruthenium , ZnS ,DSSC.

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Introduction

The growing global population has led to an increased demand for clean and renewable energy for sustainable development in various regions of the world. Recent statistics indicate that many countries rely on limited and non-renewable resources, exacerbating global warming and environmental pollution [1].Dye-sensitive solar cells (DSSCs) are among the most promising sources for renewable energy devices.These materials are characterized by their environmental friendliness, low cost, and excellent conversion efficiency [2].Dye-sensitized solar cells (DSSCs) have received considerable scientific attention since Oregano and Gratzel published a report in 1991 describing the first of these cells with an efficiency of 7% [3].Dye-sensitized solar cells are photochemical cells, and their appeal has increased due to their low processing costs,ease of manufacture, and acceptable efficiency. Electron transfer in these cells occurs using a redox medium [4]. The main basic reactions operating in dual photovoltaic cells depend on the photocatalyzed charge transfer reaction through the interfaces of the contact materials in the devices and the materials in the electrochemical devices, and this requires the reconfiguration of energy levels to become correlated with each other [5]. The electron transfer reaction stays very main crucial and basic reactions for varouse physical devices properties. It occurred by different methods such that; photo induce, thermally excitation , laser induced and chemical methods[6]. Electron transfer can play a central role in many applications of photo-induced reactions in electrochemistry,solar energy conversion cells and photocatalysis [7]. Marcus introduces a simple theory to understanding mechanism of electron transfer occured in molecules devices as well as solar energy conversion .Marcus R. introduced an electron transfer theory for charge transfer reactions in homogeneous donor-acceptor system[8].Several decades, theory of electron transfer was developing due to variety tools time resolved, spectroscopy, analytical theory and computer simulation methods [9]. Hadi and Hazim introduce a model of charge transfer in solid interact with molecule depending on transition theory [10]. However, the electron transfer processes played main role in molecule contact with semiconductor in many fields .The electron transport challenges and gains more attention for the effect of potential on the rate foe electron transfer from donor to an acceptor states in systems [11].However, although electron transport has been exploited in many devices, understanding the mechanism of electron transport is still under investigation [12]. The study and research of electron transfer across contact surfaces between two materials depends on the compatibility of the energy levels of the two materials in the system.Furthermore, the transfer of electrons is limited by potential at the interface [13].The proximity of the molecule's energy levels to the energy level of the solid material (semiconductor or metal) is a fundamental rule for the transfer of electrons in the system [14]. Zinc sulfide (ZnS) is studied because of its multiple applications in electric lighting, light-emitting diodes,sensors,infrared windows, and lasers, thanks to its thermal stability and outstanding chemical and morphological properties [15]. However, zinc sulfide (ZnS) is characterized by its low cost, low toxicity, and relative abundance in nature. It is an n-type semiconductor ,it has zinc blende and hexagonal structure (wurtzite ZnS) with a wide energy gap of approximately 3.6 electron volts.

In this work , the effect of concentration on efficiency in the N3 sensitized dye contact to ZnS semiconductor is studied using theoretical approach depend on evaluation the transition energy,strength coupling and concentration

Theory

The electronic transition for contact N3 - ZnS device may be written as [17].

$$T_{et} = \frac{4\pi^2}{h}\sum|\langle H_s\rangle|^2 \rho_e(E) \ldots\ldots\ldots\ldots(1)$$

Where h and $\langle H_s\rangle$ are Blank constant and coupling and $\rho_e(E)$ is effective of electronic density in syste ,it gives by [18].

$$\rho_e(E) = D_N \frac{l_Z}{(\frac{6}{\pi})^{1/3}} \ldots\ldots\ldots\ldots(2)$$

Where D_N and l_Z are activate density and length path in ZnS . The activate density of state is [19].

$$D_N = \langle\hat{\rho}_{NZ}\rangle \rho_N(E) \rho_a^{-2/3} \ldots\ldots\ldots\ldots (3)$$

Where $\langle\hat{\rho}_{NZ}\rangle$ is the electronic density of state, $\rho_N(E)$ is density in N3 dye and ρ_a is atomic density of ZnS . Inserting Eq.(3) in Eq.(2) to given .

$$\rho_e(E) = \langle\hat{\rho}_{NZ}\rangle \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}} \rho_N(E) \ldots\ldots\ldots\ldots(4)$$

The density of state in N3-ZnS system is [20].

$$\langle\hat{\rho}_{NZ}\rangle = \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \ldots\ldots\ldots\ldots (5)$$

Where $T_{SD}(\boldsymbol{eV})$ and ΔU^0 are the transition energy and driving force energy .

Inserting Eq.(5) in Eq.(4) to obtained

$$\rho_e(E) = \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}} \rho_N(E) \ldots\ldots\ldots\ldots(6)$$

Then the electronic transition in Eq.(1) with Eq.(6) gives .

$$T_{et} = \frac{4\pi^2}{h} \sum |\langle H_s\rangle|^2 \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}} \rho_N(E) \ldots\ldots\ldots\ldots(7)$$

The current density $J(E)$ in N3-ZnS for DSSCs is

$$J(E) = \frac{qT_{et}F(E)}{A} \ldots\ldots\ldots(8)$$

Where q is charge of electron ,F(E) is Fermi function and A is Area of cell ,substituting Eq.(7) in Eq.(8) and simply to results

$$J(E) = \frac{q}{A}\frac{4\pi^2}{h} |\langle H_s\rangle|^2 \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}} \sum F(E)\,\rho_N(E)) \ldots\ldots\ldots(9)$$

The summation in Eq. (9) is given [21].

$$\sum F(E)\rho_N(E) = [A] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(10)$$

Where $[A]$ is concentration in (cm^{-3}). The Eq.(9) with Eq. (10) produced .

$$J(E) = \frac{q}{A}\frac{4\pi^2}{h} |\langle H_s\rangle|^2 \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}} [A] \ldots\ldots\ldots(11)$$

The atomic density ρ_a in ZnS is function of nature concentration N_e at the Fermi level and Fermi energy E_F,it gives by [21].

$$\rho_a = \frac{3}{2D_n}\left(\frac{N_e}{E_F}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(12)$$

The fill factor for N3-ZnS solar cell is ratio relative to J-V curve's maximum power ,it is a function of the maximum flow current density J_m and maximum voltage V_m. and gave by[22].

$$FF = \frac{J_mV_m}{J_SV_o} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(13)$$

where J_S and V_o are short-circuit current and open circuit voltages. The efficiency of N3-ZnS solar cell can write as [18].

$$\eta = \frac{FFJ_SV_o}{I_0}\% \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(14)$$

where I_o is incident light intensity

Transition energy $T_{SD}(\boldsymbol{eV})$ of system is given by [23].

$$T_{SD}(\boldsymbol{eV}) = \frac{q^2}{8\pi\varepsilon_\circ}\left[\frac{1}{R}\left[\frac{1}{{n_s}^2} - \frac{1}{\epsilon_s}\right] - \frac{1}{2D}\left[\left(\frac{n_{Sem}^2-n^2}{n_{Sem}^2+n^2}\right)\left(\frac{1}{n^2}\right) - \frac{\epsilon_{Sem}^2-{\epsilon_s}^2}{\epsilon_{Sem}^2+{\epsilon_s}^2}\frac{1}{{\epsilon_s}^2}\right]\right] \ldots(15)$$

Where q and $\varepsilon_\circ$ are the electric charge and permittivity , n_s , n_{Sem} ,ϵ_s and $\epsilon_{Sem}$are the refractive index and dielectric constant for both solvent and semiconductor , $\boldsymbol{R}$ and **D** are radius of dye and distance from molecule to semiconductor . Radius of molecule is given by approach formula [24].

$$D(nm) = \left(\frac{3}{4\pi}\frac{MW}{N_A\rho_m}\right)^{\frac{1}{3}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(16)$$

Where MW, N_A and ρ_m are molecular weight ,Avogadro number and density of material .

Results

The current density was investigated and studies for N3 contact to ZnS theoretically using MATLAP software program . The current density in N3-ZnS system influence by transition energy. The transition energy of media surrounded N3 and ZnS is function of dielectric and refractive index for both materials . The radii of N3 dye and ZnS can the using Eq.(16) by insert the molecular weight

($705.64\frac{\text{g}}{\text{mol}}$[25], $97.46\frac{\text{g}}{\text{mol}}$[26]) and density ($1.36\ \text{g}/cm^3$[25], $4.079\ \text{g}/cm^3$[27]) , results 5.9 A^0, and 2.12Å for N3 dye and ZnS .

The overall transition energy $T_{SD}\,(\boldsymbol{eV})$ can calculate using Eq.(15) for the N3-ZnS cell by taking the refrective index (1.372[28], 2.356[27]) and dielectric constant (6.02) [28] , 8.9[27])of the Ethanol solvents and for the system N3-ZnS with taken the radii [5.9 and 2.11]Å for RuN3 and ZnS , refractive index and dielectric constant of the semiconductor ZnS [27] and the distance between N3 and ZnS ,result is 0.37eV.

Next, the atomic constant can calculate used Eq.(12) inserting $N_e = 1.4 \times 10^{14} cm^{-3}$, $E_F = 4.52eV$ and $D_n = 8$ (state /eV) of ZnS to result $5.32\ \times 10^{18} m^{-3}$. $J(E) = \frac{q}{A}\frac{4\pi^2}{h}|\langle H_s\rangle|^2 \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}}[A]$ ………(11)

The current density $J(E)$ for N3 ZnS with ethylen solvent calculates using Eq.(11) taken coupling $\langle H_s\rangle$=0.08,0.09,.10,0.20,0.30,0.40,0.50,0.60,0.70,0.80,0.90,1.00,1.10,1.20 and 1.3 $\times 10^{-1}$ eV, $T_{SD}(0.37eV$, $l_Z = 3A^o$[22], $\rho_a = 5.32 \times 10^{18} m^{-3}$ taken two concentration $[A] = (3{,}5) \times 10^{18} cm^{-3}$ [23] and results computed using MATLAP program, results show in the Table (1)

Table 1. Results of current density $\boldsymbol{J(\ mA/cm^2)}$for N3-ZnS with ethylen solvent.

Concentration			
$3 \times 10^{18} cm^{-3}$		$5 \times 10^{18} cm^{-3}$	
J(m A/cm^2)	V(Voltage)	J(m A/cm^2)	V(Voltage)
0.00	0.804	0.00	0.813
1.36	0.763	2.43	0.772
2.22	0.746	3.42	0.753
3.17	0.719	4.18	0.725
4.56	0.685	5. 36	0.691
5.36	0.663	6.73	0.678
6.15	0.585	7.39	0.592
7.34	0.523	8.77	0.534
8.62	0.475	9.25	0.482
9.81	0.419	10.72	0.428
10.31	0.365	11.62	0.374
11.38	0.310	12.77	0.326
12.66	0.275	13.23	0.287
13.55	0.229	14.70	0.237
14.14	0.175	15.29	0.187
15.53	0.139	16.76	0.1
17.653	0	18.738	0

Indeed, the voltage corresponding of N3-ZnS solar cell has been estimated using strength with MATLAP program, results show in the Table (2)

Table 2. The J-V characteristic of N3-ZnS solar cell**.**

Concentration			
$3 \times 10^{18} cm^{-3}$		$5 \times 10^{18} cm^{-3}$	
J(m A/cm^2)	V(Voltage)	J(m A/cm^2)	V(Voltage)
0.00	0.804	0.00	0.813
1.36	0.763	2.43	0.772
2.22	0.746	3.42	0.753

3.17	0.719	4.18	0.725
4.56	0.685	5. 36	0.691
5.36	0.663	6.73	0.678
6.15	0.585	7.39	0.592
7.34	0.523	8.77	0.534
8.62	0.475	9.25	0.482
9.81	0.419	10.72	0.428
10.31	0.365	11.62	0.374
11.38	0.310	12.77	0.326
12.66	0.275	13.23	0.287
13.55	0.229	14.70	0.237
14.14	0.175	15.29	0.187
15.53	0.139	16.76	0.1
17.653	0	18.738	0

Furthermore , the photocurrent characteristics of N3-ZnS solar cell limites by increasing concentration, strength coupling and current density. The J-V characteristic can show in Table (2).

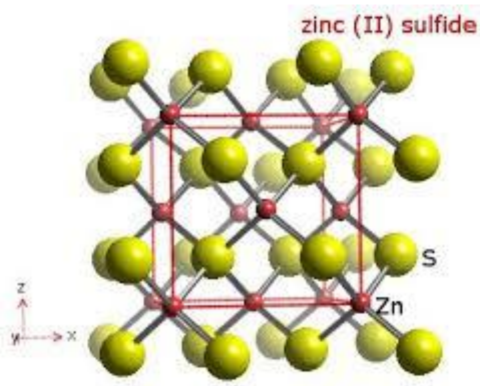

Figure 1. The zinc blende ZnS structure.

Figure 1. The current density versus voltage at a) 3×10^{18}(cm^{-3}) and 5×10^{18}(cm^{-3}).

Fill factor can estimate using Eq.(13) and efficiency can evaluate using Eq. (14) respectively using results in table (2) as well as Figure 1, results list in the Table (3) for N3-ZnS devices.

Table 3. The $J_{Sc}(mA/cm^2)$, V_{oc}(V), $J_m(mA/cm^2)$, V_m (V), fill factor FF and efficiency of N3-ZnS devices

Variables	The electronic concentration	
	$3\times10^{18} cm^{-3}$	$5\times10^{18} cm^{-3}$
$J_{Sc}(mA/cm^2)$	17.653	18.738
V_{oc} Volt	0.804	0.813
$J_m(mA/cm^2)$	8.62	9.25
V_m Volt	0.475	0.482
FF	0.289	0.292
Efficiency	4.09 %	4.448 %

Discussion

Due to the numerical results using MATLAB software for transition energy $T_{SD}(eV)$,current density $J(E)$ and characteristic J-V for electron transfer from the excited state in N3 dye to the conduction band in ZnS presented using transfer theory in the N3-ZnS system. It is calculated for varouse strength coupling in range $[0.08eV \leq \langle H_s \rangle \leq 1.3 \text{ eV}] \times 10^{-1}$ at 300K, with the inclusion of the effective density, atomic density and the driving energy as well as two carrier concentration of ZnS $[A] = (3 \text{ and } 5) \times 10^{18} cm^{-3}$, respectively. The transition energy$T_{SD}(0.37eV)$ has been calculated using the optical and dielectric constants of ethylen solvent and Zns , which influenced the energy transport . Table 1, the current density $\boldsymbol{J(mA/cm^2)}$ under many strength coupling and two concentration at finite transition energy 0.73eV, which are critical parameters for the current density J. These parameters indicated the current density behavior of the N3-ZnS system. The evolution of current density is shown in Table 1, where it observes that current density increases with the increases both strength coupling and concentration , with values ranging from 0.08 eV to 1.3 eV, it reach to maximum 16.76 ($\boldsymbol{mA/cm^2}$) with concentration $5 \times 10^{18} cm^{-3}$corresponding to current density 15.53 ($\boldsymbol{mA/cm^2}$) with concentration $3 \times 10^{18} cm^{-3}$, respectively. While the minimum current density reach to 1.36($\boldsymbol{mA/cm^2}$) and 2.43($\boldsymbol{mA/cm^2}$) for concentration $3 \times 10^{18} cm^{-3}$ and $5 \times 10^{18} cm^{-3}$. This indicated the electron transfer increases with increases concentration and coupling and vice versa. Additionally, the current density increases as increases the coupling $\langle H_s \rangle$ of the N3-ZnS system. However, the current density $J_{Sc}(mA/cm^2)$ is 17.653 as the concentration $3 \times 10^{18} cm^{-3}$ comparing to 18.738 at $5 \times 10^{18} cm^{-3}$. It observes that the current density $J\left(\frac{mA}{cm^2}\right)$ remains relatively increases and shows little variation with changes in strength coupling ranging from 0.08eV to 1.3 eV. The interactions between N3 dye and ZnS include covalent bonds, and the transition energy $T_{SD}(eV)$ of system plays a crucial role in electron transfer. This indicates that electron transport occured under good alignment of energy levels of N3 dye and ZnS with different scoupling and two concentration and transition energy 0.37eV and band alignment. Furthermore, the fill factor and efficiency in Table 3 shows a clear relationship with flow current density and concentration, as concentration energy increases from $3 \times 10^{18} cm^{-3}$ to $5 \times 10^{18} cm^{-3}$, the efficiency increases from 4.09 % to 4.448 % . Specifically, the increases concentration from $3 \times 10^{18} cm^{-3}$ to $5 \times 10^{18} cm^{-3}$, the current density $J_{Sc}(mA/cm^2)$ and $J_m(mA/cm^2)$ increase from $J_{Sc}(17.653(mA/cm^2))$ to $J_{Sc}(18.738(mA/cm^2))$ and $J_m(mA/cm^2)$ from 8.62 mA/cm^2 to 9.25 mA/cm^2. This show that as the efficiency increases from4.09% to 4.448% , the electron transport cross interaface of N3-Zns. However, the FF less increases with increase concentration from 0.289 to 0.292. The stability of N3-ZnS solar cell played an important role in electron transport and strongest depending on the morphological as well as structural properties of N3 and ZnS materials.

	The electronic concentration	
Variables	$3 \times 10^{18} cm^{-3}$	$5 \times 10^{18} cm^{-3}$
$J_{Sc}(mA/cm^2)$	17.653	18.738
V_{oc} Volt	0.804	0.813
$J_m(mA/cm^2)$	8.62	9.25
V_m Volt	0.475	0.482
FF	0.289	0.292
Efficiency	4.09 %	4.448 %

$$J(E) = \frac{q}{A} \frac{4\pi^2}{h} |\langle H_s \rangle|^2 \frac{e^{-\frac{(T_{SD}+\Delta U^0)^2}{4T_{SD}k_BT}}}{(4\pi T_{SD}k_BT)^{\frac{1}{2}}} \rho_a^{-2/3} \frac{l_Z}{(\frac{6}{\pi})^{1/3}} [A] \text{ ....(11)}$$

Conclusion

In conclusion, current density, fill factor and efficiency calculation indicate that current density in N3-ZnS cell influenced by the concentration as well as coupling of energy levels between N3 dye and ZnS , enhancment both transition energy and the charge transfer in the N3-ZnS system. The overall efficiency calculation, as a function of transition energy, current density, concentration and coupling strength, yields to improved in the electron transport reaction from N3 dye to ZnS . The consideration of concentration and coupling are the main important in the calculation of current density, particularly in high concentration and coupling. Thus indicates the N3 dye was good senstizer dye for ZnS ,it provides good tool to provide more knowledge used to investigation the mechanism of electron transfer in the N3-ZnS system.

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