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Theoretical Study and Calculation of the Efficiency Of N3-Dye-Sensitized Solar Cell Based on Zinc Sulfide Semiconductor

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Abstract :

In this paper, we explore the efficiency of ruthenium N3 contact-based ZnS semiconductor in dye-sensitized solar cells DSSCs using charge transport from excited N3 molecules to the conduction band in ZnS. An ethanol solvent was used to immerse the N3 dye and ZnS in DSSC device under assume continuum energy levels of N3 dye and ZnS in the solar cell device. The current and current density are calculation depends on semi empirical approach model for DSSC device and depends on calculate the reorganization energy using MATLAP program .The J-V characteristics have been calculated under irradiation (100 mW/cm²) and room temperature T (300) K .Two concentrations concentrations [C] (5×10^{17} and 6×10^{17}) $1/cm^3$ are used to calculate the currentdensity, (J–V) characteristics. The results show increases in current density with increases concentration and coupling, J-V characterization revealed to give the high energy conversion efficiency for the DSSC by sensitizer. Specifically, the ruthenium-620-TiO2 device showed a fill factor of 0.252 and a reach efficiency of 20%

Keywords: Efficiency N3, Zinc Sulfide, Current ,charge transfer, Solar cell.

دراسة نظرية وحساب كفاءة الخلية الشمسية المصبوغة بصبغة N3 المعتمدة على أشباه الموصلات من كبريتيد الزنك

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مستخلص:

في هذه الورقة، نسكتشف كفاءة أشباه الموصلات ZnS القائمة على تلامس الروثينيوم N3 في الخلايا الشمسية الحساسة للصبغة باستخدام نقل الشحنة من جزيئات N3 المثارة إلى نطاق التوصيل في Zns . تم استخدام مذيب الإيثانول لغمر صبغة N3 و ZnS في جهاز DSSC تحت افتراض مستويات الطاقة المستمرة لصبغة N3 و Zns في جهاز الخلية الشمسية. يعتمد حساب التيار وكثافة التيار على نموذج النهج شبه التجريبي لجهاز DSSC ويعتمد على حساب طاقة إعادة التنظيم باستخدام برنامج MATLAP . تم حساب خصائص J-V تحت الإشعاع (100 mW / cm²) ودرجة حرارة الغرفة (300) K . تم استخدام $(5X10^{17}$ s[C]، $6X10^{17}$ $\frac{1}{cm^3}$) لحساب كثافة التيار وخصائص (J-V) . اضهرت النتائج زيادة في كثافة التيار مع زيادة التركيز والاقتران، وقد أظهرت خصائص J-V كفاءة تحويل طاقة عالية لخلايا DSSC باستخدام المُحسِّس. وعلى وجه التحديد، أظهر جهاز الروثينيوم –620–TiO2 عامل تعبئة قدره 0.252 وكفاءة وصول قدرها 20٪..

Introduction

Electron transfer is an inherent mechanism in various scientific disciplines such as photosynthesis, electrical technology, and solar cell devices [1]. Electron transfer research has focused on transport reactions in chemistry, biology, and physics. Marcus introduced the classical electron transfer theory in the 1950s based on a simple donor-acceptor model. Marcus' theory, used to discuss charge transfer in molecular systems, led to qualitatively correct conclusions [2].The mechanism of electron transfer across different material interfaces plays a fundamental role in achieving optimal efficiency in various technological devices. Enhancing the technological efficiency of solar devices largely depends on the electron transfer behavior at interfaces [3]. Electron transfer reactions are a direct reaction in materials due to the donor-acceptor system. The basic charge transfer is always considered to be based on redox reactions. It is rarely referred to as a reaction involving the transfer of an electron, not necessarily a single electron [4]. Markus introduced a classical theory of charge transfer in the 1990s to describe charge transfer in a chemical reaction using thermodynamic postulates, and it has become a useful tool especially in chemistry as well as physics with materials [5]. Electron transfer has been greatly expanded due to experimental aspects in various types of research in the theoretical approach to self-exchange reactions [6]. Marcus was awarded the Nobel Prize in 1992 for his theory of electron transport, which led to the development of Marcus's charge transfer rate theory. It is related to the charge transport proposed by Ehring's theory due to the charge transfer relationship between the reorganization energy and the driving force energy [7]. More recently, electron transfer has been a key reaction process in photocatalysis, light harvesting, molecular electronics, and solar cell devices [8]. The electron transfer process upon contact of dyes with semiconductors has been essential for progress in highly efficient solar cells [9]. Dye-sensitized solar cells (DSSCs) In solar cell devices, light absorbed by molecules is converted to an excited state, causing a shift in

the state of the semiconductor's energy levels [10]. In turn, molecules present in the dye can prevent electron recombination by coupling the anode-redox system [11]. The N3 dye, known as Cis-bis(isothiocyanato)bis(2,2′-bipyridyl-4,4′-dicarboxylato) ruthenium(N3), is the oldest ruthenium dye for electron transfer in dye-sensitized solar cells (DSSCs). It has an exceptional ability to absorb light and efficiently transfer charge to the conduction band of the semiconductor in DSSCs [12]. Zinc sulfide (ZnS) has become a vital semiconductor in solar cells due to its wider range, good physical properties, and electrical and thermal stability that allows it to perform well at the interface of the semiconductor and the dye [13-14]. The aim of this research is to calculate the efficiency of a N3 ruthenium dye based on ZnS semiconductor in DSSC device depend on charge transfer reaction.

Theory

The efficiency of solar cell η can be calculated using [15].

$$\eta = \frac{J_{oc}V_{oc}.F.F}{I} \qquad (1)$$

Where J_{OC} and V_{OC} are short current and open circuit voltage, F.F is filling factor and I is light power density.

The filling factor F.F defined as max power and the production power, it evaluates using [15].

$$FF = \frac{V_m I_m}{V_{oc} J_{oc}} \qquad (2)$$

Where Vm and Jm are the maximum power voltage and current density, respectively. The current of DSSC can be calculated using an expression given by [17].

$$J_o(mA) = \frac{4\pi^2 e}{h} |\langle C_C \rangle|^2 \sqrt[3]{\left(\frac{\pi}{6}\right)} l_s \rho_S^{-2/3} \frac{e^{-\frac{\left(\lambda_N^C + \Delta V^c\right)^2}{4\lambda_N^C k_B T}}}{2\sqrt{\pi \lambda_N^C k_B T}} \int_0^\infty F(E)\rho_D(E)dE \qquad (3)$$

Where h is Planck's constant, $\langle C_C \rangle$ is coupling constant, l_S is length of charge transfer into semiconductor, $\rho_S\ (E)$ is density of charge through heterogenous solar cell, $\lambda_N^C(eV)$ is reorganization energy , driving force ΔV^c and $\rho_D\ (E)$ is density of state in dye .The solution integral is [18].

$$\int_0^{\infty} F(E)\rho_D(E)dE = [C] \qquad (4)$$

Where $[C]$ is concentration. Inserting Eq.(4) in Eq.(3) to get.

$$J_o(mA) = \frac{4\pi^2 e}{h} |\langle C_C \rangle|^2 \sqrt[3]{(\frac{\pi}{6})} l_s \rho_S^{-2/3} \frac{e^{-\frac{\left(\lambda_N^C + \Delta V^C\right)^2}{4\lambda_N^C k_B T}}}{2\sqrt{\pi \lambda_N^C k_B T}} [C] \qquad (5)$$

The current density coefficient is given by [19].

$$J_c(mA) = \frac{J_o(mA)}{A} \qquad (6)$$

Where A is the area of the solar cell. Inserting Eq.(5) in Eq.(6) to produce

$$J_o(mA) = \frac{4\pi^2 e}{Ah} |\langle C_C \rangle|^2 \sqrt[3]{(\frac{\pi}{6})} l_s \rho_S^{-2/3} \frac{e^{-\frac{\left(\lambda_N^C + \Delta V^C\right)^2}{4\lambda_N^C k_B T}}}{2\sqrt{\pi \lambda_N^C k_B T}} [C] \qquad (7)$$

The reorganization energy $\lambda_N^C(eV)$ can write as [20].

$$\lambda_N^C(eV) = \frac{e^2}{8\pi\varepsilon_\circ D}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] - \frac{e^2}{16\pi\varepsilon_\circ R}\left[\frac{n_C^2 - n^2}{n_C^2 + n^2}\frac{1}{n^2} - \frac{\varepsilon_C^2 - \varepsilon^2}{\varepsilon_C^2 + \varepsilon^2}\frac{1}{\varepsilon^2}\right] \qquad (8)$$

here $\varepsilon_\circ$ is permittivity, D and R are radius and distance between dye and semiconductor electrode, ε and n are dielectric constant and refractive index of solvent, ε_C and n_C are dielectric and refractive index of ZnS. The radius is function of molecular weight M and density ρ, it can be evaluated using [21].

$$D = A(\frac{M}{N\rho})^{\frac{1}{3}} \qquad (9)$$

where A is constant $(\frac{3}{4\pi})^{\frac{1}{3}}$ and N is Avogadro number.

Result and discussion

Current was calculated using the charge transport reaction from excited N3 dye to conduction band in ZnS in solar cells. In first, the reorganization energy is determining the current, it is a function of the properties of the N3 dye and ZnS. It refers to the optical and electrical properties of the devices. It

is limited by the dielectric and refractive index of the solvent with ZnS, the radius of the ZnS and N3 molecule, and the distance between them. The radii of N3 dye and ZnS semiconductor using Eq.(9) with taken the molecular weight ($705.64\frac{g}{mol}$ [22], $97.46\frac{g}{mol}$ [23]) and mass density ($1.36\ g/cm^3$ [22], $4.079\ g/cm^3$ [23]) of N3 dye and ZnS to results 5.9 A^0, and 2.11 A^0.The reorganization energy in Eq (8) can be using to calculate using the radius value 7.5 A^0 and 1.96 A^0 5.9 A^0, and 2.11 A^0. for N3 and *ZnS*, the distance R = 8.01 A^0, , refractive index and dielectric constant of the semiconductor ZnS [23] and the distance between N3 and ZnS ,results were showing in table (3).and taking 1.36 and 24.55 [24] from the refractive index and dielectric constant of ethanol solvent to obtain the results λ_N^C=0.487 eV.The atomic density ρ_S can be taken ($5X10^{12}$)cm^{-3}. The current $J_o(mA)$ of DSSC with ethanol solvent calculates using Eq.(5) using reorganization energy 0.487 eV, length path l_S= 3A^0, , coupling $\langle C_C \rangle$ =(0.3,0.4,0.5,0.6,0.7, 0.8,0.9,1,1.1,1.2,1.3,1.4,1.5,and 1.6) $X10^{-1}$(eV/state), with taken concentration [c] (5 and 6) $X10^{17}\frac{1}{cm^3}$ and using MATLAB software program, the results are listed in Table (1)

TABLE 1. Current $J_0(mA)$ calculation for N3-ZnS DSSC with **ethanol** solvent.

coupling $\langle C_c \rangle$ (eV/ state	Concentration carrier	
	$5 \times 10^{17}\frac{1}{cm^3}$	$6 \times 10^{17}\frac{1}{cm^3}$
0.3	0.7	0.8
0.4	1.3	1.6
0.5	1.8	2.4
0.6	2.3	3.2
0.7	3.1	3.9
0.8	3.7	4.7
0.9	4.3	5.5
1.0	4.9	6.3
1.1	5.5	7.1
1.2	6.1	7.8
1.3	6.7	8.6
1.4	7.3	9.4
1.5	7.9	10.1
1.6	8.5	10.9

Table 1.show that the current duo to charge transfer occurred from N3 to inject in the conduction band of ZnS and increases with increasing concentration from (0.7to 8.5)mA at $[c]\,(5)\times 10^{17}\frac{1}{cm^3}$ to values (0.8 to 10.9) mA at $[C]\,(6)\times 10^{17}\frac{1}{cm^3}$ by 7Increasing the concentration in DSSCs resulted in an increase in cell current and efficiency. Results in Table 1 show increased current in the solar cell device by increasing the concentration to improve the transfer of electrons. It reduces the resistive losses and increases the current in DSSC. Current in Table 1. Increases with coupling increases between the N3 dye molecule and the ZnS semiconductor. Then the current density J_c (mA/cm^2) can estimate using Eq (6) usingresults show in Table (1) and the area A (0.20 cm^2), results list in Table (2).

TABLE 2. Current density J_c (mA/cm^2) Calculation for N3-ZnS DSSC with **ethanol** solvent.

coupling $\langle C_c \rangle$ (eV/ state)	Concentration carrier	
	$5\times 10^{17}\frac{1}{cm^3}$	$6\times 10^{17}\frac{1}{cm^3}$
0.3	4.9	5.1
0.4	8.7	10.1
0.5	12.6	14.9
0.6	15.4	19.7
0.7	19.2	24.6
0.8	23.1	29.5
0.9	26.8	34.6
1.0	30.7	39.4
1.1	34.5	44.3
1.2	38.3	49.2
1.3	42.1	54.1
1.4	45.9	60.1
1.5	49.8	64.9
1.6	53.6	69.8

Current density J_c (mA/cm^2) increases with increases coupling as wellas concentration , as shown the current density increased due to increase car-

rier from $5X10^{17}$ to $6X10^{17}$ as well as increasing the coupling from 0.3 (eV/ state) to 1.6 (eV/ state) .The increasing in indicates the increasing the density in the ZnS to results high current density, because more electrons from the N3 dye are injected into the ZnS conduction band. However, increase the concentration can be allowing injection of electrons to results increase current density. Furthermore, high concentration may improve the transfer of charge cross of ethanol media for ZnS semiconductors. Increasing coupling between the dye and ZnS indicated increasing in current density and produced increases in efficiency. Due to using results in table 2, the J -V of N3 based ZnS in DSSC with **ethanol** showing in table (3).

TABLE 3. J -V characteristics of N3 based ZnS in DSSC.

Current density of electrons transfer(mA/cm^2)		
Carrier concentration (1/cm^3)		
$5 \times 10^{17} \frac{1}{cm^3}$		$6 \times 10^{17} \frac{1}{cm^3}$
V(Volt)	Current density(mA/cm^2)	Current densitym(A/cm^2)
0.79	0	0
0.80	4.9	5.1
0.76	8.7	10.1
0.71	12.6	14.9
0.67	15.4	19.7
0.65	19.2	24.6
0.54	23.1	29.5
0.51	26.8	34.6
0.46	30.7	39.4
0.43	34.5	44.3
0.37	38.3	49.2
0.32	42.1	54.1
0.28	45.9	60.1
0.22	49.8	64.9
0.17	53.6	69.8
0.0	57.7	74.9

The J-V property is limited by increasing concentration with coupling, and increases with increasing coupling and concentration in the N3 based ZnS solar cell. Moreover, the current-voltage characteristics show in Table (3).

The J -V characteristic in table 3 used to evaluate fill factor and efficiency of device by sing both Eq.(2) and Eq.(1) for Fill factor and efficiency using results in table (3), results list in the Table (4) for DSSC solar cell .

Table 4. The photovoltaic parameters of the N3 based in ZnS in DSSC.

Variables	The concentration carrier m^{-3}	
Concentration	$35x10^{23}$	$45x10^{23}$
J_{oc} (mA/cm^2)	57.7	74.9
V_{oc} Volt	0.80	0.80
J_m (mA/cm^2)	34.5.	44.3
V_m Volt	0.43	0.43
F.F	0.321	0.317
efficiency	14.8	19.04

The voltage and current density in the open-circuit are found to be (0.43) Volt and (34.5, 44.3) mA/cm2 where open circuit voltages V_{oc} is (0.8) Volt and short-circuit current J_{OC} is (57.7.,74.9)(mA/cm^2), respectively. It means when increasing the coupling produced increases the current density and results in a high short circuit J_{OC} $(mA/cm^2$ (57.7 and 74.9) because increases injection more electrons being resulting in a high current density. At concentration of $5X10^{17}cm^{-3}$, the fill factor was 0.321 and the efficiency was 14.8 and increases efficiency to become 19.05 when increasing concentration $6X10^{17}cm^{-3}$. The efficiency increased from 14.8 to 19.05 by a factor of 4.15 with increasing concentration and increasing the current density but also the overall efficiency. It can be observed that changes in current density J_c $(mA/cm^2$ supports more transfer to transfer from the excited state in N3 to the conduction band of ZnS electrode

Conclusion

An efficiency of N3 dye with ZnS in a DSSC solar cell device calculates theoretically based on charge transport. The performance exam used two concentrations and calculate current, current density, F.F, and overall efficiency to understanding the behaviour and its effectiveness as a photovoltaic system. The J–V characteristics of the N3 dye based ZnS DSSC device show that the efficiency is affected by the increases current density and concentration. At a concentration $5X10^{17}$ cm^{-3}, the DSSC exhibited current density J_{OC} $(57.7\ mA/cm^2)$ and voltage (0.8 V), with fill factor (FF = 0.312), resulting efficiency of 14.8%. comparing, at a concentration of $6X10^{17}$ cm^{-3}, the J_{OC} 74.9 mA/cm^2, V_{OC} (0.8) Volt V, FF = 0.312, and efficiency of 19.05%. The increases efficiency observed at $6X10^{17}$ cm^{-3}, indicated an enhanced transfer and light absorption.

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