Study of Charge Transfer in N719 Dye Contact with CdS Nanoparticles

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Abstract

In this paper, the charge transfer from the N719 to CdS in solar cell is studied and calculated using the analysis charge transfer theory. The charge transfer rate was calculated using the donor-acceptor model based on the quantum transfer theory in DSSC solar cells. We estimate the influence transition energy and strength coupling parameters in N719-CdS DSSC. For 1-Butanol, and Ethanol solvents, the rate over N719-CdS interface was found to be varied between higher and low. The electronic rate is most occurred with butanol and sufficiently lowering with Ethanol.

Keywords: Charge Transfer, Solar Cell, N719 Dye , CdS , Electronic Rate.

الخلاصة

تهدف الدراسة الى حساب انتقال الشحنة من N719 إلى CdS في الخلايا الشمسية باستخدام نظرية تحليل انتقال الشحنة. تم حساب معدل انتقال الشحنة باستخدام نموذج المانح–المستقبل بناءً على نظرية الانتقال الكمومي في خلاياDSSC الشمسية. قمنا بتقدير تأثير طاقة الانتقال ومعلمات قوة الارتباط فيN719–CdS في خلاياDSSC. بالنسبة لمذيبات ١–بيوتانول والإيثانول، وُجد أن المعدل عبر واجهةN719–CdS يتفاوت بين قيم مرتفعة ومنخفضة. وكان المعدل الإلكتروني الأعلى يحدث مع البيوتانول، بينما ينخفض بشكل ملحوظ مع الإيثانول.

الكلمات المفتاحية: انتقال الشحنة، الخلية الشمسية، صبغة،N719 كبريتيد الكادميوم CdS ,المعدل الإلكتروني.

Introduction

The increased environment problems and energy crisis would being necessary for exploration of clean energy and renewable materials [Wei، W،2022 ،191]. The renewable energy technology was vital part to reduce risks posed and green-house gases emitted by global warm. Convert to renewable energies sources of electric has been a vital parts of solving to many risks problems in world [Rosengarten، G ،2022، 119–140]. The solar cell was using to generate electric and it is best option for the sustainable energy requirement of the world [Upadhyaya،H.M، 2011، 1580-1608]. It was an essential diverse entirety to solve problems energy crisis that would eventually replacing fossil fuels energy sources in increasing resources [Baroni ،S,2013، 014709]. The dye-sensitized solar cells DSSCs convert light into electricity depended on using broadband semiconductor together with dye-sensitized molecules [Reshak،A.H ،٢٠١٥,2859-2871]. In the DSSCs, the photons were absorbing to excited dye and electrons can be injected into the conduction band to reach the collector [Swami,S.K،2022, 44170–44179]. As such, the charge transfer can occur from the donor energy surface to the acceptor energy surface and required a alignment of energy levels states [AL-Obaidi,R.I.N،2009,77–91]. The charge transfer reaction from the donor state to acceptor state in system without changing in the bond. It occurs by thermal , chemical and photons induced [Fadhil, M. Z,2020, 184-193].It was a fundamental role in variety physical, chemistry and electronic molecules [Gallego,J.M ،2017, 105-145].The classical charge transfer described by Marcus' ,it utilizes in deferent photovoltaic and in chemistry[Al-Agealy, H. J ,2020, 040010]. In solar cell devices, the charge transfer cross interfaces of materials has important for optimum device technology. It become an important process to understand the mechanism operation of the solar cells [Dalton, L. R,2008, 28-32]. Hadi etal refer to the main parameter reorganization energy and to use for understanding the charge transfer mechanism in variety electronic devices [Hassooni, M. A, 2014, 2454]. In this paper, we investigated and calculated the charge transfer rate at N719-CdS devices due to a theoretical model. The charge transfer rate calculated for N719 contact to CdS with two solvents using the MATLAB program.

Theory

The charge transfer rate can be given by [Abbas ،S.R،2020،8780- 8789].

$$R_{ET} = \frac{(2\pi)^2}{h}\int_0^{\infty} F(E)|C|^2\,\langle\hat{\boldsymbol{\rho}}_{\mathbf{ij}}\rangle dE\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where h is Dirac constant , F(E) is Fermi function , C is coupling strength , $\langle\hat{\boldsymbol{\rho}}_{\mathbf{ij}}\rangle$ is density of state for charge transfer and E is the energy .The density of state of charge [Mohammed،R.L، 2021،012019].

$$\langle\hat{\boldsymbol{\rho}}_{\mathbf{ij}}\rangle = \sqrt{\frac{1}{4\pi T_j k_B T}}\; e^{-\frac{(T_j+\Delta U^0)^2}{4\nabla_j k_B T}}\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Where T_j is reorganized energy , k_B is Boltzmann constant , ΔU^0 is free energy and T is temperature .inserting Eq.(2) in Eq.(1) to results

$$R_{ET} = \frac{(2\pi)^2}{h}\int_0^{\infty} F(E)|C|^2\sqrt{\frac{1}{4\pi T_j k_B T}}\; e^{-\frac{(T_j+\Delta U^0)^2}{4\nabla_j k_B T}} dE\ldots\ldots\ldots\ldots\ldots(3)$$

The reorganized energy of the dye contact to semiconductor is [Hassooni, M. A,2014, 2454].

$$T_j(\mathbf{eV}) = \frac{e^2}{8\pi R\varepsilon_\circ}\left[\frac{1}{n^2}-\frac{1}{\varepsilon}\right] - \frac{e^2}{16\pi r\varepsilon_\circ}\,[(\frac{n_S^2-n^2}{n_S^2+n^2})(\frac{1}{n^2}) - \frac{\varepsilon_S^2-\varepsilon^2}{\varepsilon_S^2+\varepsilon^2}\frac{1}{\varepsilon^2}]\ldots(4)$$

where e and $\varepsilon_\circ$ are charge and permittivity, n and ε are refractive index and dielectric constant,R is radius of dye, **r** is distance between dye and the semiconductor , n_S and ε_S are refrective index and dielectric constant of semiconductor. The radius R is a function of molecular weight M , density of material ρ and Avogadro number N and given by [Fadhil ،M.Z،2020، 184–193].

$$R(nm) = (\frac{3}{4\pi}\frac{M}{N\rho})^{\frac{1}{3}}\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

The Fermi distribution energy for electrons in system is given by [Killian ،P،2007، 56-62].

$$F(E) = \frac{1}{1+e^{\frac{E}{k_B T}}}\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

Inserting Eq.(6) in Eq.(3) to obtaine

$$R_{ET} = \frac{(2\pi)^2}{h}|C|^2\sqrt{\frac{1}{4\pi T_j k_B T}}\; e^{-\frac{(T_j+\Delta U^0)^2}{4\nabla_j k_B T}}\int_0^{\infty}\frac{dE}{1+e^{\frac{E}{k_B T}}}\ldots\ldots\ldots\ldots\ldots(7)$$

The solution integral in Eq.(7) ,the Eq.(7) become

$$R_{ET} = \frac{(2\pi)^2}{h}|C|^2\sqrt{\frac{1}{4\pi T_j k_B T}}\ e^{-\frac{(T_j+\Delta U^0)^2}{4\nabla_j k_B T}} \ln 2(e^{-\frac{E}{k_B T}}+1)^{-1} \ldots\ldots.. (8)$$

Results

The reorganization energy can calculate during charge transfer process of N719 donor and CdS acceptor states system using Eq. (4). Radii calculated for N719 Molecule dye and CdS semiconductor using equation in Eq. (5) as function of mass density and molecular weight. The radii estimate directly by insert molecular weight and density (M=1188.55 g/mol density $\rho = 1.52\ \frac{g}{cm3}$) [Mudhafar J. A، ٢٠٢٤، ١٨٣ -١٩٢] of N719 dye and molecular weight and density of CdS(M=144.64g/mol and $\rho = 4.826\frac{g}{cm3}$) [W. M.Haynes,2014, 365], results are 6.769 A° and 2.256 A^0 for N719 and CdS.

Table (1): The physical properties [Ali، M.J، 2024، 183-192] of N719 dye molecules

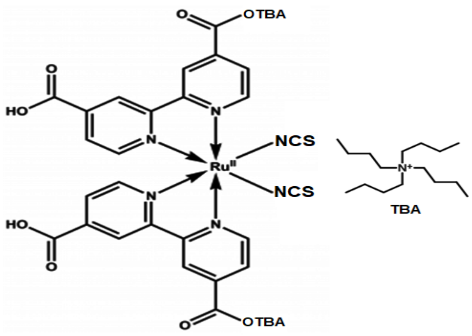
Name of dye	Di-tetrabutylammonium cis-bis(isothiocyanato)bis(2,2′-bipyridyl-4,4′-dicarboxylato)ruthenium(II)	
Molecular formula	C58H86N8O8RuS2	
Molar Mass g/mol	1188.55	
Density g/cm^3	1.36	
Melting point	> 300c°	
HOMO	-6.01 eV	
LUMO	-3.64 eV	
Calculated radius	5.65A°	

Table (2): Properties of CdS semiconductor [Haynes ,W,2014 , 365]

Properties	Value
Crystal	Hexagonal, cubic
Lattice conmnstant	A=5.653A
Molecular weight	144.64 g/mol
Mass density	4.826 g/cm^3
Dielectric constant	8.9
Refrective index	2.61
Energy gab	2.42 eV
Electron affinity	4.2eV

The reorganization of energy is the main part of the charge transfer process, it can use to understand the charge transfer features. it can calculated using continuum hypothesis of energy levels of materials in the system .It carried out by Eq.(4) by insert the dielectric constant ,refractive index from table (3) ,radii of N719 and CdS ,distance between CdS and N719 and taken using MATLAB program ,results are shown in table (3).

Table (3): Results of calculated the reorganization energy for N719 /CdS devices.

Solvents	Refractive index(n) [Haynes, W، 2014, 1065]	Dielectric constant (ε) [Haynes, W, 2014, 1065]	T_j(eV)
1-Butanol	1.399	17.51	0.354
Ethanol (EtOH)	1.359	24.55	0.393

The charge transfer rate calculates using Eq. (12) with MATLAB program at T=300k. To evaluate the charge transfer rate of electrons can be carried out using strength coupling in range $|H|^2 = (0.4,0.45,0.50,0.55,0.60,0.65,0.70,0.75,0.80) \times 10^{-11} (eV)^2$The driving energy $\Delta E^0$of the electron transfer is taken from 0eV to 0.8 eV with energy supplied of system 5.3 eV Results are tabulated in tables (4) and (5).

Table (4): Results of electrons transfer rate for N719-CdS at $\Delta U^0 = 0.2$eV.

Strength coupling $\|C\|^2 x10^{-11}$ $\|eV\|^2$	The electronic current I(Amper)	
	1-Butanol	Ethanol
0.1	1.468E-06	1.230E-06
0.2	2.93E-06	2.312E-06
0.3	4.357E-06	3.729E-06
0.4	5.7863E-06	4.738E-06
0.5	7.183E-06	5.848E-06
0.6	8.599E-06	6.257E-06
0.7	10.923E-06	7.467E-06
0.8	11.433E-06	8.676E-06
0.9	12.375E-06	9.886E-06
1	14. 656E-06	10.210E-06
1.1	15.658E-06	11.210E-06
1.2	16. 999E-06	12.311E-06
1.3	18.9845E-06	13.412E-06

Table (5): Results of electrons transfer rate for N719-CdS at $\Delta U^0 = 0.4$eV.

Strength coupling $\|C\|^2 x10^{-11}$ $\|eV\|^2$	The electronic current I(Amper)	
	1-Butanol	Ethanol
0.1	2. 618E-06	2.430E-06
0.2	3.793E-06	4.762E-06
0.3	5.657E-06	5.879E-06
0.4	6.788E-06	6.118E-06
0.5	8. 823E-06	8.418E-06
0.6	9.798E-06	10.457E-06
0.7	11.323E-06	12.987E-06

0.8	12.483E-06	14.196E-06
0.9	13.875E-06	16.236E-06
1	15. 756E-06	18.342E-06
1.1	16.878E-06	20.010E-06
1.2	17. 879E-06	22.301E-06
1.3	19.9445E-06	24.122E-06

Discussion

The electronic characteristic of the N719 Dye contact to CdS in devices has been influenced by the electron transfer rate due to the reorganization energy $T_j(\mathbf{eV})$, driving energyΔU^0 (eV) , strength coupling C(eV) at temperature T=300K . The charge transfer rate is evaluated for N719 molecule bounds to the CdS semiconductors due to reorganization energy $T_j(\mathbf{eV})$, its reorganization the configuration to begin the electron transfer and the energy of overlapping coupling each other to continues transfer of electrons cross interface .The reorganization energy $T_j(\mathbf{eV})$ in table (3) was showing increased with increased dielectric constant and decrease refrective index .It reach to maximum 0.393eV with Ethanol (EtOH)to reach and reach minimum 0.354eV with 1-Butanol solvents .The charge transfer rate relative to reorganization energy ,it increases with decrease reorganization energy with increases driving energy from 0.2 to 0.4 eV .However, the charge transfer rate has been depended on the strength coupling ,it increases with increases coupling and vice versa . It can clear s howing from Tables 4 and 5 that charge transfer rate of electron more probability for N719 Contact to CdS systems is higher with ethanol solvent comparing with 1-Butanol has lower rate at driving force energies (0.2 and 0.4) eV .This indicates charge transition rate increases with the ethanol solvents . tables (4) and (5) show the charge transfer become more probability with decrease potential barrier in system , it depends on the energy levels and structure both N719 and CdS materials .However ,the results of rate of charge transfer shows increasing with increasing the strength coupling and vice versa . Furthermore , the charge transfer increases with increases overlapping strength coupling of coupling and reach to maximum with $|C|^2 = 1.30 \times 10^{-11}(eV)^2$ with two solvents.

Conclusions

In conclusion , the charge transfer calculation of N719-CdS system carried out using quantum consideration of charge transfer theory .The charge transfer rate of N719-CdS has been proportional to reorganization energy , driving force and strength coupling by increasable with decreasesable with two solvents. The charge transfer rate increases with increases the overlapping electronic coupling. The charge transfer rate at N719-CdS system is active with butanol at driving energy 0.2 eV at lower driving force energy comparing with ethanol become active with system at large driving force energy 0.4 eV .1-Butanol solvent is the most active to charge transfer process at lower driving force energy. The results of charge transfer rate show that CdS is an active alignment with N719 dye for charge transfer reaction .

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