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Studies of the electron transfer in the N719 dye Contact to Cadmium Selenide CdSe Semiconductor

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Abstract
In this paper, the probability of electron transfer reaction at N719 dye contact into CdSe semiconductor interfaces evaluates and studied using quantum transition energy to determine the performance of N719-CdSe r cells device. The electronic characteristics of an N719-CdSe heterojunction cell device studies and investigated used quantum analytical model for electronic transition from N719 to CdSe. A theoretical investigation of interfacial electronic transfer reaction and analyzes in terms of the overlapping coupling, concentrataion and orientation transition energy. Results clarify the influence of electron transfer probablity on overlapping coupling,concentration energy as well as orentation transition energy parameters. Energy levels of both N719 dye and CdSe assumed continuum in heterojunction surround by ethyl alcohol as polar region. The electron transfer reaction characteristics of the N719-CdSE. device calculate at standard T=300k.The probability off electron transfer reaction characteristics of N719-CdSe device calculate in two different concentrations as well as variety values of coupling.The probability of electron tranbsfer reaction parameters of N719-CdSe device found increases with increases overlapping coupling and concentration and to be larger concentration $8 \times 10^{24} \frac{1}{m^3}$ compared with low for concentration $4 \times 10^{24} \frac{1}{m^3}$. Higher probablity of N719-CdSe. at concentration$8 \times 10^{24} \frac{1}{m^3}$ was leading to suggested for using in variety application of solar cell in low-cost, and high-performance.

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Introduction

Over the past century, the world – due to its dependence on petroleum fuels – has suffered from increasing challenges of pollution, warming, reduce natural sources and climate changing [1-2].There is a growing trend towards adopting sustainable energy as an alternative to oil derivatives, as a result of environmental degradation caused by pollution and non-renewable energy sources, as well as the increasing risks that threaten biodiversity and the ecosystem [3].In this context, solar energy is a very attractive option among future renewable energy sources; it provides a clean and environmentally friendly source, and is characterized by its abundance and accessibility [4]. Among the variety renewable energy source technologies, photovoltaic (PV) cell technology receives considerable more attention for convert ability solar energy into electricity [5]. With increasing production rates and reducing costs, new cells based on dye-sensitized solar cells (DSSCs) have emerged as one of the main important field in solar energy technologies, due to the optical properties and cost [6]. DSSC cells are a third-generation photovoltaic solar cell with greater appeal due to their flexible use, cost, and readily available manufacture [7].Addition, challenges arise related to electronic transfer across interfaces, as well as to controlling dielectric and contacting interfaces within

device, in order to reach full manufactures levels; this required aligning the energy levels to become similar to each other [8]. Hadi *et al*. pointed out that matching energy states are crucial factor in the electron transfer process, as compatible energy levels must be available in solar cell devices [9]. In fact, electron transtion reactions occur in a variety of heterojunction devices within different generations of solar cells, affecting their photophysical properties [10].Classical Marcus theory is the cornerstone for understanding electron transport mechanisms and remains a powerful theory for explaining the transition from initial to final state across interfaces in solar cell devices [11]. The cadmium selenide CdSe stays the most promising and common material in DSSCs cell according to strong absorption, electronic properties,band gap availability in the visible region [12]. The CdSe material has a band gap of 1.7 electron volts, which allows it to absorb radiation primarily, making it suitable for a variety of applications. It has been observed that cadmium selenide (CdSe) can be made sensitive to visible refion by chemical bonding molecules to surfaces, which helps accumulate this energies [13]. On other hand, the mechanism of action of DSSCs in converting photons into electricity depends on three stages: First, the excitation of the N719 dye by absorbing light, which leads to the transfer of electrons to conduction band in CdSe; second is regeneration oxidized dye and electrons were trantion to complete the circuit in third steps [14]. Process of electronic transfer which use to improvement overall solar cells efficiency by improving their performance depending on the nature of materials used in manufacturing these cells [15]. N719 dye ican classify as an organic complex dye based on rhothonium complexes, and is a best photosensitizer for dye-sensitized solar cells (DSSCs) due to its wide absorption spectrum and high light absorption capacity, as well as other properties such as chemical and thermal stability, and outstanding electronic and optoelectronic properties [16].The N719 organic dye remaines more attractive sensitised complex dyes use widly in solar cell, has form di-(tetrabutylammonium-cis-bis-(isothiocyanato)bis-(2,2′-bipyridyl-4,4′-dicarboxylato),ruthenium (II), [17]. The aim of this work is to studythe electron transfer and calculate the transition rate reaction process in the N719 dye contact with cadmium selenide CdSe based DSSCs and provided more knowledge to electronic transfer behaviour that occcured from N719 to conduction band of CdSe

Theory

Electron can move from initial state in N719 dye to a final state in CdSe semiconductor. The electronic transition probability $T_N^C(E)$ for electron transfer from N719 dye to state in conduction band in CdSe is [18].

$$T_N^C(E) = \frac{2\pi}{\hbar} |\langle H_{CD}\rangle|^2 \rho_{CD}(E) \quad (1)$$

Where $\langle H_{CD}\rangle$is overlapping coupling and $\rho_{Cd}(E)$ is activation electronic density in N719-CdSe system, it gives by [19].

$$\rho_{CD}(E) = \rho_{CdSe} \frac{l_{CdSe}}{(\frac{6}{\pi})^{1/3}} \quad (2)$$

Where ρ_{CdSe} refers to electronic density for CdSe and $l_{CdSe}$is active length.Electronic density in CdSe can express by [20].

$$\rho_{CdSe} = \rho_{N719}(E)\langle\widehat{\boldsymbol{\rho}}\rangle \boldsymbol{\rho}_{CdSe}^{-2/3} \quad (3)$$

Where $\rho_{N719}(E)$ define density of state in N719, ρ_{CdSe9} refers to CdSe atomic density and $\langle\widehat{\boldsymbol{\rho}}\rangle$ define density of N719-CdSe states,its written as [20].

$$\langle\widehat{\boldsymbol{\rho}}\rangle = \frac{e^{-\frac{(\lambda_N^C + \Delta U^o)^2}{4\lambda_N^C k_B T}}}{\sqrt{4\pi\lambda_N^C k_B T}} \quad (4)$$

where λ_N^C is orentation transition energy, ΔU^o is potential and T is temperature.Insert Eqs.(3),(4) and (5) in Eq.(2), results.

$$T_N^C(E) = \frac{2\pi}{\hbar} |\langle H_{CD}\rangle|^2 \rho_{N719}(E) \boldsymbol{\rho}_{CdSe}^{-2/3} \frac{l_{CdSe}}{(\frac{6}{\pi})^{1/3}} \frac{e^{-\frac{(\lambda_N^C + \Delta U^o)^2}{4\lambda_N^C k_B T}}}{\sqrt{4\pi\lambda_N^C k_B T}} \quad (5)$$

Under assuming $F(E) = F_N(E) - F_C(E)$ for continuum system,the Eq. (6) can be integrated over energy E to give.

$$T_N^C(E) = \frac{2\pi}{\hbar} |\langle H_{CD}\rangle|^2(E) \boldsymbol{\rho}_{CdSe}^{-2/3} \frac{l_{CdSe}}{(\frac{6}{\pi})^{1/3}} \frac{e^{-\frac{(\lambda_N^C + \Delta U^o)^2}{4\lambda_N^C k_B T}}}{\sqrt{4\pi\lambda_N^C k_B T}} \int_0^E \rho_{N719} F(E)\, dE \quad (6)$$

The integral can solve to give [19].

$$\int_0^E \rho_{N719} F(E)\, dE = C_s \quad (7)$$

Where C_s refers to concentration on CdSe's surface in (cm^{-3}). Eq.(7) together Eq. (8) yield.

$$T_N^C(E) = \frac{2\pi}{\hbar} |\langle H_{CD}\rangle|^2(E) \boldsymbol{\rho}_{CdSe}^{-2/3} \frac{l_{CdSe}}{(\frac{6}{\pi})^{1/3}} \frac{e^{-\frac{(\lambda_N^C + \Delta U^o)^2}{4\lambda_N^C k_B T}}}{\sqrt{4\pi\lambda_N^C k_B T}} C_s \quad (8)$$

The atomic density $\boldsymbol{\rho}_{CdSe}$ be afunction of concentration N_e at Fermi level, Fermi energy E_F, and number of states D_n,it is given by [19].

$$D_S = \frac{3}{2}(\frac{N_e}{D_n E_F}) \quad (9)$$

The orientation transition energy λ_S^B (eV) for system is [21].

$$\lambda_N^C(eV) = \frac{e^2}{8\pi\varepsilon_\circ}[\frac{1}{D}[\frac{1}{n^2} - \frac{1}{\varepsilon}] - \frac{1}{2R}[\frac{n_c^2 - n^2}{n_c^2 + n^2}\frac{1}{n^2} - \frac{\varepsilon_c^2 - \varepsilon^2}{\varepsilon_c^2 + \varepsilon^2}\frac{1}{\varepsilon^2}]] \quad (10)$$

where e $\varepsilon_\circ$, D and R are charge,permittivity,radius of N719 and CdSe and the distance between them, n, ε, n_c and ε_c are refractive index and dielectric constant of solvent and CdSe.The radius D is [22].

$$D = (\frac{3}{4\pi})^{\frac{1}{3}}(\frac{m}{N\rho})^{\frac{1}{3}} \quad (11)$$

where molecular weight (m), Avogadro number (N), and material density ρ.

Results and Discussion

Electronic transition probability $T_N^C(E)$ can be determined on the basis of quantum charge transfer theory for the donor N719 dye contact with acceptor CdSe in N719-CdSe cell.the orientation transition energy is critical effected with concentration as well as strength coupling on the values of probability of transition.The orientation transition energy is a general parameters in probability of electron transfer reaction. It is providing an electronic tool to polar media information for the understanding reaction of electron-transfer and can occur or not.It is indicated the electron transfer reaction behaviour and define the optical togother electronic properties of N719-CdSe.Orientation transition energy parameters combine dielectric and refractive index of CdSe, solvent with structure of N719 dye as well as radii of N719 molecule and CdSe with distant between them. Radii of N719 and CdSe evaluate using Eq.(12) by inserting the molar weight M= 1188.5 g/mo l [23] and (M=191.3g/mol [24] with density $\rho = 1.5\ \frac{g}{cm3}$ [23]and $\rho = 5.81\frac{g}{cm3}$ of N719 and $CdSe$ respectively to result 7.47 A^0 and 1.96$A^0$for N719 and $CdSe$.The orientation transition energy estimates using Eq.(11) by inserte radii of N719, CdSe, distance,refractive index 2.5 [24] and dielectric constant 10.65 [24] of $CdSe$, refractive 1.36 [25] and ethyl alcohol dielectric constant 24.6 [25], results $\lambda_N^C(eV) = 0.415\ eV$.Density of states for CdSe estimated by inserti concentration $N_e = 6 \times 10^{16} cm^{-3}$ and Fermi energy $E_F = 2.7eV$ and $D_n = 8$ state /eV) in Eq.(10) to results $\rho_{CdSe} = 5.81 \times 10^{24}\ \frac{1}{m^3}$.

The electronic transition probability $T_N^C(E)$ occured from N719 dye to $CdSe$ with ethyl alcohol solvent has calculated using Eq.(9) by insert using$\lambda_N^C(eV) = 0.415\ eV$, activate length $l_{CdSe} = 3A^0$ [24], overlapping coupling $|\langle H_{CD}\rangle|^2$=0.13.0.26,0.39,0.52,0.65,0.78,0.91, 1.14, 1.27,1.40.,1.53,1.66,1.79,1.92and *2.05 x10−2* |eV|², atomic densityρ_{CdSe} == $5.81 \times 10^{24} 1/m^3$ and concentration $C_s = (4\ and\ 8) \times 10^{24}\ \frac{1}{m^3}$ via MATLAP program, results are in Tables (1) and (2) and ploted in figures (1) and (2) for N719-CdSe devices.

TABLE 1. Results of electronic transition probability $T_N^C(E)$(1/sec) for N719/$CdSe$with ethyl alcohol at concentration

$$4 \times 10^{24} m^{-3}$$

overlapping coupling $\langle H_{CD}\rangle$ *x10*$^{-2}$eVElectronic transition probability $T_N^C(E) \times 10^{11}(\frac{1}{\text{sec}})$

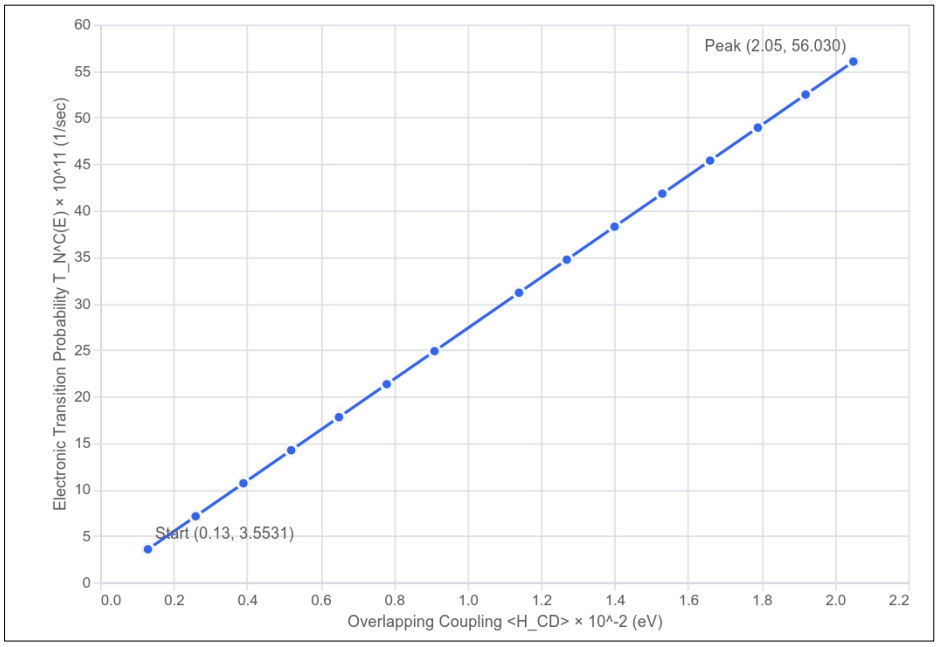


Fig 1: The behaviour of electronic transition probability $T_N^C(E) \times 10^{11}\left(\frac{1}{sec}\right)$rs $\langle H_{CD}\rangle(eV)$

For N719 / CdSe devices with concentration $4 \times 10^{24} 1/m^3$. The electronic transition probability $T_N^C(E)$ in in both Tables (1) and (2) are dependent on orientation transition energy,overlapping coupling, concentration and effected by N719,CdSe and ethyl alcohol materials in solar materials properties cell. The probability $T_N^C(E)$ related to orientation transition that's depending on refractive index togother ethyl alcohol polarity.

The data in table 1 and figure 1 demonstrates a linear and directly proportional between the electronic transition probability and overlapping coupling energy H_{CD} \rangle\). As the increases in coupling $\langle H_{CD}\rangle$ from 0.13 *x10*$^{-2}$ eV to 2.05 *x10*$^{-2}$ eV, the probability $T_N^C(E)$ will be increased steadily from $(3.5531 \times 10^{11}(\frac{1}{\text{sec}}))$ to $(56.030 \times 10^{11}(\frac{1}{\text{sec}}))$

Table 2: Results of electronic transition probability $T_N^C(E)$(1/sec) for N719/$CdSe$with ethyl alcohol at concentration $8 \times 10^{24} m^{-3}$

overlapping coupling $\langle H_{CD} \rangle$ *x10*$^{-2}$ eV	**electronic transition probability $T_N^C(E) \times 10^{11}(\frac{1}{\text{sec}})$**
0.13	7.116
0.26	14.2124
0.39	21.318
0.52	28.424
0.65	35.532
0.78	42.638
0.91	49.744
1.14	62.316
1.27	68.422
1.40	76.528
1.53	.83.634
1.66	90.742
1.79	97.848
1.92	104.954
2.05	112.060

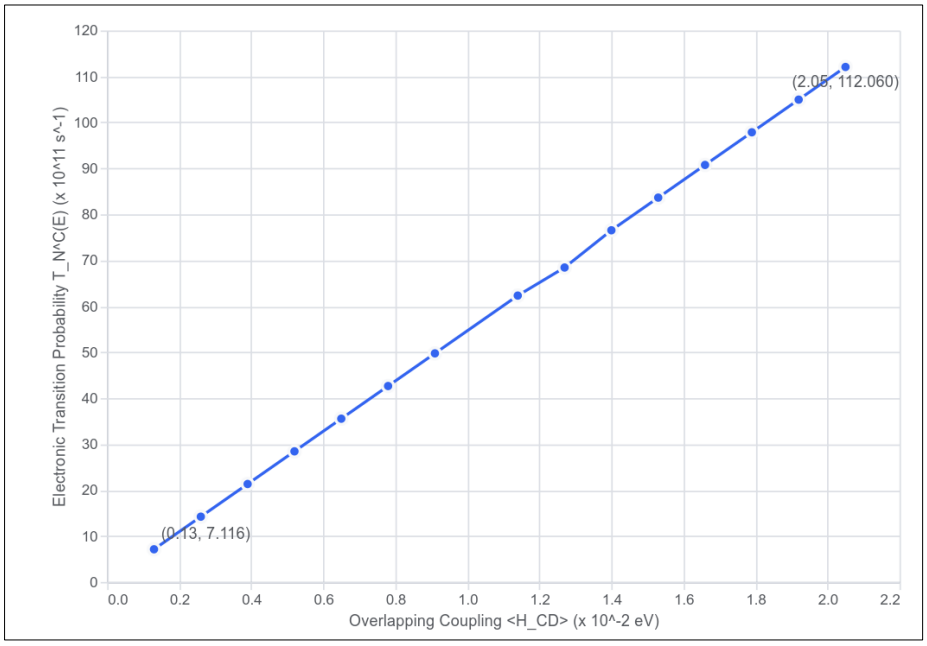


Fig 2: The behaviour of electronic transition probability $T_N^C(E) \times 10^{11} \left(\frac{1}{sec}\right)$rs $\langle H_{CD} \rangle (eV)$

For N719 / CdSe devices with concentration $8 \times 10^{24} 1/m^3$. Tables 1 and 2 show results of probability $T_N^C(E)$ were increasing upon increased overlapping coupling and concentration, as seen the probability $T_N^C(E)$ increases alternatively with increases concentration from $4 \times 10^{24}$to 8×10^{24} and increased overlapping couploing in range (0.13 to 2.05) $x10^{-2}$ eV. increases probablity with increases overlapping coupling (\(\langle H_{CD} \rangle\)) indicate that greater overlap between the N719 dye wavefunctions (donor) and CdSe wave founction (acceptor) in continuumstates. This stronger interference between wave functions reduces the barrier effect to electron transfer, thus enhancing the probability of electron transfer between different states.The probability $T_N^C(E)$ in table (2) with concentration 8×10^{18} increases about two times than probability $T_N^C(E)$ with concentration 4×10^{24} with ethyl alcohol. More important, the increasing in concentration indicates to transfer more electrons and probability $T_N^C(E)$ become more probable to cross interface of N719-CdSe cell device

In contrast, the probability behavior in Figures 1 and 2 indicates that the probability of transition—as a function of the overlapping coupling energy—remains almost constant, because the temperature, the orientation-dependent transition energy, and the density of states all remain constant, while the value of \(\langle H_{CD} \rangle\) is changed.

. In fact, results of probability presented in two tables1 and 2 and illustrated in two figures 1 and 2 indicated to effected of the overlapping coupling H_{CD} in unit eV on transition probability$T_N^C(E)$. It has evidently that $T_N^C(E)$exhibited a strictly linearly proportional increasing with increased H_{CD}(eV),it rises from 3.5531 x 10^{11}(1/sec) at H_{CD} = 0.13 x 10^{-2}eV to 56.030 X 10^{11}(1/sec) at H_{CD} = 2.05 x 10^{-2} eV.The $T_N^C(E)/\langle H_{CD} \rangle$ ratio stay constant,it indicated to external thermal and structural parameters are kept constant.The electric transition probability $T_N^C(E)$ limits under influence of concentration as well as coupling and $T_N^C(E)$ increased when the concentration increases from $4 \times 10^{24} m^{-3}$ to $8 \times 10^{24} m^{-3}$ by two times in N719-CdSe system. The behaviour of probability of transition $T_N^C(E)$ of N719-CdSe device

evaluated using two concentration to provide more information and to understand about device performance. In concentration 4×10^{24}, both probability of electron transfer calculated amount indicates that electrons trans through the N719/ CdSe heterojunction are lowe than with concentration 8×10^{24} by percentage factor 2. This indicates to increase efficiency by twice with increasing the concentration. Increasing in concentration will be leading to an increase in transfer more electrons cross interfaces which influenced the qualities of the N719-$CdSe_2$ device.

Due to two figures 1 and 2,we observe the probability of electronic transition was supported with increased of overlapping coupling as well as concentration values. Difference electron transfer probability should be increased to reach to maxima as results to more electrons transfer from excited state in N719 to conduction band of CdSe, and by orientation transition energy reformation of electron injected efficiency.Results of electronic transition that's clears iindicated that the efficiency can increase with increasing the ctransfer of electrons of the N149/ CdSe cell device.

Conclusion

In this work, a theoretically investigated the probability of electron transfer of the N719 contact into CdSe in hetero-junction for its potential in renewable energy applications calculates theoretically due to the quantum electron transition theory. The N719-CdSe device studies under variety overlapping strength with two different concentration to explore its hetero-junction electronic characteristics which used to understand the performance device. Particular attention has be given to the ieffect of overlapaping coupling,strength coupling and orentation transition energy on the interfacial transfer mechanism of electrons. The probablity results indicated that electron transfer reaction is strongly dependent on overlapping strength,concentaration and properties of N719,CdSe and alchohle ethyl due to orentation transition energy The probalblity of electron transfer reaction characteristics of the N149-CdSe device wwas reveal changing in overall efficiency due to overlapping coupling and concentration in N149-CdSe system.

A decrease in concentration and coupling energy generally leads to an increase in activation barrier and a decreased in probability of electron transfer, which hinders the injection of electrons across the interface between the N719 dye and the cadmium selenide (CdSe) material.

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