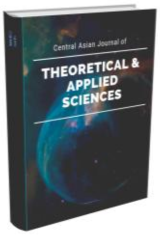

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Article

Study and Analysis of the Quantum Charge Transfer Rate in Ruthenium Dye RuN3 Contacting Semiconductors

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Abstract: In this work, the charge transfer interaction from the donor state in excited ruthenium dye RuN3 to the acceptor state in the semiconductor CdSe was elucidated. The charge transfer rate was calculated using the quantum scenario of charge transfer theory, based on the donor-receiver approach. IN this approach, the injection of the charge from the excited RuN3 dye into the conduction band of CdSe is treated as a quantum transition process subject to the effects of electronic coupling and reorganization energy.The rate of charge transfer in a RuN3-CdSe cell depends greatly on the rearrangement energy, the polarity of the solvent medium, the coupling strength, the distance between the RuN3 dye and CdSe, the atomic density, and the charge concentration. A high reorganization energy increases the probability of charge transfer and reduce reocobination charge , while a low energy increases the rate of charge injection and decreases the rate of transfer. Ethyl alcohol and methyl alcohol were used as polar media to evaluate the effects of the solvent, when in contact with RuN3 with CdSe in the device. Analysis of the reorganization energy and charge transfer rate reveals that RuN3, CdSe, and solvent properties play a crucial role in modifying charge transfer between surfaces under different solvent conditions, coupling strength, and varyied temperatures. The rate of charge transfer increases significantly with increasing temperature, overcoming the activation barrier to inject it into the conduction band of CdSe, as a result of the increased vibrational energy of the molecular system.The charge transfer reaction occurred mainly as a result of the strong bond between the RuN3 dye and CdSe, which led to increased wavefunction overlap at the interface, thus enhancing the electrical transport potential of the RuN3-CdSe device. Based on the results, the overall performance of the RuN3-CdSe device can be improved by optimizing the basic parameters of charge transport, which are governed by fundamental quantum principles, where temperature affects thermal activation, barrier reorganization energy controls, and coupling controls the quantum transport probability.

Keywords: Quantum , Charge Transfer, Rate , RuN3 dye.

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Introduction

The depletion of fossil fuel resources, increased energy consumption, and greenhouse gas emissions are among the most important environmental challenges that have prompted intensive efforts to promote renewable and clean energy sources[1]. Replacing fossil fuels with low-cost and renewable energy sources is essential to meeting the growing global demand for energy while reducing harmful effects on climate and the environment, and is one of the most prominent challenges facing the world . Sunlight provides a convenient and clean source of energy that can play a pivotal role in future energy solutions [2]. Among the various types of solar cells, dye-sensitized solar cells (DSSCs) have received increasing attention and are considered a practical option due to their low cost and high efficiency in converting sunlight into electricity[3]. Charge transfer science is a fundamental process that explains the operation of many electronic device technologies and solar cells [4]. The charge transfer has been fundamental reaction in photovoltaic cells, and it relies on photo induced transfer across molecular dye contact into semiconductor in solar cells [5]. Charge transport interactions, which are fundamental in photovoltaic devices, are discussed based on a simplified model of the Marcus theory of electron transport from the 1950s, specifically a continuum model with the assumption of a linear response[6].

Marcus theory has gained increasing attention for its pivotal role in the non-adiabatic charge transfer process, artfully addressing the distinctive electronic and physical properties at different temperatures in solar cell applications[7]. Many studies on charge transfer at the interface of electronic technological devices have received considerable attention due to their use in technological materials, with the primary goal of improving performance [8].The transfer of charge in the dye-sensitive contact layer of dye-sensitive solar cells (DSSCs) is a critical factor for enhancing efficiency, and this area, popularized by Oregano and Grätzel, has recently received increased attention as modern research focuses on improving charge transfer[9]. Hadi and his colleagues argued that reaorganization energy is a critical cofficient in the charge transport process for reconfigurate energy levels in devices.This occurs in hetrojunction devices across various device technologies[10].Quantum charge transport interactions are a fundamental process, and quantum control of charge transport dynamics in charge donor-acceptor systems is of great importance in many systems at interface surfaces ,it play a pivotal role in the development the interaction of molecules with semiconductors [11]. Furthermore, semiconductors are modified by dipole interactions between electrodes in the conduction band, which induce a change in potential that prevents recombination at the interface, and results in a shift either up or down in the conduction band depending on the electronic properties of light absorption at the LUMO level [12]. Ruthenium dye RuN3 is characterized by its superior ability to absorb light photons and inject electrons into the semiconductor's conduction band, significantly enhancing the solar energy harvesting efficiency of dye-sensitized solar cells (DSSCs)[13]. Cadmium selenide (CdSe) is defined as an inorganic semiconductor belonging to the class II-VI semiconductor group.It has become the best semiconductor in solar cell manufacturing as results to its n-type conductivity and its band gap of 1.74 eV at room temperature [14]. The CdSe semiconductor is used in solar cells due to its multiple properties, such as high absorption coefficient, wide energy gap, and high charge carrier mobility, making it an attractive candidate for use in solar cells [15].In this research, we study and analyze the quantum charge transfer rate of Ruthenium dye RuN3 when it comes into contact with CdSe semiconductors using two solvents, in order to design two types of solar cells. This is due to understanding and analyzing the challenges facing charge transfer capability between RuN3 and CdSe modules.

Theory

The quantum charge transfer rate is a key factor in determining the limiting resistance derived from the von Klitzing constant of electron tunneling between donor and acceptor states[16].The Quantum charge transport rate $R_{\mu}$is defined as the ratio of transition probability T_R on time relaxation τ ,it writes by [17].

$$R_{\mu} = \frac{|T_R|}{t} \qquad (1)$$

The transition probability T_R in **RuN3** contact with CdSe device can express by [18].

$$|T_R| = \frac{4\pi^2 t}{h}\int_0^E |\langle K_{RC}\rangle|^2\, \rho_{DA}(E_D - E_A)dE \qquad (2)$$

Where h is the Planck constant, $\langle K_{RC}\rangle$ is expectation values of strength coupling and $\rho_{DA}(E_D - E_A)$ is the density of state and E_D and dye E_A are energies in donor **RuN3** dye and acceptor in conduction band in CdSe semiconductor.Inserting Eq. (2) in Eq. (1) and introduces the Fermi density $\mathrm{F}_{(\mathrm{E})}$ for **RuN3-**CdSe cell system to results

$$R_{\mu} = \frac{4\pi^2}{h}\int_0^E |\langle K_{RC}\rangle|^2\, \mathrm{F}_{(\mathrm{E})}\rho_{DA}(E_D - E_A)dE \qquad (3)$$

The density of state $\rho_{DA}(E_D - E_A)$ in RuN3-CdSe system is [19].

$$\rho_{DA}(E_D - E_A) = \langle\boldsymbol{\widehat{\rho}_D}\rangle \rho_o^{-2/3}\, \frac{l_C}{(\frac{6}{\pi})^{1/3}}\rho_A(E) \qquad (4)$$

Where $\langle\boldsymbol{\widehat{\rho}_D}\rangle$ is effective density of electrons, ρ_o is the atomic density of the acceptor CdSe l_C is the length and $\rho_A(E)$ is the electronic density of the acceptor CdSe. The effective density of electrons, $\langle\boldsymbol{\widehat{\rho}_D}\rangle$ for electrons move from donor RuN3 dye to conduction band of CdSe acceptor is [20].

$$\langle\boldsymbol{\widehat{\rho}_D}\rangle = \frac{e^{-\frac{(\lambda_C^R + \Delta V^0)^2}{4\lambda_C^R k_B T}}}{\sqrt{4\pi\lambda_C^R k_B T}} \qquad (5)$$

Where λ_C^R(eV) is reorganization energy , ΔV^0 is driving potential , k_B is the Boltzmann constant and T is temperature. The driving potential is function as conduction band energy $\mathrm{E_c}$ and chemical potential $\mathrm{Q^o}$ for RuN3 [21].

$$\Delta V^0 = \mathrm{E_c} - \mathrm{Q^o} \qquad (6)$$

Inserting the Eq. (6) and Eq. (5) in Eq. (4) to results.

$$\rho_{DA}(E_D - E_A) = \frac{e^{-\frac{(\lambda_C^R + \mathrm{E_c} - \mathrm{Q^o})^2}{4\lambda_C^R k_B T}}}{\sqrt{4\pi\lambda_C^R k_B T}}\rho_o^{-2/3}\, \frac{l_C}{(\frac{6}{\pi})^{1/3}}\rho_A(E) \qquad (7)$$

Substituting Eq.(7) in Eq.(3) to obtain.

$$R_{\mu} = \frac{4\pi^2}{h}\int_0^E |\langle K_{RC}\rangle|^2\, \frac{e^{-\frac{(\lambda_C^R + \mathrm{E_c} - \mathrm{Q^o})^2}{4\lambda_C^R k_B T}}}{\sqrt{4\pi\lambda_C^R k_B T}}\rho_o^{-2/3}\, \frac{l_C}{(\frac{6}{\pi})^{1/3}}\mathrm{F}_{(\mathrm{E})}\rho_A(E)dE \qquad (8)$$

The expression in Eq.(8) can be simplified by

$$R_{\mu} = \frac{4\pi^2}{h}|\langle K_{RC}\rangle|^2 \frac{e^{-\frac{(\lambda_C^R + \mathrm{E_c} - \mathrm{Q^o})^2}{4\lambda_C^R k_B T}}}{\sqrt{4\pi\lambda_C^R k_B T}}\rho_o^{-2/3}\, \frac{l_C}{(\frac{6}{\pi})^{1/3}}\int_0^E \mathrm{F}_{(\mathrm{E})}\rho_A(E)\; dE \qquad (9)$$

The integral in Eq.(9) results to [22].

$$\int_0^E \mathrm{F}_{(\mathrm{E})}\rho_A(E)\, dE = [C] \qquad (10)$$

Where $[C]$ is concentration .Insert Eq. (10) in Eq.(9) to results.'

$$R_{\mu} = \frac{4\pi^2}{h}|\langle K_{RC}\rangle|^2 \frac{e^{-\frac{(\lambda_C^R + \mathrm{E_c} - \mathrm{Q^o})^2}{4\lambda_C^R k_B T}}}{\sqrt{4\pi\lambda_C^R k_B T}}\rho_o^{-2/3}\, \frac{l_C}{(\frac{6}{\pi})^{1/3}}[C] \qquad (11)$$

The reorganization energy λ_C^R(eV) of RuN3-CdSe system is [23].

$$\lambda_C^R(\mathrm{eV}) = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{r}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] + \frac{1}{2D_D}\left[\left(\frac{\varepsilon_{Sem}^2 - \varepsilon^2}{\varepsilon_{Sem}^2 + \varepsilon^2}\,\frac{1}{\varepsilon^2} - \frac{n_{Sem}^2 - n^2}{n_{Sem}^2 + n^2}\right)\left(\frac{1}{n^2}\right)\right]\right] \qquad (12)$$

where e , ε_0 , r and D_D are charge**,** permittivity , radius of RuN3 or CdSe and distance between RuN3 and CdSe, S_{sem} are s, $n_{sem}$and n are the dielectric constant and refractive index of the semiconductor and solvents. The radius of the dye molecule is [24].

$$r(nm) = (\frac{3}{4\pi}\,\frac{M}{N\rho})^{\frac{1}{3}} \tag{13}$$

Where M is the molecular weight, N_A is Avogadro's number, and ρ is the mass density.

Results

A quantum charge transfer rate has the most important criteria to understand efficiency . The quantum charge transfer rate can understand depends on the studies the behavior of charge transfer reaction occured in the RuN3 -CdSe interface.Theoretical quantum computational approach used to calkculate the cjharge transfer rate based on the donor-acceptor picture with assumes the energy levels in RuN3 donor and CdSe acceptor are continuum . The charge transfer rate ulation were presented for RuN3-CdSe system with ethyl alcohol and methyl alcohol solvents using MATLAB software.

The rate of quantum charge transfer from the excited RuN3 dye to the conduction band in the CdSe semiconductor was calculated using the parameters of reorganization energy, coupling force, driving force, and activation potential, which are key parameters in the charge transfer process. The reorganization energy plays a crucial role in limiting the charge transfer reaction rate from RuN3 dye to CdSe, and has been evaluated using equation (12).Based on the expression in Eq.(13),the radii of RuN3 and CdSe can estimate using Molecular weight 705.64 g/mol[25] for RuN3 and 191.37 g/mol[26] for CdSe and mass density 1.36 g/cm^3 [25] for RuN3 and 5.81 g/mol[26] for CdSe, radii results are found that 5.39 Å for RuN3 dye and 3.45 Å for CdSe .The reorganization energy can evaluated using Eq.(12) taking the radii 5.39 Å and 3.45 Å for RuN3 dye and CdSe ,as well as the refractive index 2.5[27] and dielectric constant 9.7 [28]of CdSe and taking account the refrective index (1.36 and 1.33) and dielectric constant (23.40 and 32.70) for Ethyl alcohol (**C_2H_5OH**) and Methyl alcohol (CH_3OH) solvents [29] and the distance between RuN3 and CdSe (8.84 Å),results are 0.54eV and 0.59eV for RuN3-CdSe-(**C_2H_5OH**) and RuN3-CdSe-(CH_3OH) respectively.The quantum charge transfer rate R_μ calculates as a function of the reorganization energy λ_C^R(0.54eV and 0.59eV), atomic density ρ_o, strength coupling$\langle K_{RC}\rangle$ 0.5,0.75,1,1.25,1.5,1.75,2,2.25,2.5,2.75,3,3.25,3.5,3.75,4] x10^{-6} eV/state [30], conduction energy $\mathrm{E_c}$,RuN3 potential $\mathrm{Q^o}$, length path $\boldsymbol{l}_C(3A)$ [31]and concentration $[C]$ $2 \times 10^{18} cm^{-3}$ using Eq.(11) for the RuN3-CdSe cell talken the temperature T=300,305 and 310K . Results show in tables (1)) for RuN3-CdSe-(**C_2H_5OH**) device and Table (2) for RuN3-CdSe-(CH_3OH) device at three temperatures T=300K,305K and 310 K,respectivelly.

Table 1. Results quantum charge transport $R_\mu(\frac{1}{Sec})$for hetrojunction RuN3-CdSe-(**C_2H_5OH**) device at different temperatures.

$\langle K_{RC}\rangle x10^{-6}$ eV/ state	Temperatures		
	305K	**310**	305K
0.50	7.256E+11	1.269E+12	2.129E+12
0.75	1.633E+12	2.855E+12	4.791E+12
1.00	2.902E+12	5.076E+12	8.517E+12
1.25	4.535E+12	7.931E+12	1.331E+13
1.50	6.531E+12	1.142E+13	1.916E+13
1.75	8.889E+12	1.555E+13	2.608E+13

2.00	1.161E+13	2.030E+13	3.407E+13
2.25	1.469E+13	2.570E+13	4.312E+13
2.50	1.814E+13	3.173E+13	5.323E+13
2.75	2.195E+13	3.839E+13	6.441E+13
3.00	2.612E+13	4.568E+13	7.665E+13
3.25	3.066E+13	5.362E+13	8.996E+13
3.50	3.556E+13	6.218E+13	1.043E+14
3.75	4.082E+13	7.138E+13	1.198E+14
4.00	4.644E+13	8.122E+13	1.363E+14

Table 2. Results quantum charge transport $R_{\mu}(\frac{1}{Sec})$ for hetrojunction RuN3-CdSe-(CH_3OH) device at different temperatures.

$\langle K_{RC} \rangle x10^{-6}$ eV/ state	Temperatures		
	305K	**310K**	**315K**
0.50	5.094E+11	8.953E+11	1.509E+12
0.75	1.146E+12	2.014E+12	3.395E+12
1.00	2.037E+12	3.581E+12	6.036E+12
1.25	3.184E+12	5.595E+12	9.432E+12
1.50	4.584E+12	8.057E+12	1.358E+13
1.75	6.240E+12	1.097E+13	1.849E+13
2.00	8.150E+12	1.432E+13	2.415E+13
2.25	1.031E+13	1.813E+13	3.056E+13
2.50	1.273E+13	2.238E+13	3.773E+13
2.75	1.541E+13	2.708E+13	4.565E+13
3.00	1.834E+13	3.223E+13	5.433E+13
3.25	2.152E+13	3.782E+13	6.376E+13
3.50	2.496E+13	4.387E+13	7.394E+13
3.75	2.865E+13	5.036E+13	8.488E+13
4.00	3.260E+13	5.730E+13	9.658E+13

Discussion

Based on the expression for the redevelopment energy in Equation (12) and the results, it was shown that the dielectric constant and refractive index of CdSe, ethanol, and methanol used in the RuN3-CdSe system are affected. The redevelopment energy was found to increase to 0.59 eV with Ethyl alcohol (C2H5OH) compared to 0.54 eV with Methyl alcohol (C2H5OH) when the dielectric constant increases from 23.40 for Ethyl alcohol (C2H5OH) to 32.70 for Methyl alcohol (CH3OH) solvents . However, the readjustment energy increases as the refractive index decreases from 1.36 for ethanol (C2H5OH) to 1.33 for methanol (CH3OH). Specifically, the rate of quantum charge transfer depends on the rearrangement energy, coupling strength, and concentration, as well as the atomic density and path length in CdSe, temperature and also on the structure and properties of the RuN3-CdSe, C2H5OH, and CH3OH solvents. Table 1 show the highest value for the quantum charge transport 4.644E+13 at 305K,8.122E+13 at 310K and 1.363E+14 at 315K were recorded for Ethayn alchohole at strength coupling 0.50eV, while the lowest value7.256E+11 at 305K 1.269E+12 at 310K and 2.129E+12 at 315K werre recorded for strength coupling 4.00eV. These results indicate that increasing the bonding strength and temperature leads to an increased charge transfer rate, and vice versa. The quantum charge transfer rates mentioned in Table 1, which range between (7.256×10^{11}, 1.269×10^{12}, and 2.129 ×

10^{12}) and (4.644×10^{13}, 8.122×10^{13}, and 1.363×10^{14}) at different temperatures (305, 310, and 315) Kelvin, and under the influence of a single driving force, highlight the greater effect of temperature.The high temperature (315 K) facilitates the passage of electrons through the activation barrier at the contact surfaces between the RuN3 dye and CdSe, resulting in a rapid injection of charge from the conduction band of the excited RuN3 dye into the CdSe.It is governed by a cobination ofmaterial stability, kinetics, and thermodynamics. However,increasing the temperature may lead to changes in the properties of cadmium sulfide (CdSe), which may slightly improve charge mobility, but increases electron recombination, which is often a major drawback.

On the other hand, the results in table(2) show same behaviour of charge transport reaction but lower than in Table(1) ,in range between (5.094E+11,8.953E+11 and 1.509E+12) and (3.260E+13 , 5.730E+13 and 9.658E+13) at different temperatures (305, 310, and 315) Kelvin under the same driving force, highlight the greater effect of temperature .These results show the effect of the reorganization energy, with the highest value recorded in the case of Methyl alcohol (CH3OH) at 0.59 electron volts, while the lowest value was recorded in the case of Ethyl alcohol (C2H5OH) at 0.54 electron volts. The RuN3-CdSe device using Ethyl alcohol (C2H5OH) exhibited a higher charge transport rate than the device using Ethyl alcohol (C2H5OH) . In Table 1, at temperatures of 305 K, 310 K, and 315 K, with a concentration of 2×10^{20} m^{-3} and an effective driving force of 0.22 eV, the quantum charge transfer rate in the RuN3-CdSe device using ethanol was highest compared to the RuN3-CdSe device using methanol, while the charge transfer rate in the RuN3-CdSe device using methanol was lowest, as shown in Table 2. Compared to the results in Tables 1 and 2, the Ethyl alcohol solvents used in this RuN3-CdSe system, at the same concentration, operating energy, and coupling strength, exhibited the lowest charge transfer rate, at 5.094×10^{11} at 0.50 eV. As expected, the charge transfer rate increased with increasing coupling strength and decreased with increasing redevelopment energy. Comparing the both solvents at the same strength coupling shows that decreases in the solvent's reorganization energy is offset by an increase in the quantum charge transfer rate.However, the results confirm that the charge transfer rate can increase with increasing coupling of the energy levels of RuN3 and CdSe and decreasing the reorganization energy, consistent with the electronic transition theory. In both Tables 1 and 2, the charge transfer rate at higher temperatures indicates that an increase of approximately three times compared to the charge transfer rate at 305 K for the same charge transfer parameters. This indicates that increasing temperature energy facilitates charge transfer and significant enhancement by promoting activation over the barrier. As in both Tables 1 and 2, the charge transfer rate continues to increase with increasing temperature as well as coupling strength and decreasing reorganization energy.

Conclusion

In conclusion, based on the results of the quantum charge transfer rate depends on the donor-acceptor framework and quantum transition theory, the highest charge transfer rate is achieved when the RuN3-CdSe device is operated in an Ethyl alcohol (C2H5OH) solvent environment characterized by low reorganization energy and high temperature. The results clearly show that the charge transfer rate in the RuN3-CdSe device is strongly affected by the rearrangement energy and temperature, as well as the coupling strength, in both of the solvents studied:Ethyl alcohol (C2H5OH) and Methyl alcohol (CH3OH) solvents. The reorganization energy refers to the physical compatibility between the excited state energy levels of the donor in RuN3 and the acceptor state in the conduction band of CdSe.

A decrease in reorganization energy means an increase in charge transfer rate, as a result of a better energy match between the excited state of RuN3 and CdSe. At high temperatures of around 315 K, the charges have sufficient thermal energy to transport charges across the interface between the photoexcited RuN3 dye and reach the conduction band in CdSe with greater efficiency. Comparison between ethyl alcohol ((C2H5OH) and methyl alcohol ((CH3OH) solvents shows that the RuN3-CdSe device using ethyl alcohol has a charge transfer rate approximately twice that of the device using methyl alcohol , resulting in improved charge injection dynamics. This improvement is physically attributed to the lower reorganization energy and the favorable polarity properties of ethyl alcohol, which reduces the reorganization barrier and improves the bonding strength at the interface. In general, the study confirms that optimal charge transport in RuN3-CdSe devices is governed by physical factors, including low reorganization energy, high coupling strength between RuN3 and CdSe, and high temperature. These factors collectively determine the charge injection efficiency in RuN3-CdSe systems.

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