International Journal of Latest Research in Engineering and Technology (IJLRET)
ISSN: 2454-5031
www.ijlret.com || Volume 11 - Issue 11 || November 2025 || PP. 01-09

A Study of the Influence of Temperature on Electron Transfer of an Ruthenium Complex Donor in Contact with ZnS Semiconductor in Dye-Sensitized Solar Cell

Haider Mushina Obeed[1,a)], Hadi J.M. Al-Agealy[2,b)]
[1]*Department of Medical Physics, College of Applied Medical Science, Shatrah University, Thi-Qar , 64001, Iraq*
[2]*Department of Physics, College of Education for Pure Science Ibn-ALHaitham, University of Baghdad, Baghdad-Iraq*

Abstract: In this paper, a theoretical study has been presented on influence of temperature on process of charge transport reaction based on the quantum transition from the donor excited state of ruthenium to the conduction band in zinc sulfide (ZnS) semiconductors. This study uses reorganization energy to evaluate the transport properties of four types of polar solvents, including ethanoic acid, dimethoxyethane (DME), propanol, and methyl alcohol, around a ZnS device contacting a ruthenium N3 heterojunction, for dye-sensitized solar cell (DSSC) applications within continuum energy levels. Calculations include momentum energy, coupling strength, atomic density, concentration vector, and polarity properties related to the dielectric constant and refractive index of the solvent and ZnS. Charge transfer rate analysis of ruthenium N3-ZnS using four solvents reveals that ethanoic acid and dimethoxyethane exhibit favorable polar media for efficient charge transfer from the excited ruthenium N3 dye to the conduction band of ZnS semiconductors, compared to propanol and methyl alcohol.

Keywords: Electronic Transport, Ruthenium Complex, ZnS, Dye-Sensitized Solar Cell.

I. INTRODUCTION

In recent decades, relentless pursuit of sustainable and renewable energy sources has become crucial to meet the world's growing energy needs, while at the same time mitigating environment impacted was associating with conventional energy generated method [1]. Since Michel Grätzel and colleagues introduced the first photovoltaic (PV) cells in 1991, research in the field of dye-sensitized solar cells (DSSCs) has gained interest and achieved some notable breakthroughs due to, cost-effective, simple and scalable raw material-based manufacturing methods [2]. The operation of DSSCs is based on the electron transfer principles, i.e., the conversion of photon light energy into electricity using light-absorbing dye molecules, which play main role in initiating the electronic transport process [3]. First, light absorbs by sensitizing dye excited an electrons, which moves to conduction band of semiconductor, leaving a positive dye. Electrons then diffused through semiconductor to reach conductive surface to collect current. Further, the ions were forming by oxid diffusion through short distance from electrolyte to cathode and the regeneration cycle. Finally, the ions travel to photoanode and are oxidized back to an ion by transfer an electronic back to sensitizing material, ready to return to its neutral state [4]. The electron transfer is of great importance in various fields of science and electronic technology in addition to the DSSCS solar cell. However, in charge transfer no chemical bond is formed or broken during the transfer process besides small change in bond and angle [5].Electron transport occurs in different heterostructured devices in many different technological devices [6]. Classical theory of Marcus represents basis to understand the dynamics of the electron transport process between a state at the donor and state at the acceptor when interface between them, that occurred in various electronic technology [7]. In recently, Marcus developed a semiclassical theory for the electron transfer rate equation, and Gürtner presented it based on quantum mechanics. A non-adiabatic electron transfer reaction is considered to occur between two electronic states within the Franck-Condon approximation, which is the probability of an electron transfer from the donor to the acceptor [8]. A quantum theory of charge transport QTCT is challenged and have a main attention is being paid to effect of barrier on the rate of electronic transport between donor and acceptor states [9], it is shown in figure .1

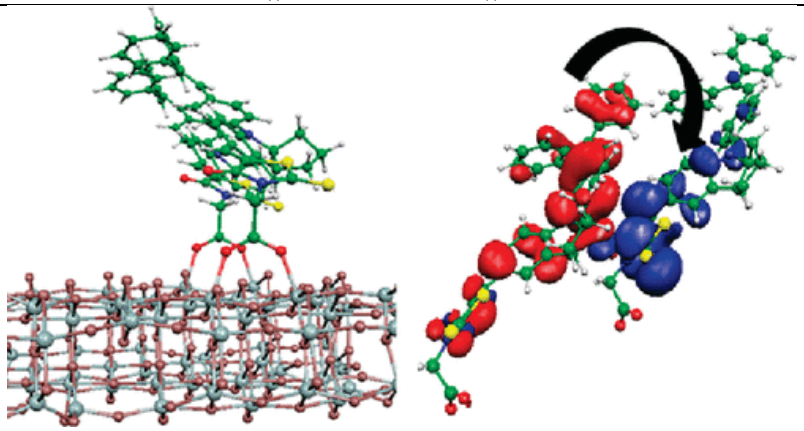

Figure 1: Schematic connection of Ruthenium contact with ZnS interfaces

In many applied electronic devices involving electron molecules, semiconductors and metals, various electron transfer processes have been found, where electrons move from the donor state to the final acceptor state [10].However, charge transport can occur in different heterogeneous structural devices in various types of solar cells, as well as technological devices [11]. The classical Marcus theory was introduced as a basis for understanding the dynamics of electron transfer between donor and acceptor states, which occurs in various devices [12]. Based on Hadi et al.'s theory, the transition energy is a fundamental and important factor in the electron transfer process, and it is necessary for the device to redirect the energy levels before transferring electrons in the devices [13]. QTCT was challenging and gained most attention for the effect of potential barrier on the charge transport rate for transfer of charge from donor to an acceptor states [8]. Many researchers are enhanced the charge transport theory based on theoretical analytical or experimental methods beside the computer simulation methods [14]. In this work, a theoretical study temperature effected on charge transport transition was summarize for ruthenium complex dye contact with zinc blend ZnS semiconductor in dye sensitized solar cell device .

II. THEORY

The coefficient of charge transport rate from initial donor dye state to final acceptor conduction band state can be utilized with [15].

$$\mathrm{K}_{i\to f} = \frac{2\pi}{\hbar}\left|\langle \mathscr{M}_{i\to f}\rangle\right|^2 \rho_{i\to f}(E) \tag{1}$$

Where $\hbar$ is Planck constant,$\mathscr{M}_{i\to f}$ is the coupling constant matrix element of donor acceptor overlapping and $\rho_{i\to f}(E)$ is density of electronic state in system, it can be written as [16].

$$\rho_{i\to f}(E) = \rho_{ef}\boldsymbol{l}_{ef}\left(\frac{6}{\pi}\right)^{-\frac{1}{3}} \tag{2}$$

Whereρ_{ef} is effective density in donor-acceptor system, $\boldsymbol{l}_{ef}$ is effective length in semiconductor. The Eq. (2) together Eq.(1) leads to .

$$\mathrm{K}_{i\to f} = \frac{2\pi}{\hbar}\left|\langle \mathscr{M}_{i\to f}\rangle\right|^2 \rho_{ef}\boldsymbol{l}_{ef}\left(\frac{6}{\pi}\right)^{-\frac{1}{3}} \tag{3}$$

However, the effective density can compute using [17].

$$\rho_{ef} = \rho_D(E)\rho_{at}^{-2/3}\langle\hat{\boldsymbol{\rho}}\rangle \tag{4}$$

Where $\rho_D(E)$ is the density of electrons in excited donor, ρ_{at} is the atomic density of semiconductor and $\langle\hat{\boldsymbol{\rho}}\rangle$ is measurment of density in donor-acceptor system given by.

$$\langle\hat{\boldsymbol{\rho}}\rangle = \frac{e^{-\frac{(\lambda_A^D+\Delta V^0)^2}{4\lambda_A^D k_B T}}}{\sqrt{4\pi\lambda_A^D k_B T}} \tag{5}$$

Where $\lambda_A^D(eV)$ is the reorganization energy, ΔV^0 is drive energy force, $k_B$is Boltzman constant as well as T is temperature. Reorganization energy $\lambda_A^D(eV)$ of the donor-acceptor around new equilibrium of system is [18].

$$\lambda_A^D(eV) = \frac{e^2}{8\pi\varepsilon_\circ}\left[\frac{1}{r}\left[\frac{1}{n^2}-\frac{1}{\varepsilon}\right] - \frac{1}{2D_{D-A}}\left[\left(\frac{n_A^2-n^2}{n_A^2+n^2}\right)\left(\frac{1}{n^2}\right) - \frac{\varepsilon_A^2-\varepsilon^2}{\varepsilon_A^2+\varepsilon^2}\frac{1}{\varepsilon^2}\right]\right] \quad (6)$$

Where e^2 is electron charge, $\varepsilon_\circ$, r and D_{D-A} are permittivity, radius of the materials in system, and distance between donor and acceptor ,n is refrective index of solvents and ε is dielectric constant ,n_A is refrective index and ε_A is dielectric constant of donor. The radius donor or acceptor can evaluate from spherical approach formula [19].

$$r(nm) = \left(\frac{3}{4\pi}\frac{M}{N\rho}\right)^{\frac{1}{3}} \quad (7)$$

Where M, **N** are molecular weight and Avogadro number, and ρ is density of material. Insert Eq. (5) and Eq. (4) into Eq. (3) using Fermi distribution function $F(E)$and integrated over all energy to produce.

$$\mathrm{K}_{i\to f} = \frac{2\pi}{\hbar}\int\left|\langle\mathscr{M}_{i\to f}\rangle\right|^2 \rho_D(E)\rho_{at}^{-2/3}\frac{e^{-\frac{(\lambda_A^D+\Delta V^0)^2}{4\lambda_A^D k_B T}}}{\sqrt{4\pi\lambda_A^D k_B T}}\boldsymbol{l}_{ef}\left(\frac{6}{\pi}\right)^{-\frac{1}{3}}F(E)dE \quad (8)$$

The constant term in Eq. (8) split out integral and simplified to

$$\mathrm{K}_{i\to f} = \frac{2\pi}{\hbar}\left|\langle\mathscr{M}_{i\to f}\rangle\right|^2 \rho_{at}^{-2/3}\frac{e^{-\frac{(\lambda_A^D+\Delta V^0)^2}{4\lambda_A^D k_B T}}}{\sqrt{4\pi\lambda_A^D k_B T}}\boldsymbol{l}_{ef}\left(\frac{6}{\pi}\right)^{-\frac{1}{3}}\int F(E)\,\rho_D(E)dE \quad (9)$$

The integral in Eq. (9) reduces to concentration of charge transfer in acceptor final state

$$\int F(E)\,\rho_D(E)dE = [C] \quad (10)$$

Substituting Eq. (10) into Eq. (9) to obtained.

$$\mathrm{K}_{i\to f} = \frac{2\pi}{\hbar}\left|\langle\mathscr{M}_{i\to f}\rangle\right|^2 \rho_{at}^{-2/3}\frac{e^{-\frac{(\lambda_A^D+\Delta V^0)^2}{4\lambda_A^D k_B T}}}{\sqrt{4\pi\lambda_A^D k_B T}}\boldsymbol{l}_{ef}\left(\frac{6}{\pi}\right)^{-\frac{1}{3}}[C] \quad (11)$$

III. RESULTS

To evaluate the effect of temperature on the charge transport process from energy state in Ruthenium complex dye to conduction band in ZnS semiconductor based dye-sensitized solar cells (DSSCs) ,was systematically study and investigated over] ranging from 25°C to 45°C. The effect of temperature on electron transport for all types of electrons in dyes, semiconductors, and electrolytes was studied and calculated using the density of states and quantum transition rate, and the characteristics of the reorganization energy in the steady state and the continuum state were calculated. In the first step, assuming charge transport from donor to an acceptor, the charge transfer rate coefficient calculated based on reorganization energies, which usually plays a most important to limit charge transport from the sensitized excited ruthenium complex to ZnS.

Reorganization energy $\lambda_A^D(eV)$ has been studied to evaluate used Eq. (6) taking into account the radius of the complex ruthenium dye and zinc sulfide (ZnS) with refractive index aa well as dielectric constant of solvent and zinc sulfide (ZnS). Radii of complex ruthenium dye and ZnS calculate using Eq.(7) with taken the molecular weight (M=705.64g/mol with density $1.36\frac{\mathrm{g}}{\mathrm{cm}\,3}$) for ruthenium complex using table (1) , M= 97.46g/mol and $\rho = 4.079\ \frac{\mathrm{g}}{\mathrm{cm}\,3}$[20]) for ZnS, results are $6.499A^o$ and $2.117A^0$for both ruthenium dye and ZnS respectively .

Table (1): Main physical properties of Ruthenium N3 dye [20-21].

Ruthenium N3 dye	
Name	Cis-bis(isothiocyanato-bis(2,2′-bipyridyl-4,4′-dicarboxylato) ruthenium(II)
synonym	Ruthenium N3
Molecular form	$C_{26}H_{16}N_6O_8RuS_2$
Molar Mass (g/mol)	705.64
Density (g/cm^3)	1.36
Melting point (C^o)	> 300
HOMO(eV)	-5.39
LUMO(eV)	-2.79
solubility	C_2H_5OH
classificate	Ruthenium, Bipyridyl-ligands, Dye-sensitized solar cells , Energy materials,donor

Calculated radius	6.499 A^o

Table (2): he properties of ZnS [22,23].

Properties	**ZnS**
Molecular Weight	97.46
Groups	Zinc(12)
	Sulfur(16)
Structure	Cubic Crystal
Lattice Constant(Å)	5.4093
Dielectric Constant	8.9
Band Gap(eV)	3.54
Density(g/cm^3)	4.079
Melting Point (°C)	1850
Refractive Index	2.356
Radius (Å)	2.116

The reorganization energy $\lambda_A^D(eV)$was derived using Equation (6) with the input of both the dielectric constant and refractive index of the solvents from Table (3) and ZnS from Table (2), and the results show in Table (3).

Table (3): The reorganization energy $\lambda_A^D(eV)$ for charge transfer from ruthenium dye to ZnS

solvents	**Formula**	**Dielectric constant (ε)[25]**	**Refractive index (n) [25]**	$\lambda_A^D(eV)$
Ethanoic Acid	CH_3 COOH	6.15	1.372	0.303
Dimethoxyethane DME	$C_4H_{10}O_2$	7.2	1.380	0.434
Propanol	$CH_3CH_2CH_2OH$	20.33	1.384	0.438
Methyl Alcohol	CH_3OH	32.7	1.330	**0.476**

Understanding charge transfer upon contact of ruthenium dye with zinc sulfide (ZnS), its effect on temperature, and its relationship to DSSC efficiency through simulations is based on a theoretical model. These simulations typically include alignment of power levels, routing, manufacturing methods, and optimization to achieve good efficiency. These processes typically involve determining the direction and adjusting the alignment by calculating the charge transfer rate $K_{i\to f}$. Thats can be calculated by applied a expression in Eq. (11) by insert the conduction band (3.66eV) , temperature from of 25°C, 35°C and 45°C ,carrier concentration [C]($1.4\times10^{20}m^{-3}$), effective length$\boldsymbol{l}_{ef}=3\times10^{-10}m$[24], atomic density $5.81\times10^{18}\frac{1}{m^3}$, strength coupling ranging ($7.25\times10^{-6}\geq\left|\langle\mathcal{M}_{i\to f}\rangle\right|^2\geq1.25\times10^{-6}$|eV|^2)and taken the Electrochemical potentialΔV^0 =3.45eV with reorganization energy from table (3) using (MATLAP) software, results summarized in the Tables (4) (5) and (6) at temperature 25°C, 35°C and 45°C .

Table (4): Results of rate ofharge transport calculated for RutheniumN3- ZnS at $\Delta V^0=0.21$ eV at 25°C.

solvents	$\lambda_A^D(eV)$	$K_{i\to f}\times\mathbf{10^{13}}(\boldsymbol{cm^2/\sec})$						
		$\left\|\langle\mathcal{M}_{i\to f}\rangle\right\|^2\times\mathbf{10^{-6}eV/state}$						
		1.25	**2.25**	**3.25**	**4.25**	**5.25**	**6.25**	**7.25**
Ethanoic Acid	0.303	**1. 764**	**3.321**	**4. 448**	**5.1455**	**6.644**	**7.689**	**8.167**
Dimethoxyethane	0.434	**2. 713**	**3.256**	**4.358**	**4.697**	**5. 396**	**6.698**	**7.676**
Propanol	0.438	**0. 896**	**1.2876**	**1.678**	**2.191**	**2.5940**	**3.145**	**3.438**
Methyl Alcohol	**0.476**	**0.828**	**1.264**	**1. 387**	**1.456**	**1.657**	**1.897**	**2.234**

Table (5): Results of rate ofharge transport calculated for RutheniumN3- ZnS at $\Delta V^0=0.21$ eV at 35°C

solvents	$\lambda_A^D(eV)$	$K_{i\to f} \times 10^{13}\ (cm^2/sec)$ $\lvert\langle \mathcal{M}_{i\to f}\rangle\rvert^2 \times 10^{-6}\ eV/state$						
		1.25	**2.25**	**3.25**	**4.25**	**5.25**	**6.25**	**7.25**
Ethanoic Acid	0.303	3.687	5.254	7.456	9.296	11.321	13.156	15. 197
Dimethoxyethane	0.434	3.214	4.789	6.456	7.981	9.698	10.181	12.945
Propanol	0.438	1.765	2.257	3.244	3.943	4.756	5.142	6.398
Methyl Alcohol	0.476	1.098	1.512	1.997	2.478	3.114	3.494	2.191

Table (6): Results of rate of harge transport calculated for Ruthenium N3- ZnS at $\Delta V^0 = 0.21$ eV at 45°C.

solvents	$\lambda_A^D(eV)$	$K_{i\to f} \times 10^{13}\ (cm^2/sec)$ $\lvert\langle \mathcal{M}_{i\to f}\rangle\rvert^2 \times 10^{-6}\ eV/state$						
		1.25	**2.25**	**3.25**	**4.25**	**5.25**	**6.25**	**7.25**
Ethanoic Acid	0.303	4.698	7.108	9.564	11.956	14. 645	16.433	18.982
Dimethoxyethane	0.434	4.118	6.270	8.357	10. 672	12.562	14.659	16.328
Propanol	0.438	1.989	3.140	4.016	5.115	6.211	7.230	8.329
Methyl Alcohol	0.476	1.376	2.031	2.571	3.321	3.983	4.667	5.785

Figures (1), (2), and (3) show the calculated electron transfer rate of ruthenium N3-ZnS at temperatures T=25°C, 35°C, and 45°C. Charge transfer rate can reveal important information regarding its potential use in solar cell applications.

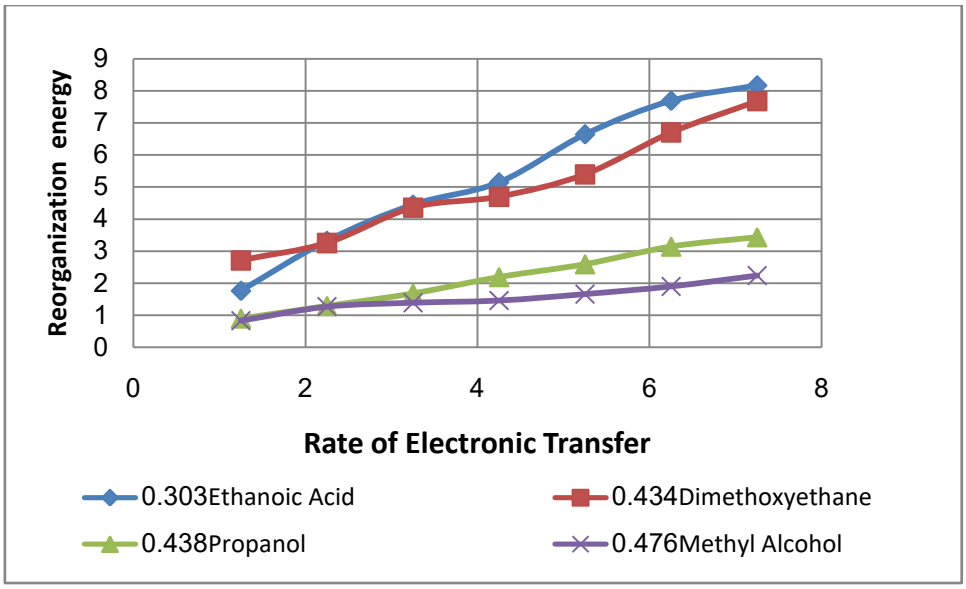

Figure (1): The rate of charge transportfor Ruthenium N3- ZnS at 25°C

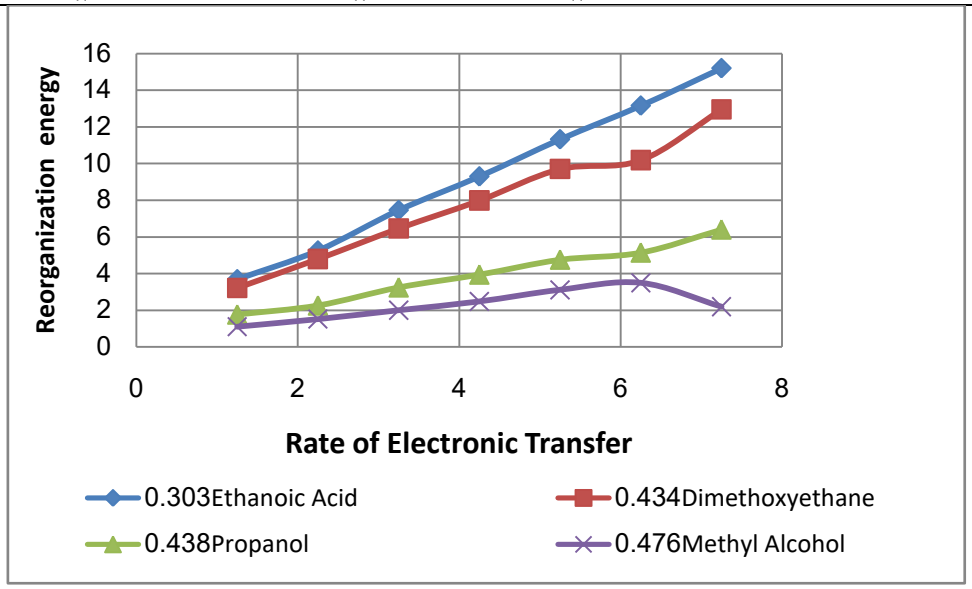

Figure (2): The rate of charge transportfor Ruthenium N3- ZnS at 35°C.

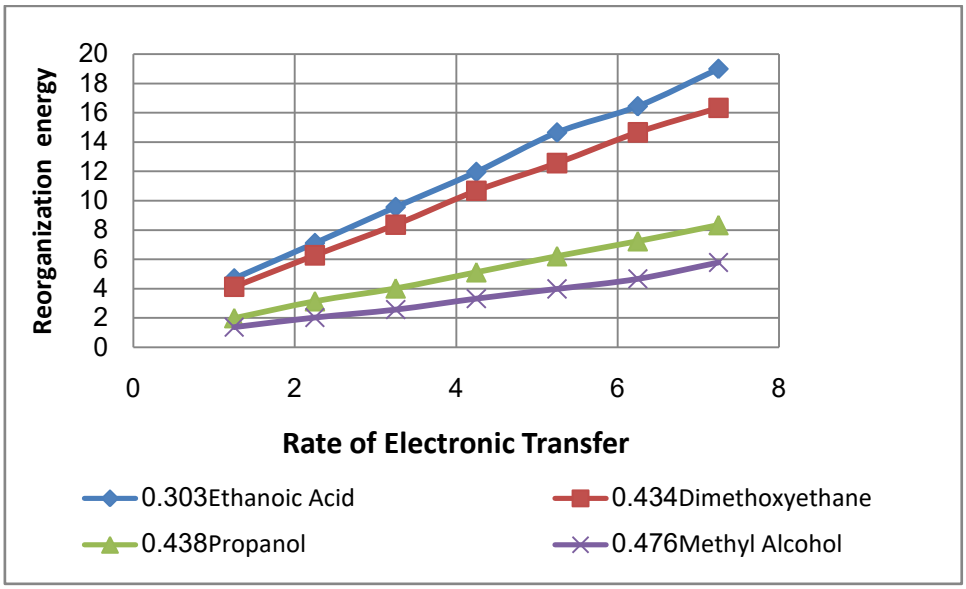

Figure (3): The rate of charge transportfor Ruthenium N3- ZnS at 45°C.

IV. DISCUSSION

The results showed reorganization energy and temperature dependent behavior in the main charge transfer rate coefficients and interface charge transfer dynamics. The reorganization energy is influenced by solvent polarity.Table (3) indicates the main results that highlight a clear dependence on the forced reorganization energy of both the refractive index and the dielectric constant of the solvents.The reorganization energy of the system using methyl alcohol solvent (0.476 eV) is higher than the reorganization energy of ethanoic acid (0.303 eV), DME (0.434 eV), and propanol (0.438 eV) solvents, indicating that the device requires more energy for orientation, which means a lower probability of charge transfer. However, the device containing ethanoic acid solvent has a low reorganization energy of 0.303 eV and results in a high $K_{i\to f}(cm^2/sec)$.The calculated rate $K_{i\to f}(cm^2/sec)$under finite temperature showed significant changes in the reorganization energy with increases in dielectric constant and decreased in the refractive index. Calculated charge transport rate under a limited temperature showed significant changes and reorganization energy-dependent behavior with increasing dielectric constant and decreasing refractive index. As shown in Tables (4), (5), and (6), the best charge transfer rate increased at (T = 25, 35, and 45) °C, with a minimum reorganization energy of 0.303 and a significant improvement with decreasing dielectric constant and more polar media.This improvement has been attributed to improved charge injection as well as reduced the resistance of charge.

However, the charge transfer rate results, derived from theoretical calculations (see Figures 1, 2, and 3), show a decrease in $K_{i\to f}(cm^2/sec)$ at the interface between ruthenium N3 and zinc sulfur, with the reorganization energy decreasing with decreasing refractive index of the solvents. There are changebale common behavoure of the relation of electronic transfer rate with reorganization energy and temperatures, the more stable of which are in figure (3). As shown in the figure(3), for the ruthenium N3-ZnS as-assumed in this study, the 45oC is dominated the increases rate of electron transfer .The results in Table (3) showed an increase in the reorganization energy of the ruthenium N3-ZnS contact system with four kinds of solvents from 0.303 with ethanoic acid to 0.476 with methyl alcohol.The rate $K_{i\to f}(cm^2/sec)$ of ruthenium N3-ZnS in Tables (4), (5) and (6) with decreasing reorganization energy depends on solvents polarity due to the refractive index as well as dielectric constant of the solvents.

The main results highlight a clear dependence on the force coupling of both the charge transfer rate and the total reorganization energy, according to the expression in Eq. (11).As expected, the charge trasport in Tables (4), (5) and (6) increased with increased force coupling and decreased reorganization energies at the same temperature.Moreover, the rates results in Tables (4) to (6) for N3 dye sensitized using ZnS devices with ethanoic acid solvent were higher than with methyl alcohol solvent due to the reorganization energy.The charge transfer rate increases with increasing force coupling from [1.25 to 7.25] and the reorganization energy decreases from 0.476 eV to 0.303 eV for four types of solvents with limited driving energy (0.21 eV).

At lower temperatures (25°C), the rate and overall charge transfer reaction were relatively modest becouse they attributed to reduced transition energy, which limited the transfer of charge and slows down the injection of charges from the donor ruthenium N3 dye into the conduction band of ZnS. On the other hand, the charge transport will be increased alternatively with increased in the temperature from 25°C, 35°C, to 45°C.As result, higher rate of the device at 45°C indicates that charge has transferred in most of the potential cross-linked heterojunction devices as the temperature increases.

Charge transfer rate data confirmed an increase in the charge transfer interaction at the ruthenium N3 dye/zinc sulfur (ZnS) interface when increased temperature from 25°C to 45°C for reaction in devices, indicating high charge separation efficiency between the two surfaces.

In fact, the charge transport rate reaches to miximum values at 45°C with lower reorganization energy , ranging ~4.698× $\mathbf{10^{13}}$(to~18.982× $\mathbf{10^{13}}$(, while at 25°C, it decreased significantly to ~(1. 764- 8.167) × $\mathbf{10^{13}}$.Indicating improved charge transport of ruthenium N3 –ZnS device largely with increased temperature and reach maximum values with all solvents at 45oC.However, this indicates that the device performance is affected by temperature rise, which is limited by recombination losses or thermal instability of the dye layer.As the temperature increased to about 45°C, the charge transfer rate in the ruthenium N3-ZnS devices improved significantly. This indicates improved charge transfer kinetics and increased velocity of charge carriers within the ZnS semiconductor matrix with a lower reorganization energy.

V. CONCLUSION

Electron transfer rate and reorganization energy calculations were performed on zinc sulfide (ZnS) sensitized with ruthenium N3 dye, to understand charge transport mechanism through the sensitized dye with increasing temperature to develop performance of solar cells sensitized with simple organic dyes. The effect of temperature on the electron transfer rate in dye-sensitized solar cells was studied. Analysis of these calculations indicates a decreasing effect of the reorganization energy in all solvents as the reorganization energy increases and the temperature decreases. Zinc-based solar cells were studied, sensitized using an organic dye ruthenium N3 and five solvents. The electron transport velocity and reorganization energy were studied at different temperatures to understand the electron transport and charge transport mechanism in ruthenium N3-ZnS device. The electron transfer rate of ruthenium N3 dye sensitized at 45°C using ethanoic acid solvent is higher than other solvents, while the carrier rate of ruthenium N3 dye sensitized at 25°C using methyl alcohol solvent is lower compared to other solvents due to the effect of reorganization energy.The electron transport properties of ruthenium N3-Zns show that low reorganization energy and high temperature modification improve electron transport, which is explained by the alignment energy levels and high polarity mechanism.Of the four solvents, ethanoic acid performs best as a sensitizer for ruthenium N3 with ZnS, while methyl alcohol solvent yields the lowest electron transfer rate in ZnS-based solar cells.

REFERENCES

[1]. Gunawardhana, P.; Balasooriya, Y.; Kandanapitiye, M.S.; Chau, Y.-F.C.; Kooh, M.R.R.; Thotagamuge, R. Optoelectronic Characterization of Natural Dyes in the Quest for Enhanced Performance in Dye-Sensitized Solar Cells: A Density Functional Theory Study. Appl. Sci. 2024, 14, 188. https://doi.org/10.3390/app14010188

[2]. Carmen Coppola, Anna Visibelli, Maria Laura Parisi, Annalisa Santucci, Lorenzo Zani, Ottavia Spiga & Adalgisa Sinicropi, A combined ML and DFT strategy for the prediction of dye candidates for indoor DSSCs, npj Computational Materials | (2025) 11:28. https://doi.org/10.1038/s41524-025-01521-9
[3]. Zulkifili, A.N.B.; Kento, T.; Daiki, M.; Fujiki, A. The Basic Research on the Dye-Sensitized Solar Cells (DSSC). J. Clean Energy Technol. 2015, 3, 382–387.
[4]. Jing Chen , Andreas L. Vishart , Stephan P. A. Sauer , Kurt V. Mikkelsen, Theoretical Investigations of Dye-Sensitized Solar Cells, JNanotechnol Nanomaterials. 2023; 4(2):38-54
[5]. AL-agealy, H. J. M., Harbbi, K. H., Hassooni, M. A., & Noori, R. I. (2013). Theoretical Study of Charge Transfer in Styryl Thiazilo Quinoxaline Dyes STQ-1, STQ-2, and STQ-3 in Organic Media System. *Baghdad Science Journal*, *10*(4), 1262-1268.
[6]. Al-Agealy, H. J., & Hassooni, M. A. (2011). Calculate of the Rate Constant of Electron Transfer in TiO2–Safranine Dye System. Ibn AL-Haitham Journal For Pure and Applied Science, 24(3).
[7]. Marcus, R. A. (2020). Electron transfer reactions in chemistry. Theory and experiment. In Protein electron transfer (pp. 249-272). Garland Science.
[8]. Kalyani Chordiya, Md. Ehesan Ali, and Mousumi U. Kahaly, Photoexcited Intramolecular Charge Transfer in Dye Sensitizers: Predictive In Silico Screening for Dye-Sensitized Solar Cell Devices, ACS Omega 2022, 7, 13465−13474. https://doi.org/10.1021/acsomega.1c06233.
[9]. Al-Agealy, H. J., & Al-Hakany, J. S. (2017). Theoretical Calculations of Rate Constant of Electron Transfer Across N3/TiO2 Sensitized Dye Interface Solar Cell. Ibn AL-Haitham Journal For Pure and Applied Science, 25(2).
[10]. Vahideh Hadigheh Rezvan ,Charge transfer complexes: a review survey, Results in Chemistry,Vol.17, 2025, 102600. https://doi.org/10.1016/j.rechem.2025.102600.
[11]. Buck, J. T., Wilson, R. W., & Mani, T. (2019). Intramolecular long-range charge-transfer emission in donor–bridge–acceptor systems. *The Journal of Physical Chemistry Letters*, *10*(11), 3080-3086.
[12]. Paulo Roberto Bueno, Quantum rate theory and electron-transfer dynamics: A theoretical and experimental approach for quantum electrochemistry, Electrochimica Acta, Vol. 466,2023, 142950 https://doi.org/10.1016/j.electacta.2023.142950
[13]. Al-Agealy, H. J., Hassoni, M. A., Ahmad, M. S., Noori, R. I., &Jheil, S. S. (2014). A Theoretical Study of Charge Transport y at Au/ZnSe and Au/ZnS Interfaces Devices. *Ibn AL-Haitham Journal for Pure and Applied Science*, *27*(1), 176-187.
[14]. Al-agealy, H. J., Alshafaay, B., Hassooni, M. A., Ashwiekh, A. M., Sadoon, A. K., Majeed, R. H., ... & Mahdi, S. H. (2018, May). Theoretical discussion of electron transport rate constant at TCNQ/Ge and TiO2 system. In *Journal of Physics: Conference Series* (Vol. 1003, No. 1, p. 012122). IOP Publishing.
[15]. Pau Besalú-Sala; Alexander A. Voityuk; Josep M. Luis Corresponding Author ; Miquel Solà, Effect of external electric fields in the charge transfer rates of donor–acceptor dyads: A straightforward computational evaluation ,J. Chem. Phys. 158, 244111 (2023)
[16]. Taif Saad Al Maadhde , Mohammad Hafizuddin Jumali ,Hadi J. M. Al-Agealy, Fatimah Binti Abdul Razak and Chi Chin Yap" An Investigation of the Fill Factor and Efficiency of MolecularSemiconductor Solar Cells" Materials Science Forum ,Vol.1039, pp
[17]. Sarmad S. Al-Obaidi1, Hadi J. M. Al-Agealy, Saadi R. Abbas "Theoretical Evaluation of Flow Electronic Rate at Au /TFB Interface "Journal of Physics: Conference Series 1879 (2021) 032096 IOP Publishing doi:10.1088/1742-6596/1879/3/032096.
[18]. Al-Agealy, H. J.M., and Hassooni, M.A. 2014. "Effect of Semiconductors Types on Electron Transmission at Metal/ Semiconductor Interface" J. Chem. Bio.Phys.SCI. Sec. C.4(3).
[19]. Hadi Jabbar Al-Agealy and TaifSaad Al Maudhady "Influence of The Polarity Function on the Probability of Transition Rate Constant (sec-1) At Metal/Molecule In Nano Scale Devices "International Journal of Application or Innovation in Engineering & Management (IJAIEM),Volume 3, Issue 5, May 2014
[20]. Wayment-Steele, H. K., Johnson, L. E., Tian, F., Dixon, M. C., Benz, L., & Johal, M. S. (2014). Monitoring N3 dye adsorption and desorption on TiO2 surfaces: a combined QCM-D and XPS study. *ACS Applied Materials & Interfaces*, *6*(12), 9093-9099.
[21]. Hassooni, M. A. (2020). Theoretical analysis of charge flow rate at dye sensitized-semiconductor interfaces cell system. *Energy Reports*, *6*, 72-78.
[22]. Firas Adel Shnain and Hadi Jabbar Alagealy, Theoretical calculation of the efficiency of dye solar cells using quantum transfer theory for solid-state dye contact with ZnO, AIP Conf. Proc. 3282, 050044 (2025)
[23]. Weber, M.J., 2018. *Handbook of optical materials*. CRC press.

[24]. Hadi J.,M. Al-Agealy and Nada A. Sabri "Theoretical studies of electronic transition characteristics of senstizer molecule dye N3-SnO2 semiconductor interface" AIP Conference Proceedings 2437(1):020062 ,2022 .