Theoretical calculation of the electronic current density in ruthenium 620 contact with TiO$_2$ semiconductor in propanol solvent

Hadi J. M. Al-Agealy[1,*], Hazim Hadi Dhayef Al-Hasan[2], Raafat Abdul Hassan Muslim[3], Mohsin A. Hassooni[1]

[1]*Department of Physics, College of Education for Pure Science -Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq.*
[2]*Ministry of Education, General Directorate of Wasit Education, Iraq.*
[3]*Center of Education, Researches-studies, Ministry of Education, Iraq.*

Corresponding author: hadi.j.m@ihcoedu.uobaghdad.edu.iq

Original Research

Abstract:

In this study, a theoretical model was presented to calculate current and current density to investigate the efficiency of the heterogeneous ruthenium 620-TiO$_2$ device using a propanol solvent. This work examines the effect of concentration carriers on the current density and performance of ruthenium 620-TiO$_2$ devices for dye-sensitized solar cells (DSSCs) in the presence of a propanol solvent based on electron transfer theory. Quantum electron transfer theory is used to describe current cross-linked 620-TiO$_2$ ruthenium devices. When the concentration is increased from 1.5×10^{24} m^{-3} to 2.5×10^{24} m^{-3}, the current density and current show a significant shift to an increase of approximately 1.66. The fill factor does not change significantly, but there are efficiency shifts of about 1.004 with increasing concentration carrier taken from the experimental literature from 1.5×10^{24} m^{-3} to 2.5×10^{24} m^{-3}.

Keywords: Current density; Ruthenium 620; TiO$_2$; Propanol solvent

---

1. Introduction

Recently, the crisis of increasing energy demand has become a global issue these days due to the increase in population. The decline in fossil fuel resources due to the increasing demand for energy supplies has exacerbated the problem [1]. Solar energy is unique from the most preferred, most abundant, least expensive, and cheapest type of renewable energy to convert electricity, but its popularity has been limited due to the high cost of traditional solar cells [2]. The photovoltaic effect is the process that converts light energy from the sun into electricity [3]. Solar photovoltaic cell technologies are divided into three generations. The first generation was crystalline silicon, which has stability and good performance. The second generation is based on amorphous silicon and inorganic semiconductors such as cadmium telluride (CdTe). Furthermore, the third generation was based on organic semiconductors, it was

based on dye-sensitized solar cells [4]. Among a variety of photovoltaics, Dye-sensitized solar cells (DSSCs) have received a lot of attention since Gratzel and O'Regan reported that dye-sensitized solar cells (DSSCs) convert light into electricity. They are still limited because of low conversion efficiencies [5]. DSSC's photovoltaic solar cell technology remains promising and is gaining wide attention due to its low cost, simple manufacturing process, and higher efficiency [6]. The dye in the DSSC solar cell absorbs light for excitation to stimulate the charge transfer from the sensitive dye to the conduction band of TiO$_2$, replenish the oxidized dye molecules by donating electrons from the redox couple in the system, and finally, the electron transfer is completed through convection [7]. The electronic transfer process is one of the most important processes that play a major role in the operating systems of DSSCs [8]. The quantum theory of electron transfer theory suggests that a greater challenge is to pay attention to the contact interface between two ma-

terials that require the transfer of an electron from the donor state to the acceptor state [9]. The donor–acceptor scenario is one of the simplest models used to discuss electron transfer that does not form or break any chemical bond in the system [10]. The electronic transfer in heterojunction interfaces occurs when electrons are moved from the donor level to the acceptor level in solar cell devices [11]. Moreover, the contact region between molecules and semiconductor systems has received more attention in various technological applications because the charge transfer process occurs across the interface [12]. The mineral-based organic dye which includes the ruthenium complex such that ruthenium 620 is a compound widely used as sunlight harvester in DSSC sensitization to achieve higher efficiencies [13].

Ruthinium 620 dye is an attractive, sensitive organic dye used in DSSCs solar cells, it has the formula [(C4H9)4N] 3[Ru(Htcterpy)(NCS)3] C69H117N9O6RuS3, Tris [N, N, N-tributyl-1-butanaminium [2, 2″6′, 2″-terpyridine]-4, 4′, 4″-tricarboxylato (3-N1, N1′, N1″ tris (thiocyanato-N-hydrogen ruthenium) [14] and the chemical structure is listed in Figure 1 [15].

Lately, the improvement in solar cell performance through the efficiency of DSSCs has increased and achieved at a more comprehensive and lower cost, which constitutes a critical condition for energy applications [16]. This work focuses on calculating the electron current density in a ruthenium 620 solar cell in contact with a TiO$_2$ semiconductor and theoretically studies the fill factor and its efficiency based on the current density.

2. Theory

To estimate efficiency, the fill factor (FF) must be calculated using a simple expression using the cell output and given by [17].

$$FF = \frac{I_{pp}V_{pp}}{I_{Sc}V_{oc}} \qquad (1)$$

where $I_{pp} V_{pp}$ is denoted by maximum power point, it determines from the power (P)-voltage (V) curves from which current density I_{pp} and output voltage V_{pp} can be obtained, I_{Sc} and V_{oc} are short-circuited current. Open circuit voltages respectively, the efficiency of DSSCs defines as the ratio of output power to its incident light power density, It is simply obtaining using Eq. (1) to give [18].

$$\eta = \frac{I_{Sc}V_{oc}FF}{P_i} \times 100\% \qquad (2)$$

Is the room temperature where P_i is incident light intensity (mW·cm^{-2}). The electronic current in solar cell devices can be determined using an expression as [19].

$$I = \frac{2\pi e}{\hbar} \frac{1}{\sqrt{4\pi\lambda k_B T}} |\langle M_D^A \rangle|^2 e^{-\frac{(\lambda+(E_{cb}-qE^o))^2}{4\lambda k_B T}} \frac{l_{Se}}{(\frac{6}{\pi})^{1/3}}$$
$$d_{Se}^{-\frac{2}{3}} \int_0^E \rho_D(E)F(E)dE \qquad (3)$$

where q is electronic charge, $\hbar$ is dirac constant, M_D^A is the strength coupling, λ is reorganization energy, E_{cb} is the conduction band, qE^o is chemiscat potential of dye, k_B is the Boltzman constant, T the room temperature, l_{se} is active

length, d_{se} is the electronic density in semiconductor, ρ_D is the density of state dye system and $F(E)$ is the Fermi distribution in donor and acceptor. Integration in Eq. (3) may be a solution to the electronic concentration n_s at the surface semiconductor's [20].

$$\int_0^E F(E)\rho_B(E)dE = n_S \qquad (4)$$

Substituting Eq. (4) in Eq. (3) to yields.

$$I = \frac{4\pi^2 q}{h} \frac{1}{\sqrt{4\pi\lambda k_B T}} |\langle M_D^A \rangle|^2 e^{-\frac{(\lambda+(E_{cb}-qE^o))^2}{4\lambda k_B T}} \frac{l_{Se}}{(\frac{6}{\pi})^{1/3}}$$
$$d_{Se}^{-\frac{2}{3}} n_S \qquad (5)$$

The reorganization energy λ (eV) is a critical parameter for electronic transfer in solar cell system, it is given by [21].

$$\lambda(\text{eV}) = \frac{e^2}{8\pi\varepsilon_0}$$
$$\left[\left(\frac{1}{D}\frac{1}{n^2} - \frac{1}{\varepsilon} \right) - \frac{1}{2R} \left(\frac{n_S^2 - n^2}{n_S^2 + n^2}\frac{1}{n^2} - \frac{\rho_S^2 - \varepsilon^2}{\rho_S^2 + \varepsilon^2}\frac{1}{\varepsilon^2} \right) \right] \qquad (6)$$

where ε_0 is permittivity, D and R are the radius of the dye molecule and the distance between dye and semiconductor, n and ε are refractive index and dielectric constant of solvent, n_s is the refractive index of semiconductor and ε_S is the dielectric constant of semiconductor [21]. The radius is function of molecular weight M and density of the material ρ, it is given in form [22].

$$D = \left(\frac{3}{4\pi}\frac{m}{N\rho} \right)^{\frac{1}{3}} \qquad (7)$$
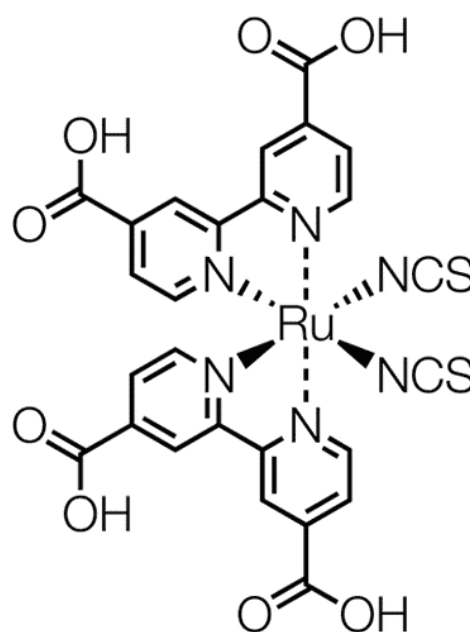
where, Avogadro number N.

Figure 1. Structure of Ruthenium 620 sensitized dye [15].

3. Results

The current density produced when TiO$_2$ contacts ruthenium 620 in the DSSC solar cell was calculated theoretically by calculating the current. In this regard, we initially evaluate the reorganization energy by using Eq. (6). Calculating the radius of ruthenium dye 620 and TiO$_2$ is based on Eq. (7) with the introduction of molecular weight $M = 1364.9$ (g/mol) [23] and $M = 79.87$ (g/mol) [24] and density $\rho = 1.28$ (g/cm^3) [23] and $\rho = 4.23$ (g/cm^3) [24] for ruthenium 620 and TiO$_2$, respectively, the results are 7.47 $\AA$ and 1.96 $\AA$ for ruthenium 620 and TiO$_2$. Reorganization energy calculated onto the ruthenium 620-TiO$_2$ solar cell with Propanol solvent used in DSSCs using Eq. (6) by inserting dielectric constant 55 and refractive 2.609 of TiO$_2$ semiconductor [24] with dielectric constant 20.33 [25] and refractive 1.3856 [25] for propanol solvent within Eq. (7) with to results $\lambda = 0.342$ eV. Then, the current through ruthenium 620-TiO$_2$ is calculated using Eq. (5), taking the carrier concentration n_s in range (1.5×10^{18} and 2.5×10^{18}) [26], semiconductor density $d_{se} = 5.8 \times 10^{18}$ (1/m^3) [20], $l_{Se} = 3\AA$ [27], the strength coupling $|\langle M_D^A \rangle|^2 = (0.1.$ to 1.5) $\times 10^{-2}$ |eV|^2 with MATLAP soft world program, results list in Table 1.

Current density I_d can be evaluated by divided the current in Table 1, on the area of solar cell (19×10^{-2} (cm^2) [28], results list in Table 2.

The current density I_d (A/cm^2) verses voltage in Volt characteristic is shown in Table 3.

The data in Table 3 can be plotted into two curves using the Log scale of current density versus volts shown in Figure 2. Figure 2 indicates the $I_d - V$ characteristic of ruthenium 620-TiO$_2$ heterojunction in solar cells for estimation of maximum current density I_{PP} and output voltage V_{PP}, they are determined from the two curves in Figure 2. The short-circuit current I_{Sc} and open circuit voltages V_{oc} to estimate both fill factor and efficiency of DSSCs defines.

The fill factor can be estimated using Eq. (1) with inserting I_{PP}, V_{PP}, I_{Sc} and V_{oc} from two curves in Figure 2, the results listed in the Table 4 also, the efficiency evaluate using
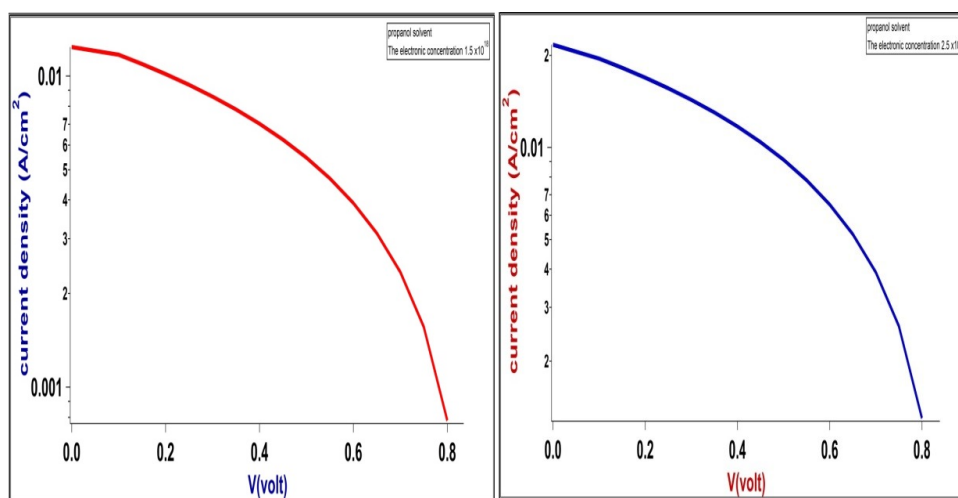
Eq. (2) with fill factor, I_{Sc} and V_{oc} results from Table 4 and Figure 2, results list in Table 4 for ruthenium 620-TiO$_2$ devices.

4. Discussion

The current density is the main parameter effect on the fill factor and efficiency of ruthenium 620 dye-TiO$_2$ in solar cells based on a quantum model with a propanol solvent and used two concentrations for carriers in a system. Table 1 refers to the current of the ruthenium 620-TiO$_2$ solar cell, which is influenced by the carrier concentration and strength coupling. The current was increased upon increasing the strength coupling from (0.1, to 1.5) $\times 10^{-2}$ |eV|^2. However, the current of the ruthenium 620-TiO$_2$ devices has been increases from 1.2337E-04 A/cm^2 to 2.0561E-04 A/cm^2 at strength coupling 0.1×10^{-2} |eV|^2 and from 1.8505E-03 A/cm^2 to 3.0842E-03 A/cm^2 at strength coupling 1.5×10^{-2}|eV|^2 with concentration change from 1.5×10^{24} (1/m^3) to 1.5×10^{24} (1/m^3).

In turn, the current density depends on the force coupling and the concentration carrier and increases as both the concentration carrier and the force coupling parameters with the propanol solvent media in the devices increase. The current density calculated revealed in two concentrations that the efficiency of ruthenium 620-TiO$_2$-based DSSCs improved slightly because of a concentration increase and a considerable increase in JSC (short circuit current) and maximum current.

It observes that when the concentration carrier of electrons has been increased from 1.5×10^{24} (1/m^3) to 2.5×10^{24} (1/m^3), the I_{Sc} enhances significantly from 12.392 to 21.672 (mA/cm^2); but, increases in the concentration from 1.5×10^{24} (1/m^3) to 2.5×10^{24} (1/m^3) resulted in a downward trend with respect to filling factor from 0.136 to 0.133. The influence of different concentrations on current and current density are shown in Tables 1 and 2 and η in Table 4. The increase in I_{Sc} values can be attributed to the modified surface characteristics of ruthenium 620-TiO$_2$ devices with polar solvent. In contrast, the increases in concentration carrier

Figure 2. Current density verses voltage characteristics of ruthenium 620 dye contact with TiO$_2$ at concentrations 1.5×10^{24} (1/m^3) and 2.5×10^{24} (1/m^3).

Table 1. The current calculates for ruthenium 620 contact with TiO_2 with propanol solvent.

$|\langle M_D^A \rangle|^2 \times 10^{-2}|$ eV$|^2$	The electronic concentration (1/m^3)	
	1.5×10^{24}	2.5×10^{24}
0.1	1.2337E-04	2.0561E-04
0.2	2.4673E-04	4.1122E-04
0.3	3.7010E-04	6.1684E-04
0.4	4.9347E-04	8.2245E-04
0.5	6.1684E-04	1.0281E-03
0.6	7.4020E-04	1.2337E-03
0.7	8.6357E-04	1.4393E-03
0.8	9.8694E-04	1.6449E-03
0.9	1.1103E-03	1.8505E-03
1	1.2337E-03	2.0561E-03
1.1	1.3570E-03	2.2617E-03
1.2	1.4804E-03	2.4673E-03
1.3	1.6038E-03	2.6730E-03
1.4	1.7271E-03	2.8786E-03
1.5	1.8505E-03	3.0842E-03

Table 2. The current density I_d (A/cm^2) for ruthenium 620 contact with TiO_2 with propanol solvent.

$|\langle M_D^A \rangle|^2 \times 10^{-2}|$ eV$|^2$	The electronic concentration (1/m^3)	
	1.5×10^{24}	2.5×10^{24}
0.1	7.8081E-04	1.3013E-03
0.2	1.5616E-03	2.6027E-03
0.3	2.3424E-03	3.9040E-03
0.4	3.1232E-03	5.2054E-03
0.5	3.9040E-03	6.5067E-03
0.6	4.6848E-03	7.8081E-03
0.7	5.4656E-03	9.1094E-03
0.8	6.2464E-03	1.0411E-02
0.9	7.0273E-03	1.1712E-02
1	7.8081E-03	1.3013E-02
1.1	8.5889E-03	1.4315E-02
1.2	9.3697E-03	1.5616E-02
1.3	1.0150E-02	1.6917E-02
1.4	1.0931E-02	1.8219E-02
1.5	1.1712E-02	1.9520E-02

provide more electrons to transfer electron cross interface from excited levels of ruthenium 620 dye to the conduction band in TiO$_2$ semiconductor.

A theoretical calculation based on electron transfer theory has been established and is a good tool for calculating current through ruthenium 620-TiO$_2$ devices. In fact, the electron is increasingly transferred across the interface of a device with high concentration and vice versa. On the other hand, the current and current density are increased with increasing coupling strength for all concentration increments in Tables 1 and 2. When the coupling strength of ruthenium 620 dye is increased, the current and current density of ruthenium 620-TiO$_2$ is larger at concentration 2.5 compared with 1.5, which indicates increased electron transfer through the ruthenium 620-TiO$_2$ device with propanol solvents. It is indeed expected that the efficiency of solar cells increases when the carrier concentration in the system increases. Furthermore, fill factor and efficiency are deter-

Table 3. Results of current density for ruthenium 620-TiO$_2$ with propanol solvent.

The electronic concentration (1/m^3)			
1.5×10^{24}		2.5×10^{24}	
V (Volt)	I_d (A/cm^2)	V (Volt)	I_d (A/cm^2)
0.835	0	0.8389	0
0.8	7.8081E-04	0.8	1.3013E-03
0.75	1.5616E-03	0.75	2.6027E-03
0.7	2.3424E-03	0.7	3.9040E-03
0.65	3.1232E-03	0.65	5.2054E-03
0.6	3.9040E-03	0.6	6.5067E-03
0.55	4.6848E-03	0.55	7.8081E-03
0.5	5.4656E-03	0.5	9.1094E-03
0.45	6.2464E-03	0.45	1.0411E-02
0.4	7.0273E-03	0.4	1.1712E-02
0.35	7.8081E-03	0.35	1.3013E-02
0.3	8.5889E-03	0.3	1.4315E-02
0.25	9.3697E-03	0.25	1.5616E-02
0.2	1.0150E-02	0.2	1.6917E-02
0.15	1.0931E-02	0.15	1.8219E-02
0.1	1.1712E-02	0.1	1.9520E-02
0	1.2392E-02	0	2.1672E-02

Table 4. Results of photovoltaic parameters of the for ruthenium 620-/TiO$_2$ DSSC with propanol solvent.

Variables	Value	
concentration (1/m^3)	1.5×10^{24}	2.5×10^{24}
I_{Sc} (mA/cm^2)	12.392	21.672
V_{oc} (Volt)	0.835	0.8389
I_m (mA/cm^2)	1.9561	3.324
V_m (Volt)	0.7234	0.7278
$F.F$	0.13675	0.133065
Efficiency	1.415%	2.4192%

mined by the current-voltage characteristic. As can be seen in Table 4, the filling factor and estimated efficiency are based on the current density calculated in units (mA/cm^2), and the current versus voltage are listed in Table 3 and Figure 2. The data results presented as curves in 2A and 2B show that in pure propanol solvent, the average open circuit photovoltage V_{PP} (Volt) and current I_{PP} (mA/cm^2) are re-estimated from Figure 2 and inscribed in Table 4. The two curves closely matched the observed behavior through theoretical values of efficiency of about 1.415% with concentration and 2.419% with concentration compared with experimental conversion efficiency in the 1.26% – 1.61% [1].

5. Conclusion

In this study, a theoretical calculation of current density was introduced to study the fill factor and efficiency of the heterogeneous ruthenium 620-TiO$_2$ device with propanol solvent for its potential in photovoltaic solar cell applications. The effects of concentration and strength coupling were examined by simulation with a propanol solvent. The concentrations were upshifted from 1.5×10^{24} (1/m^3) to 2.5×10^{24} (1/m^3) but the fill factor values shifted in less changed. The efficiency results showed that increasing the amount of carrier concentration on ruthenium 620-TiO$_2$ increases the current density and leads to increased efficiency. The efficiency calculated found that the device with concentration 2.5×10^{24} (1/m^3) possessed 1.7% higher ($\eta = 2.419\%$) compared to the device with concentration 1.5×10^{24} (1/m^3) that possessed ($\eta = 1.4150\%$) mainly due to enhanced current density.

References

[1] A. Siddika, M. Sultana, M. S. Bashar, S. Tabassum, S. Aziz, and M. A. Ali Shaikh. "Improved performance of dye sensitized solar cell by exploration of photoanode and ruthenium based dye.". *Opt Mater (Amst)*, **125**, 2022.

[2] A. Singh, Y. K. Saini, A. Kumar, S. Gautam, D. Kumar, V. Dutta, H. K. Lee, J. Lee, and S. K. Swami. "Property modulation of graphene oxide incorporated with TiO$_2$ for dye-sensitized solar cells.". *ACS Omega.*, **7**, 2022.

[3] Mohd. R. S. Shaikh. "A review paper on electricity generation from solar energy.". *Int J Res Appl Sci Eng Technol. V*, , 2017.

[4] H. Soonmin, Hardani, P. Nandi, B. S. Mwankemwa, T. D. Malevu, and M. I. Malik. "Overview on different types of solar cells: An update.". *Applied Sciences (Switzerland)*, **13**, 2023.

[5] S. Suhaimi, M. M. Shahimin, Z. A. Alahmed, J. Chysky, and A. H. Reshak. "Materials for enhanced dye-sensitized solar cell performance: Electrochemical application.". *Int J Electrochem Sci.*, **10**, 2015.

[6] J. Dou, Y. Li, J. Wu, Y. J. Chang, and M. Wei. "Improving the photovoltaic performance of Zn$_2$SnO$_4$ solar cells by doping Sr2+/Ba2+ ions: Efficient electron injection and transfer.". *Solar Energy.*, **165**:122–130, 2018.

[7] T. H. Syed and W. Wei. "Technoeconomic analysis of dye sensitized solar cells (DSSCs) with WS$_2$/carbon composite as counter electrode material.". *Inorganics (Basel)*, **10**, 2022.

[8] J. S. H Al-Hakany and Hadi J. M. Al-Agealy. "Theoretical calculations of rate constant of electron transfer across N$_3$/TiO$_2$ sensitized dye interface solar cell. ". *Ibn AL- Haitham Journal For Pure and Applied Science*, **25**:160–169, 2012.

[9] H. J. M. Al-Agealy, B. Alshafaay, M. A. Hassooni, A. M. Ashwiekh, A. K. Sadoon, R. H. Majeed, R. Q. Ghadhban, and S. H. Mahdi. "Theoretical discussion of electron transport rate constant at TCNQ/Ge and TiO$_2$ System. ". *J Phys Conf Ser*, , 2018.

[10] M. A. Hassooni. "Theoretical analysis of charge flow rate at dye sensitized-semiconductor interfaces cell system. ". *Energy Reports.*, **6**, 2020.

[11] H. J. Al-Agealy and M. A. Hassooni. "Calculate of the rate constant of electron transfer in TiO$_2$–safranine dye system. ". *Ibn AL-Haitham Journal For Pure and Applied Science*, **24**, 2010.

[12] M. Grätzel. " Review dye-sensitized solar cells. ". *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*, **4**:145–153, 2003.

[13] M. Tahir, I. U. Din, M. Zeb, F. Aziz, F. Wahab, Z. Gul, Alamgeer, M. R. Sarker, S. Ali, S. H. M. Ali, and I. Kymissis. "Thin films characterization and study of N749-black dye for photovoltaic applications.". *Coatings.*, **12**:1163, 2022.

[14] Q. Feng, H. Wang, G. Zhou, and Z.-S. Wang. "Effect of deoxycholic acid on performance of dye-sensitized solar cell based on black dye.". *Frontiers of Optoelectronics in China*, **4**:80–86, 2011.

[15] T. S. Kamatchi, P. Kalaivani, P. Poornima, V. V. Padma, F. R. Fronczekc, and K. Natarajan. "New organometallic ruthenium(ii) complexes containing chelidonic acid (4-oxo-4H-pyran-2,6-dicarboxylic acid): synthesis structure and in vitro biological activity. ". *RSC Adv.*, **4**, 2014.

[16] F. Kabir, M. M. H. Bhuiyan, M. R. Hossain, H. Bashar, M. S. Rahaman, M. S. Manir, S. M. Ullah, S. S. Uddin, M. Z. I. Mollah, R. A. Khan, S. Huque, and M. A. Khan. "Improvement of efficiency of dye sensitized solar cells by optimizing the combination ratio of natural red and yellow dyes.". *Optik (Stuttg).*, **179**, 2019.

[17] S. H. Bendary, A. A. Hashem, and S. A. Mahmoud. "High efficiency dye-sensitized solar cells with a novel two dimensional Cd-V-LDH photoanode.". *Front Mater.*, **10**, 2023.

[18] T. S. Al Maadhede, M. H. Jumali, H. J. Al-Agealy, C. C. Yap, and Y. Al-Douri. "Improved performance of D149 dye-sensitized ZnO-based solar cell under solvents activation effect. ". *The European Physical Journal Plus*, **138**:325, 2023.

[19] T. S. Al Maadhede, M. H. Jumali, H. J. M. Al-Agealy, C. C. Yap, A. D. Ayada, and A. H. Shaban. "Effect of solvents on performance of Alq3/ZnO solar cells: A theoretical approach. ". *Energy Reports*, **9**, 2023.

[20] N. N. Abd Ali, H. J. Al-Agealy, and H. M. Moghaddam. "Theoretical calculation of the fill factor of N749/TiO$_2$ solar cells.". *Ibn AL-Haitham Journal For Pure and Applied Sciences*, **36**:145–158, 2023.

[21] N. N. A. Ali and H. J. M. Al-Agealy. "A theoretical model for efficiency N749 black dye-sensitized solar cell based on TiO$_2$ photoanode.". *AIP Conf. Proc.*, **3018**, 2023.

[22] H. J. M. Al-Agealy, M. A. Hassooni, R. Q. Ghadhban, M. A. Obaid, and A. J. Saud. "Theoretical calculation of electronic rate at cis-bisisothiocyanatobis (2,2′-bipyridyl-4,4′-dicarboxylato) ruthenium(II) N3 dye contact to GaAs semiconductor. ". *AIP Conference Proceedings*, **2845**, 2023.

[23] C. Bauer, G. Boschloo, E. Mukhtar, and A. Hagfeldt. "Interfacial electron-transfer dynamics in Ru(tcterpy)(NCS)3-sensitized TiO$_2$ nanocrystalline solar cells.". *J Phys Chem B.*, **106**:12693–12704, 2002.

[24] M. A. R. Mohsin and H. J. M. Al-Agealy. "Theoretical calculation of the electronic current at N$_3$ contact with TiO$_2$ solar cell devices. ". *AIP Conference Proceedings*, **2437**:020060, 2022.

[25] W. M. Haynes. " Handbook of Chemistry and Physics.". *CRC Press*, , 2014.

[26] M. Sotoudeh, M. Abbasnejad, and M. R. Mohammadizadeh. "First principles study of hydrogen doping in anatase TiO$_2$.". *EPJ Applied Physics*, **13**:67, 2014.

[27] N. A. Sabri and H. J. M. Al-Agealy. "Theoretical studies of electronic transition characteristics of sensitizer molecule dye N$_3$-SnO$_2$ semiconductor interface.". *AIP Conference Proceedings*, **2437**:020062, 2022.

[28] G. Koyyada, R. Kumar Chitumalla, S. Thogiti, J. H. Kim, J. Jang, M. Chandrasekharam, and J. H. Jung. "A new series of EDOT based Co-sensitizers for enhanced efficiency of cocktail DSSC: a comparative study of two different anchoring groups. ". *Molecules*, **24**:3554, 2019.