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Study of the Charge Transfer Rate and Injection Dynamic of Indoline Dye Contacting TiO_2 in a Sensitized Solar Cell

Mohamad Hady Mahdi[1*] **and Hadi J.M.Al-Agealy**[2*]
[1,2]Department of Physics College of Education for Pure Sciences (Ibn-ALHaitham), University of Baghdad, Baghdad, Iraq
*Corresponding Author

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Abstract

In this study, the theoretical framework relied on the quantum charge (electron) transfer theory to investigate and calculate the probability of transfer and charge transport behavior in the heterojunction D102/TiO_2 device. Electronic transport characteristics were calculated using MATLAB simulations, assuming continuum levels for both the D102 dye and the TiO_2 semiconductor. The transition rate of the D102/TiO_2 heterojunction was found to depend on the reorganization energy, strength of coupling, heterojunction, and intrinsic D102 and TiO_2 properties. The charge transition process was examined over a range of strength couplings (0.387–1.244) × 10^{-3} eV/state and concentrations in the range (2–7) × 10^{30} cm^{-3} using DCM and butanol solvents at room temperature. The results indicate that the transition rate increases with increased reorganization energy, strength coupling, and concentration. Under identical coupling and concentration conditions, the D102/TiO_2 with butanol demonstrates a significantly high transition rate (≈12%) compared to the D102/TiO_2 device with the DCM solvent. The enhancement of electron transport in D102/TiO_2 suggests that it is suitable for improved transfer in heterojunction D102/TiO_2 applications.

Keywords: Charge Transfer, Indoline, D102 dye, TiO_2.

1. Introduction

As energy transitions have been paid attention to in terms of ongoing challenges and technological dimensions of energy transitions, societal changes are needed and sustainable implementation strategies to transition to sustainable renewable energy with better environmental protection [1].Transporting energy has been produced from fossil fuels to renewable energy sources, playing a main important role in the reduction of emissions from greenhouse gases, which is crucial to mitigate climate change[2]. Solar energy is now a pivotal component of the global transition to renewable energy sources. Recently, according to the International Renewable Energy Agency (IRENA), installed solar photovoltaic (PV) capacity worldwide reached 1,418 gigawatts (GW) at the end of 2023, representing 36.7% of the world's renewable sources. Growth underscores rapidly [3]. Moreover, a variety of photovoltaic PV energy technologies could be invented and developed to convert photon light into electricity, which has been primarily for the benefit of society[4]. One such technology is dye-sensitized solar cells (DSSCs), which are photovoltaic devices that use a photocatalytic reaction to produce electrical energy using organic dyes (photosensitizers) and semiconductors[5]. Solar cells come in several generations, each with its own advantages, disadvantages, and unique characteristics. First-generation deals with silicon cells, which are less expensive, more reliable, and efficient. The second generation consists of thin-film cells. The third generation includes organic cells and dye-sensitized solar cells[6] .

Both Gratzel and Oregano addressed the issue of dye-sensitized solar cells (DSSCs), which have gained increasing attention in recent years because of easy manufacturing, low cost, and

transparency with sustainability compared to inorganic cells[7] .DSSCs offer an economical and practical alternative to first- and second-generation solar cells, they can be a main option due to their ability to reduce costs and improve efficiency in different applications with less environmental impact[8] .

The general features of DSSC cells are that light is absorbed by the sensitizing dye to become excited, and then the charge is transferred to the conduction band in the semiconductor to convert the light photons into electricity in the cell. Electrons move through the interface due to the geometric structure of solar cells to convert electrical current into direct current (DC) [9]. However, charges can move across interfaces and become independent charge carriers when dye comes into contact with semiconductors in heterojunction devices [10]. In solar cell devices, charges can transfer across the contact of the dye with oxide semiconductor interfaces when charges move from the donor excited dye state to the receiving conduction band state in the semiconductor across the interface between them[11]. In 2023 A study presented a mathematical scenario for studying the electron current in devices with a heterogeneous structure, which depends on the reorganization energy and alignment of the energy levels of the materials in the device[12].

Induline D102 is one of the most common metal-free induline dyes used as a sensitizer in dye-sensitized solar cells due to its chemical and thermal stability, low cost, superior optical and electronic characteristics, best photoresponse, and higher extinction parameters [13,14]. The chemical compound D102 is known as 2-[(5Z)-5-(4-4-(2,2-diphenylethenyl,phenyl]-2,3,3a,8b-tetrahydro-1H-cyclopenta[b]indol-7-yl],methylidene]-4-oxo-2-sulfanylidene-1,3-thiazolidin-3-yl]acetic acid and has the forma C37H30N2O3S2 [15].

A charge transfer reaction involves an absorption of light by sensitizing D102 to become an excited dye, then a charge will be transferred to the conduction band of titanium dioxide (TiO_2) in a photochemical phenomenon, and then their transfer to its electrodes will generate an electric current[16] .The efficiency of this process depends on the alignment of the energy levels of two materials at the interfaces, the conductivity of the material, and the shape of the membrane [17]. Furthermore, dye sensitization has received greater attention due to its use in dye-enhanced solar cells applicable because of its low cost, environmental friendliness, and performance in the field of energy, as well as sustainable and renewable energy[18].

Strength coupling, energy level alignment, and dye-semiconductor contact reorganization energy are key factors describing the charge transport process in a heterojunction [19]. In addition, titanium dioxide (TiO_2) is used as a biophotonic anode due to its high absorption of photons in ultraviolet (UV) radiation, its non-toxicity, low cost, ease of use in DSSC cells, and relative higher energy conversion[20].

This paper is aiming to study and calculate the transfer rate in indoline D102 dye contacting the TiO_2 heterojunction using a quantum theory of charge transfer. The reorganization energy, strength coupling, density of state, and concentration are calculated and discussed in the D102-TiO_2 heterojunction interfaces.

2.Materials and Methods

In the charge transport reaction from the excited states in the D102 dye to the conduction band in TiO_2 in heterojunction D102/ TiO_2, as shown in the **Figure 1-a** and structure of D102 dye in **Figure 1-b** [21].

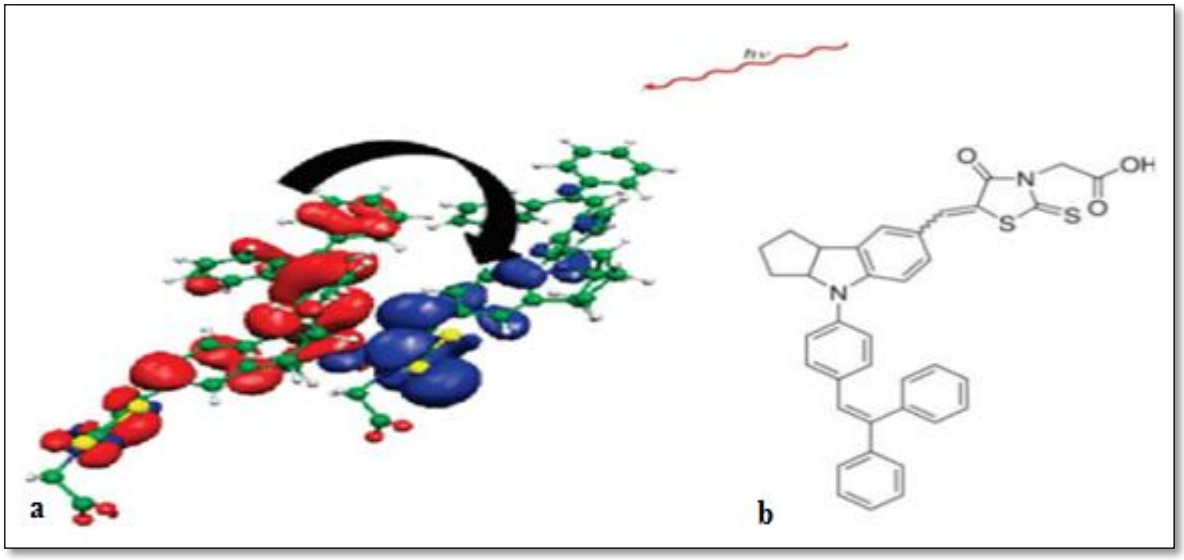

Figure 1. a) Charge transfer process from excited-D102 dye to TiO_2 , b) structure of D102 dye.

The density of state is given as a function of the effective path of charge in a semiconductor and effective density by expression [22]:

$$\delta(E_D - E_T) = (\frac{6}{\pi})^{-\frac{1}{3}} l_c D_T(E) \quad \textbf{(1)}$$

where $E_D$and E_T are donor energy (D102 dye) and acceptor energy in (TiO_2). However, total effective density $D_T(E)$ for the charge transport reaction is [23].

$$D_T(E) = \frac{D_{D102}(E)}{\rho_T^{2/3}} \langle \hat{\rho}_{\frac{D}{T}} \rangle \quad \textbf{(2)}$$

Where $D_{D102}(E)$ and $\langle \hat{\rho}_{D/T} \rangle$ defines electronic density in D102 dye and expectation of density electronic state in D102/TiO2 heterojunction, ρ_T refers to TiO_2 atomic density. Insert **Equation (2)** in **Equation (1)** results.

$$\delta(E_D - E_T) = (\frac{6}{\pi})^{-\frac{1}{3}} l_c \frac{D_{D102}(E)}{\rho_T^{2/3}} \langle \hat{\rho}_{D/T} \rangle \quad \textbf{(3)}$$

The expected electronic density in D102/ TiO_2 in the heterojunctio can be defined by relation [24].

$$\langle \hat{\rho}_{D/T} \rangle = \frac{1}{2\sqrt{\pi \Lambda_{D/T} k_B T}} e^{-\frac{(\Lambda_{D/T} + \Delta^0 U)^2}{4\Lambda_{D/T} k_B T}} \quad \textbf{(4)}$$

Where $\Lambda_{D/T}$ refers to reorganization energy, k_B and T are the Boltzman constant and temperature as well as $\Delta^0 U$ is driving energy that is given as follows [25].

$$\Delta^0 U = E_c - qE^o \quad \textbf{(5)}$$

Where E_c and qE^o are the conduction band energy of TiO_2 and the chemical potential for D102 dye. Substitute **Equation (5**) beside **Equation (4)** into **Equation (3)**, obtain.

$$\delta(E_D - E_T) = (\frac{6}{\pi})^{-\frac{1}{3}} l_c \frac{D_{D102}(E)}{\rho_T^{2/3}} \frac{1}{2\sqrt{\pi \Lambda_{D/T} k_B T}} e^{-\frac{(\Lambda_{D/T} + E_c - qE^o)^2}{4\Lambda_{D/T} k_B T}} \quad \textbf{(6)}$$

The probability transition of electrons that move from the D012 state to the conduction band in TiO2 is given by [26].

$$T_D^T(E) = \frac{4\pi^2}{h} \sum \left| \langle \hat{H}_{\frac{D}{T}}(E) \rangle \right|^2 \delta(E_D - E_T) \quad \textbf{(7)}$$

where $h(6.626 \times 10^{-34} \text{joule.seconds})$ and $\langle \hat{H}_{\frac{D}{T}}(E) \rangle$ represent Planck's constant and strength coupling. Insert **Equation (6)** in **Equation (7**) to give:

$$T_D^T(E) = \frac{2\pi^2}{h\sqrt{\pi\Lambda_{D/T}k_BT}}\sum\left|\langle\widehat{H}_{\frac{D}{T}}(E)\rangle\right|^2 \left(\frac{6}{\pi}\right)^{-\frac{1}{3}} l_c \frac{D_{D102}(E)}{\rho_T^{2/3}}\, e^{-\frac{(\Lambda_{D/T}+E_c-qE^o)^2}{4\Lambda_{D/T}k_BT}} \quad \textbf{(8)}$$

Furthermore, we can introduce the Fermi- Dirac $F_o(E)$ for the distribution of electrons in the D102/TiO2 heterojunction as a function of the conduction band E_C and electronic energy E in the system and give it by [27].

$$F_o(E) = \frac{1}{\left(e^{\frac{(E_C-E)}{k_BT}}+1\right)} \quad \textbf{(9)}$$

Insert **Equation (9)** in **Equation (8)** and integrate over energy E to product:

$$T_D^T(E) = \frac{2\pi^2}{h\sqrt{\pi\Lambda_{D/T}k_BT}} \left(\frac{6}{\pi}\right)^{-\frac{1}{3}} \int_0^E \left|\langle\widehat{H}_{\frac{D}{T}}(E)\rangle\right|^2 l_c \frac{D_{D102}(E)}{\rho_T^{2/3}}\, e^{-\frac{(\Lambda_{D/T}+E_c-qE^o)^2}{4\Lambda_{D/T}k_BT}} dE \quad \textbf{(10)}$$

The integral in **Equation (10)** can solve to the results [28].

$$\int_0^E \left|\langle\widehat{H}_{\frac{D}{T}}(E)\rangle\right|^2 l_c \frac{D_{D102}(E)}{\rho_T^{2/3}}\, e^{-\frac{(\Lambda_{D/T}+E_c-qE^o)^2}{4\Lambda_{D/T}k_BT}} dE = \frac{\left|\langle\widehat{H}_{\frac{D}{T}}(E)\rangle\right|^2 l_c}{\rho_T^{2/3}}\, e^{-\frac{(\Lambda_{D/T}+E_c-qE^o)^2}{4\Lambda_{D/T}k_BT}} [C_o] \quad \textbf{(11)}$$

Insert **Equation (11)** in **Equation (10)** to reduce.

$$T_D^T(E) = \frac{2\pi^2}{h\sqrt{\pi\Lambda_{D/T}k_BT}} \left(\frac{6}{\pi}\right)^{-\frac{1}{3}} \frac{\left|\langle\widehat{H}_D(E)\rangle\right|^2 l_c}{\rho_T^{2/3}}\, e^{-\frac{(\Lambda_{D/T}+E_c-qE^o)^2}{4\Lambda_{D/T}k_BT}} [C_o] \quad \textbf{(12)}$$

The number of states N_T in TiO_2 as function density of states σ_T and atomic density ρ_T of TiO_2 ,it calculates by [29] .

$$N_T = \sigma_T \rho_T \quad \textbf{(13)}$$

The Fermi energy E_F of TiO_2 is a function of carrier density N_e and density of states σ_T of TiO_2, gives by [29].

$$E_F = \frac{3}{2}\left(\frac{N_e}{\sigma_T}\right) \quad \textbf{(14)}$$

The atomic density ρ_T can be calculated using both **Equation (13)** and **Equation (14)**

$$\rho_T = \frac{2N_TE_F}{3N_e} \quad \textbf{(15)}$$

In contrast, the reorganization energy $\Lambda_{D/T}$of the D102/TiO_2, heterojunction as a function of the radius R of the D102 dye and distance between the D102 and TiO_2 $R_{D/T}$, it is given by[30].

$$\Lambda_{\frac{D}{T}}(eV) = \frac{e^2}{8\pi R\epsilon_\circ}\left(\frac{1}{n^2}-\frac{1}{\epsilon}\right) - \frac{e^2}{16\pi R_{D/T}\epsilon_\circ}\left(\frac{n_S^2-n^2}{n_S^2+n^2}\frac{1}{n^2} - \frac{\epsilon_S^2-\epsilon^2}{\epsilon_S^2+\epsilon^2}\frac{1}{\epsilon^2}\right) \quad \textbf{(16)}$$

Where e^2 $\epsilon_\circ$, n_S , ϵ_S , n and ϵ are the electronic charge, permittivity, refractive indices, and dielectric constants of TiO_2 and the solvent. Radii of D102 and TiO_2 can be estimated using the molecular weight MW, density ρ_m and Avogadro number N using approach [31].

$$R = \left(\frac{3}{4\pi N}\right)^{\frac{1}{3}}\left(\frac{MW}{\rho_m}\right)^{\frac{1}{3}} \quad \textbf{(17)}$$

The indoline D102 dye have MW(79.87g/mol, and density $\rho = 4.23\frac{g}{cm3}$while the TiO_2 semiconductor have MW 614.78 g/mol, density $\rho = 1.32\ \frac{g}{cm3}$ and refrective index 2.609 and dielectric constant 55 in D102/TiO_2 heterojunction with two solvents Dichloromethane (DCM) and 1-Butanol have refractive indices (1.4241 and 1.3993), and dielectric constants (8.93 and 17.51) respectivelly . TiO_2 have $N_T(1.4\times10^{14}\frac{electron}{cm^3})$, Fermi energy $E_F(4.52eV)$, and N_e $(8\frac{state}{eV})$ for TiO_2,with $l_c = 3$ Å [32-39].

3. Results

A mathematical calculation of probability transition $T_D^T(E)$of charge transfer was presented for electron transition across interface from excited donor the D012 state to an acceptor in the conduction band for TiO_2 using **Equation (12)**.

Transition $T_D^T(E)$ is strongly affected by the force coupling, reorganization energy, driving energy, chemical potential of the D102 dye, and concentration carrier. Calculating the reorganization energy is one of the important criteria for determining the probability of charge transfer in a d102/TiO_2 junction. The presented calculation of reorganization energy under assumed continuum energy levels for both the D102 dye and TiO_2 using the D102/TiO2 device with Dichloromethane (DCM) and 1-Butanol solvents, respectively.

Due to the spherical approach, the radii of the TiO_2 semiconductor indoline and D102 dye in the D102/TiO_2 hetrojunction can be evaluated using **Equation (17)** with the inserted molecular weight MW(79.87g/mol, and 614.78 g/mol), and density $\rho = 4.23\frac{\text{g}}{\text{cm3}}$, $\rho = 1.32\ \frac{\text{g}}{\text{cm3}}$, for TiO_2 and D102, respectively, and takes the Avogadro number (6.02×10^{23} molecule /mol), the results give 1.956 A^0 and 5.694 A^0 for TiO_2 and D102. Due to the continuum model, the reorganization energy $\Lambda_{\frac{D}{T}}(eV)$ of charge transition produces in D102/TiO_2 device Presented using **Equation (16).**

The D102/TiO2 reorganization energy represents to the energy required to reorganize the surrounding medium, including the solvent and the D102 dye, when a charge is transferred from the D102 dye molecule to the TiO2 titanium dioxide upon absorption of a photon. The reorganization energy $\Lambda_{\frac{D}{T}}(eV)$ has been the main parameter used to limit and study the probability of charge transition $T_D^T(E)$ as a function of the polarity of solvents and materials according to the use of dielectric and refractive indices of DCM and Butanol solvents, TiO_2, and the radius of D102 and distance between D102 and TiO_2 using **Equation (16)** and taking into account the radii (5.694 $A^0$and 1.956 A^0) for D102 and TiO_2, the refractive indices (1.4241, 1.3993 and 2.609), and dielectric constants (8.93, 17.51 and 55) for Dichloromethane (DCM) and 1-Butanol solvents and TiO_2.

The reorganization energy calculation taken **Equation (16)** results in 0.362 eV, and 0.442eV for D102/TiO_2 with DCM and Butanol, respectively.

However, the density ρ_T can be categorized as interstructure in TiO_2, with the former exerting a more significant impact on the charge transport process.

It estimates using **Equation (14)** by taking $N_T(1.4 \times 10^{14}\frac{electron}{cm^3})$, Fermi energy $E_F(4.52eV)$, and N_e $(8\frac{state}{eV})$ for TiO_2, to get the results $4.17 \times 10^{24}\frac{1}{cm^3}$. The ρ_T density can be described as the quantity of electron transport associated with the change in the structure and energy levels of the involved in the electron transfer process.

The probability transition of electrons $T_D^T(E)$ from the D012 dye to the TiO_2 semiconductor in a heterojunction with DCM and Butanol solvents has been calculated using **Equation (12)** using the reorganization energies (0.362 eV and 0.442eV) with a coupling strength ranging from $\widehat{H}_{\frac{D}{T}}(E)$ ranging $0.387 \times 10^{-3}eV \leq \widehat{H}_{\frac{D}{T}}(E) \leq 1.244 \times 10^{-3}$eV and taking into account TiO_2 $l_c = 3$ Å [39], $\rho_T(4.17 \times 10^{24}\frac{1}{cm^3})$ and concentration $[C_o]$ from $2\times 10^{30}\ \frac{1}{cm^3}$ to $7 \times 10^{30}\ \frac{1}{cm^3}$.

The transition $T_D^T(E)$ results using MATLAB software list in **Table 1** and **Figure 2** for D102-TiO_2 with a DCM solvent and **Table 2** and **Figure 3** for D102-TiO_2 with a Butanol solvent.

Table 1. Results of probability transition $T_D^T(\frac{1}{s})$ calculation using Dichloromethane(DCM) solvent.

$\langle \widehat{H}_{\frac{D}{T}} \rangle x10^{-3}$ eV/ state	$[C] \times 10^{24} \frac{1}{m^3}$					
	2	3	4	5	6	7
0.387	1.556E+12	2.333E+12	3.111E+12	3.889E+12	4.667E+12	5.444E+12
0.500	2.010E+12	3.015E+12	4.019E+12	5.024E+12	6.029E+12	7.034E+12
0.591	2.376E+12	3.563E+12	4.751E+12	5.939E+12	7.127E+12	8.314E+12
0.670	2.693E+12	4.040E+12	5.386E+12	6.733E+12	8.079E+12	9.426E+12
0.741	2.978E+12	4.468E+12	5.957E+12	7.446E+12	8.935E+12	1.042E+13
0.806	3.240E+12	4.860E+12	6.479E+12	8.099E+12	9.719E+12	1.134E+13
0.866	3.481E+12	5.221E+12	6.962E+12	8.702E+12	1.044E+13	1.218E+13
0.921	3.702E+12	5.553E+12	7.404E+12	9.255E+12	1.111E+13	1.296E+13
0.974	3.915E+12	5.872E+12	7.830E+12	9.787E+12	1.174E+13	1.370E+13
1.024	4.116E+12	6.174E+12	8.232E+12	1.029E+13	1.235E+13	1.441E+13
1.072	4.309E+12	6.463E+12	8.618E+12	1.077E+13	1.293E+13	1.508E+13
1.118	4.494E+12	6.741E+12	8.988E+12	1.123E+13	1.348E+13	1.573E+13
1.161	4.667E+12	7.000E+12	9.333E+12	1.167E+13	1.400E+13	1.633E+13
1.204	4.839E+12	7.259E+12	9.679E+12	1.210E+13	1.452E+13	1.694E+13
1.244	5.000E+12	7.500E+12	1.000E+13	1.250E+13	1.500E+13	1.750E+13

Table 2. Results of probability transition $T_D^T(\frac{1}{s})$ calculation using Butanol solvent.

$\langle \widehat{H}_{\frac{D}{T}} \rangle x10^{-3}$ eV/state	$[C] \times 10^{24} \frac{1}{m^3}$					
	2	**3**	**4**	**5**	**6**	**7**
0.387	1.970E+13	2.955E+13	3.940E+13	4.925E+13	5.910E+13	6.895E+13
0.500	2.545E+13	3.818E+13	5.091E+13	6.363E+13	7.636E+13	8.909E+13
0.591	3.009E+13	4.513E+13	6.017E+13	7.521E+13	9.026E+13	1.053E+14
0.670	3.411E+13	5.116E+13	6.821E+13	8.527E+13	1.023E+14	1.194E+14
0.741	3.772E+13	5.658E+13	7.544E+13	9.430E+13	1.132E+14	1.320E+14
0.806	4.103E+13	6.155E+13	8.206E+13	1.026E+14	1.231E+14	1.436E+14
0.866	4.408E+13	6.613E+13	8.817E+13	1.102E+14	1.323E+14	1.543E+14
0.921	4.688E+13	7.033E+13	9.377E+13	1.172E+14	1.407E+14	1.641E+14
0.974	4.958E+13	7.437E+13	9.917E+13	1.240E+14	1.487E+14	1.735E+14
1.024	5.213E+13	7.819E+13	1.043E+14	1.303E+14	1.564E+14	1.824E+14
1.072	5.457E+13	8.186E+13	1.091E+14	1.364E+14	1.637E+14	1.910E+14
1.118	5.691E+13	8.537E+13	1.138E+14	1.423E+14	1.707E+14	1.992E+14
1.161	5.910E+13	8.865E+13	1.182E+14	1.478E+14	1.773E+14	2.069E+14
1.204	6.129E+13	9.194E+13	1.226E+14	1.532E+14	1.839E+14	2.145E+14
1.244	6.333E+13	9.499E+13	1.267E+14	1.583E+14	1.900E+14	2.216E+14

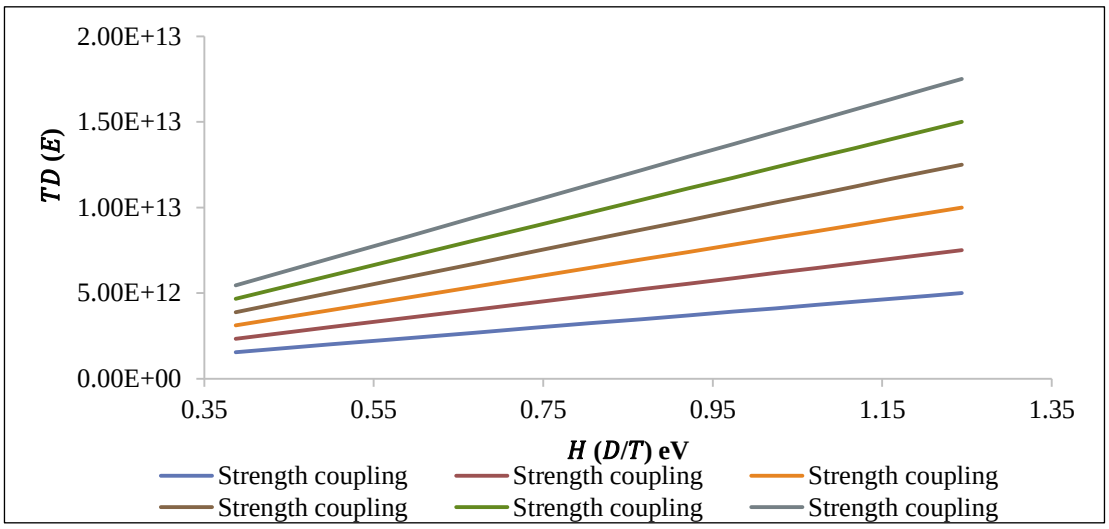

Figure 2. The probability transition $T_D^T(E)$ in unit $(\frac{1}{s})$ with for D102/TiO2 with DCMsolvent

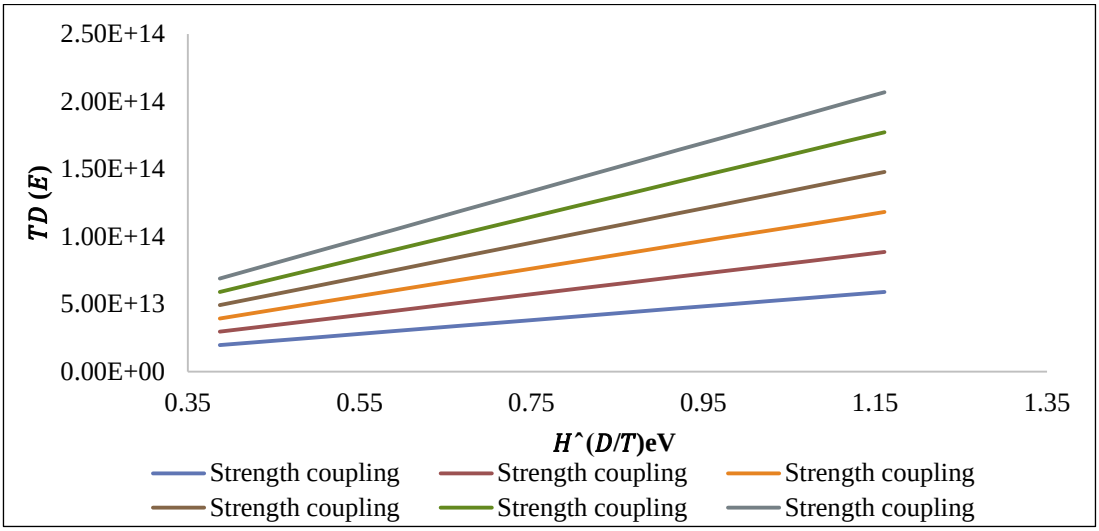

Figure 3. The probability transition $T_D^T(E)$ in unit $(\frac{1}{s})$ with for D102/TiO2 with Butanol solvent

4. Discussion

To study the charge transport behavior in the D105/TiO_2 heterojunction device, the charge transport rate was calculated and examined for D105/TiO_2 using two solvents, DCM and butanol. The probability of transfer can be obtained using a quantitative model of the donor-receiver model, from which the relevant transfer coefficients were extracted. In the D105/TiO_2 heterojunction device, the charge transfer rate from excited D102 dye to the conduction band in the TiO_2 photoanode has been calculated using two Dichloromethane (DCM) and Betanol solvents. Reorganization energy is an effective tool for measuring the levels of reorganization energy and maintaining charge neutrality at the interface. It is related to charge transfer in a heterojunction device.

A low reorganization energy indicates less efficient charge separation and a lower probability transition, as it allows a small fraction of the transition electron transfer to contribute and vice versa. It is important to note that the reorganization energy was affected by the polarity of the solvents, which must be taken into account when evaluating the transfer of electrons from D102 molecules to the TiO_2 conduction band, ultimately leading to an improvement in the overall performance of the charge transfer process in the heterojunction device.

Reorganization energy can be interpreted as a reorientation process to adjust the energy level configuration in both D102 and TiO_2 conduction bands prior to the electron transfer process taking place. The estimated theoretical reorganization energy depends heavily on the refractive index and dielectric constant for the solvent. Specifically, reorganization energy shows that it increases with increasing dielectric strength and decreases with increasing refractive index. High rearrangement energy typically facilitates the transfer of more electrons from the D102 dye to unoccupied TiO_2 states.

The current rearrangement energy values for the studied D102/ TiO_2 systems indicate that the lowest rearrangement energies were obtained using dichloromethane (DCM) (0.362 eV) for D102/TiO_2 and 0.442 eV when using 1-butanol solvents with D102/TiO_2. In contrast, the highest transition coefficient was found with 1-butanol0.442 eV for the D102/TiO_2 system. The lower electron transfer rate from D102 to TiO_2 using DCM solvents, compared to D102 to TiO_2 using butanol solvents, is attributed to the lower rearrangement energy associated with poor energy level alignment in the D102/TiO_2 system, as shown in Tables (1) and (2). The best electronic transfer performance was occurring with the butanol solvent, due to improved alignment between the energy levels of D102 and the conduction band of TiO_2.

The potential coefficient was calculated as a function of the TiO_2 band gap (3.03 eV) [40] and the electrochemical potential E^o=-3.64-(-6.01)=-2.37eVeV) of the D102 dye, and it increases with decreasing electrochemical potential of the dye and increasing band gap energy. However, the electron transfer rate in DCM solvent was much lower than in butanol solvents under strong coupling. The results show that transition rate increases with increases in strength coupling as well as concentration. Understanding the effect of force coupling on transfer rate coefficients requires considering both the readjustment energy and the potential. The potential and readjustment energy determine how well the solvent is suited to efficiently transferring charge.

The result indicates that the transfer rate is limited by the coupling strength and the concentration at the D102/ TiO_2, interface. The transfer rate approaches its maximum when the concentration is a mixture of $7 \times 10^{24} \frac{1}{m^3}$, which also corresponds to an increase in the number of transferable electrons.

The charge transition was increased with increased strength coupling and vice versa. This indicates that the strong bond between the D102 dye and titanium dioxide (TiO2), or the high degree of reactivity, leads to more efficient charge transfer because the systems involved are energetically compatible. In the case of D102/TiO_2, it is important to show that the transition of electrons shows essentially a maximum charge transport occurs, with maximum strength coupling. The effect of strength coupling on transition rate can never be neglected; increasing the strength coupling can enhance the transition in D102/ TiO_2system, with a maximum reached at a coupling strength of $1.24\times 10^{-3} \frac{eV}{state}$.

As shown in result, the transition rate increases by more than twelve with increasing strength coupling. In general, the maximum transfer rate is achieved when the highest value of rearrangement energy, power coupling, and concentration is reached, as in butanol, where the transfer of electrons between the dye D102 and the titanium dioxide (TiO_2) conduction band is energy-favorable.

5. Conclusion

The probability of charge transport characteristics for the D102 junction with TiO_2 in the D102/TiO_2 heterojunction device was investigated using quantum transport theory. The D102/TiO_2 system was studied in DCM and butanol solvents at various concentrations ranging from $2 \times 10^{30} \frac{1}{cm^3}$to $7 \times 10^{30} \frac{1}{cm^3}$ and at varying coupling strengths ranging from $0.387\times 10^{-3} \frac{eV}{state}$ to $1.244 \times 10^{-3} \frac{eV}{state}$ to explore its effect on the electronic response behavior.

The results of the transition rate indicated that butanol with D102/TiO_2 had a stronger effect on electron transport processes compared to the DCM solvent. This enhancement is attributed to butanol's modification of the redistribution energy, which affected electronic density, barrier, and driving energy coefficients.

Charge transfer rate in the D102/TiO_2 device depends significantly on the reorganization energy, strength coupling, and concentration. Increasing coupling strength, along with the concentration and reorganization energy, enhances the electron transport at the interface, thus improving the electron transport characteristics of the D102/TiO_2 device. In general, the transition rate and value of the reorganization energy in the D102/TiO_2 with DCM solvent are lower than those in the D102/TiO_2 with butanol solvent (~12%) at similar coupling strengths and concentrations, as reflected in the observed charge transfer in the D102/TiO_2.

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Conflict of Interest

The author declares no conflicts of interest.

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Ethical Clearance

As a theoretical study with no human or animal subjects, ethical approval was unnecessary.

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