

# Charge Transfer from Indoline Dye Contact to Zinc Selenide: Analytical Study

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## ABSTRACT

In this research paper, we study the processes of charge transfer from the Indoline dye to zinc selenide (ZnSe) are carried out by chemical solvents through using a simple model of quantum which is concerned with the behaviour of electrons transfer. Different solvents such as Chloroform, Methyl Acetate, Butanol, Methanol Ethyl Ketene and Ethanol are commonly used to discuss the system's rate of charge transfer. It is a matter of fact that the rate of charge transfer can be various due to the increased sufficient orientation energy. Besides, this paper will show that the rate of the charge transfer is high when the orientation energy is low and the process of transfer interaction from Indoline dye to a ZnSe become active with ethanol solvent which has low orientation energy. Hence, this work proposes a theoretical scenario to calculate the rate of the charge transfer in sensitization of Indoline dye in contact with ZnSe semiconductor. In addition, the results indicate that the rate of the charge transfer decreases with the increase in its potential in which it is expected that the motivation has more experimentally worked pointing to the realization of Indoline dye-based dye cell.

**Keywords:** Charge Transfer, Indoline Dye, Zinc selenide.

## Introduction

The interaction of charge transition occurs between two electronic state donors and acceptors as there are the fundamental processes of optoelectronic and solar cell devices [1]. The solar cells become essential elements of the variety entirely of solving that will be eventually a clean energy resource and they would replace the fossil fuels resource [2]. In recent years, the critical challenges of energised scenarios have led to considerable energy. One of the most assisted researches in solving global energy problems is nanoscience and nanotechnology in addition to the discovery of more sources of energies [3]. The dye cell (DS) was a type of photo-induced electrochemical cell, which was more attractive attention in resulting in wide-ranging operative advantage low-cost materials, printable, flexible usage and accessible manufacturing technology [4]. Hadi et al were studying the charge transfer in heterostructure materials by depending on orientation energy under the alignment energy levels for materials in system devices. Electrons' ability to transfer from one material to another requires the closed alignment of energy levels stated in both materials [5]. The process of charge transfer in heterostructure materials transfers from energy state in donor to energy state in acceptor for contact donor and acceptor to each other [6]. A molecule's energy states are unoccupied and occupied orbitals, respectively. The molecule orbital energies will be changed relative to the solid's surface [7]. However, the molecule/semiconductor interface devices are active field research in applied technological devices due to electronic transition processes through materials' interfaces. Furthermore, the devices of DSs have been dominated photosensitise through using inorganic contact with solid materials. It is realised that the photo induced electron transition reaction is separated by dye molecule as light-absorbing material with semiconductors which has a wide bandgap [8]. The processes of charge transfer have main processes in the molecule/semiconductor photovoltaic system; in other words, the electrons will transition gradually from the initial donor electronic energy state to the final acceptor electronic state of the semiconductor [9]. Recently, the increased power conversion efficiency with more than 15%, is achieved and coupled with the ability to grow on a more extensive scaling with a low cost while solar cell makes a crucial case for energy applications [10]. Moreover, the process has an essential aspect in utilizing sensitised dyes that have broad absorbed spectra to absorb more photons of light to be more efficient energies in electric conversion [11]. Additionally, the indoline dye is the organic attractive sensitised dye used in the solar cell. The pure organic indoline dye is a more efficient complex and its 9% efficiency and excitation lifetimes by depending on the concentration of solvent [12]. It is notable to mention that its chemical formula is (C<sub>42</sub>H<sub>35</sub>N<sub>3</sub>O<sub>4</sub>S<sub>3</sub>). Its chemical structure is illustrated in Figure (1).

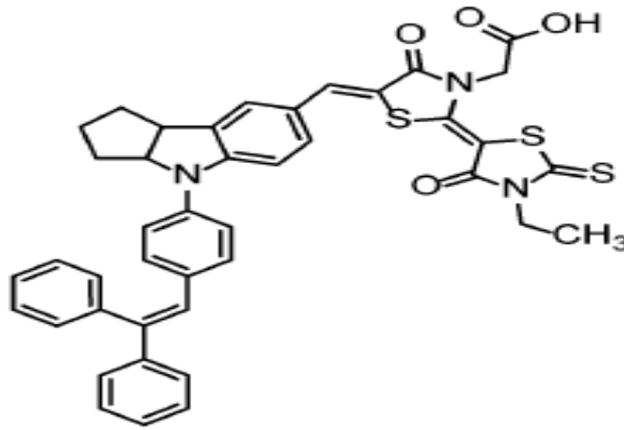


Figure (1): The chemical structure of indoline dye [13].

The ZnSe is so significant semiconductor that it is used in technical optoelectronic. It can be also used in photovoltaic cells. It is a significant technological material because of its potential applications in different electronic and optical devices and as a buffer material it is used in heterojunction solar cells[14]. Zinc selenide can be defined as a single crystal that is used in different devices, including; thin film, bioimaging, laser resonators and photovoltaics [15]. However, ZnSe semiconductor has photocatalytic activity since it has a suitable band energy material ( 2.67 eV) [16]. The paper also will study and analyse the processes of the mechanism of charge transfers in heterostructure indoline dye in contact with zinc selenide devices by using a simple quantum scenario. The scenario of charge transfers is illustrated in figure (2). The absorption photons sensitise dye to interfacial electronic transition from the electronically excited state of dyes to the conduction band of semiconductor (CB) within a few hundred femtoseconds.

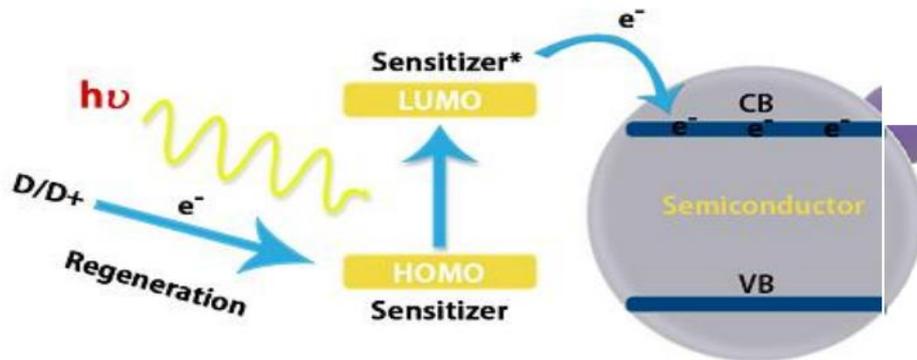


Figure (2): Illustrated of energy levels in D149/ZnSe devices[17].

**Theoretical Scenario**

The rate of the charge transfer in range energy is E and E + dE in the transition process from donor to an acceptor[18]:

$$\beta_{ET} = \frac{2\pi}{\hbar} \sum_{S=1, D=1}^{\infty} F(E) |\langle K_{SD}(\epsilon) \rangle|^2 \rho_{SD} \delta(E_S - E_D) dE \dots \dots \dots (1)$$

When  $F(E)$  is the Fermi occupation function,  $|\langle K_{SD}(\epsilon) \rangle|$  is a coupling constant,  $E_S$  and  $E_D$  are the electronic energies in the initial and final state. Moreover, the density of states  $\rho_{SD}$  for system is given by expectation value[19]:

$$\langle \rho_{SD} \rangle = \sqrt{\frac{1}{4\pi\Lambda_{SD}k_B T}} e^{\frac{-(\Lambda_{SD}+G^0)^2}{4\Lambda_{SD}k_B T}} \dots \dots \dots (2)$$

When  $\Lambda_{SD}$  is the orientation energy,  $G^0$  is the driving energy force and T is the room temperature. The orientation energy  $\Lambda_{SD}$  of system is [20]:

$$\Lambda_{SD}(eV) = \frac{e^2}{8\pi\epsilon_0} \left[ \frac{1}{D} \left( \frac{1}{n^2} - \frac{1}{\epsilon_{s0}} \right) - \frac{1}{2R} \left( \frac{n_S^2 - n^2}{n_S^2 + n^2} \frac{1}{n^2} - \frac{\epsilon_S^2 - \epsilon_{s0}^2}{\epsilon_S^2 + \epsilon_{s0}^2} \frac{1}{\epsilon_{s0}^2} \right) \right] \dots \dots \dots (3)$$

When  $e$  and  $\epsilon_0$  are the charges of electron and vacuum permittivity, D and R are the radius of dye and the distance from dye to

semiconductor,  $n$  and  $\epsilon_{so}$  are refractive index and dielectric constant of solvents,  $n_s$  and  $\epsilon_{so}$  are refractive index and dielectric constant of semiconductor. The radius of the dye  $D(nm)$  is given by approach formula function of molecular weight  $M$  and mass density  $\rho$  [21]:

$$D(nm) = \left(\frac{3}{4\pi} \frac{M}{N\rho}\right)^{\frac{1}{3}} \dots \dots \dots (4)$$

When  $N$  is Avogadro number, the Eq. (2) should be inserted in Eq. (1) to obtain:

$$\beta_{ET} = \frac{2\pi}{\hbar} \sum_{S=1, D=1}^{\infty} F(E) |\langle K_{SD}(\epsilon) \rangle|^2 \sqrt{\frac{1}{4\pi\Lambda_{SD}k_B T}} e^{-\frac{(\Lambda_{SD}+G^0)^2}{4\Lambda_{SD}k_B T}} \delta(E_S - E_D) \dots \dots \dots (5)$$

The activation density for dye-semiconductor system  $\rho_a(E)$  is [21][22].

$$\rho_a(E) = \delta(E_S - E_D) = \rho_S \frac{l_c}{\rho_m^{2/3} \left(\frac{\epsilon}{\pi}\right)^{1/3}} \dots \dots \dots (6)$$

When  $\rho_S$  : the density of electrons in the semiconductor,  $l_c$  is the coupling length and  $\rho_m$  is the atomic density of semiconductor. Inserting Eq.(6) in Eq.(5) to results:

$$\beta_{ET} = \frac{2\pi}{\hbar} \sum_{S=1, D=1}^{\infty} F(E) |\langle K_{SD}(\epsilon) \rangle|^2 \sqrt{\frac{1}{4\pi\Lambda_{SD}k_B T}} e^{-\frac{(\Lambda_{SD}+G^0)^2}{4\Lambda_{SD}k_B T}} \rho_S \frac{l_c}{\rho_m^{2/3} \left(\frac{\epsilon}{\pi}\right)^{1/3}} \dots \dots \dots (7)$$

The charge transfer rate was decay due to distance by  $C$  and given by [23].

$$\beta_{et} = \frac{\beta_{ET}}{c} \dots \dots \dots (8)$$

Inserting Eq. (7) in Eq. (8) and are integrated to obtain:

$$\beta_{et} = \frac{2\pi}{\hbar} \frac{1}{c} \sqrt{\frac{1}{4\pi\Lambda_{SD}k_B T}} \frac{l_c}{\rho_m^{2/3} \left(\frac{\epsilon}{\pi}\right)^{1/3}} \int |\langle K_{SD}(\epsilon) \rangle|^2 e^{-\frac{(\Lambda_{SD}+G^0)^2}{4\Lambda_{SD}k_B T}} \rho_S(E) F(E) dE \dots \dots (9)$$

The driving force energy of electrons is:

$$G^0 = E_c - E^o \dots \dots \dots (10)$$

Where  $E_c$ , the conduction is a band of semiconductor and  $E^o$  is the potential of the dye. The potential of contact materials in system is given:

$$U_C(E) = \frac{(\Lambda_{SD}+(E_c-E^o))^2}{4\Lambda_{SD}} \dots \dots \dots (11)$$

Inserting Eq. (11) in Eq. (9) and remove out the coupling and exponential to get the results:

$$\beta_{et} = \frac{2\pi}{\hbar} \frac{1}{c} \sqrt{\frac{1}{4\pi\Lambda_{SD}k_B T}} \frac{l_c}{\rho_m^{2/3} \left(\frac{\epsilon}{\pi}\right)^{1/3}} |\langle K_{SD}(\epsilon) \rangle|^2 e^{-\frac{(\Lambda_{SD}+G^0)^2}{4\Lambda_{SD}k_B T}} \int \rho_S(E) F(E) dE \dots \dots (12)$$

The solution integral in Eq.(10) reduce to concentration of electrons  $N(E)$  [24]:

$$\int \rho_S(E) F(E) dE = N(E) \dots \dots \dots (13)$$

The charge transfer in Eq. (13) with Eq.(12) is given as:

$$\beta_{et} = \frac{2\pi}{\hbar} \frac{N(E)}{c} \sqrt{\frac{1}{4\pi\Lambda_{SD}k_B T}} \frac{l_c}{\rho_m^{2/3} \left(\frac{\epsilon}{\pi}\right)^{1/3}} |\langle K_{SD}(\epsilon) \rangle|^2 e^{-\frac{(\Lambda_{SD}+G^0)^2}{4\Lambda_{SD}k_B T}} \dots \dots \dots (14)$$

However, the activation energy at the contact for two materials can be estimated theoretically through using [25]:

$$G_C(E) = \frac{hc}{\lambda} - \Lambda_{SD} \dots \dots \dots (15)$$

When  $c$  and  $\lambda$  are the velocity of light and wave length of absorption spectrum of dye.

## Results

Depending on simple quantum scenario, the rate of the charge transfer in indoline dye which is contacted with ZnSe devices is influenced by orientation energy. Its function both polarity radii and contact distance from dye to ZnSe. The radii of indoline dye and ZnSe is calculated by using Eq.(4) with molecular weight ( $M=0.741 \frac{kg}{m^3}$  and  $M=0.144 \frac{kg}{m^3}$ ) and mass density[26] ( $\rho = 0.214 \frac{kg}{m^3}$  and  $\rho = 0.542 \frac{kg}{m^3}$ ) for indoline dye and ZnSe respectively, the results would be  $D_m=5.16 \text{ \AA}$  and  $2.193 \text{ \AA}$  for indoline dye and ZnSe. The orientation energy is calculated by using Eq.(3) and MATLAB program through using the radii of indoline dye and ZnSe, refractive and dielectric constant of solvents as it is shown in Table (2) with dielectric and refractive index of ZnSe semiconductor results are also shown in table (2).

**Table1: Properties of ZnSe semiconductor[27].**

Molecular weight g/mol	144.35
Dielectric Constant	9.2
Mass density (g/cm <sup>3</sup> )	5.42 g/cm <sup>3</sup>
Crystal structure	Cubic
Refractive index	2.89
Lattice constant(Å)	5.6676 Å
Radius calculated(Å)	2.193778
Energy gab eV	2.58 eV
Group	Zinc – 12 and Selenium - 16
Refractive index	2.5688
Electron concentration (1/cm <sup>3</sup> )	2×10 <sup>20</sup> cm <sup>-3</sup>
Electron affinity (eV)	4.2

Table 2: The calculation of the orientation energy  $\Lambda_{SD}$ (eV) of indoline dye in contact with ZnSe.

Solvent	refractive index (n) at 20 C	static dielectric constant (ε) at 20 C	The orientation energy $\Lambda_{SD}$
Chloroform	1.446	4.81	0.248946
Methyl Acetate	1.3593	7.3	0.397170
Butanol	1.397	17.51	0.478561
Methanol Ethyl Ketene	1.3788	18.8	0.496887
Ethanol	1.359	23.40	0.526165

In contrast to the activation energy which can be estimated by using Eq.(15) the results of orientation energy in table (2) with absorption energy by spectrum in ref.[28] the results are shown in Table (3 ).

As can be seen, the potential of system can be calculated through using Eq. (11) with taking values of electrochemical potential (3.5, 3.3,3.1,2.9,2.7,2.5 and 2.3) eV. The results are shown in table (4).

The rate of the charge transfer  $\beta_{et}$  in indoline dye to ZnSe semiconductor with (Chloroform, Methyl Acetate, Butanol, Methanol Ethyl Ketene and Ethanol) solvents are evaluated by using Eq.(14) with taking the results of orientation energy in the table (2), in which coupling constant  $\langle K_{SD}(\epsilon) \rangle = 2, 4, 6, 8, 10, 12$  and  $14 \times [10]^{-3}$  eV, length coupling  $l_c = 3 \text{Å}$  [19] the driving force energy 0.99., 1.19 eV, atomic density is 0.29 for ZnSe and electron concentration NSe (E) in the table(1) by using MATLAB program. Results have been listed in Table (5) and table (6) for indoline dye in contact to ZnSe devices.

**Table 3: Results of activation energy  $G_c$ (eV) of indoline dye in contact to ZnSe system.**

V λ nm	Absorption energy	Solvent				
		chloroform	Methyl Acetate	Butanol	Methanol Ethyl Ketene	Ethanol
300	4.133	3.851177	3.701177	3.620293	3.601604	3.571925
350	3.542	220.50	3.110177	3.029293	3.010604	2.980925

400	3.099	269.56	2.667177	2.586293	2.567604	2.537925
450	2.755	318.56	2.3231770	2.242293	2.223604	2.193925
500	2.479	367.56	2.047177	1.966293	1.947604	1.917925
550	2.254	416.56	1.822177	1.741293	1.722604	1.692925
600	2.066	1.784177	1.634177	1.553293	1.534604	1.504925
650	1.907	1.625177	1.475177	1.394293	1.375604	1.345925
700	1.771	1.489177	1.339177	1.258293	1.239604	1.209925
750	1.653	1.371177	1.221177	1.140293	1.121604	1.091925
800	1.549	1.267177	1.117177	1.036293	1.017604	0.987925

**Table 4: Results of potential energy  $U_C$  (eV) of indoline dye in contact to ZnSe system along with  $E_{CB} = 3.66$  eV**

Solvent	$\Lambda_{SD}$ (eV)	The driving force energy $G^0$ (eV)						
		3.8	3.6	3.4	3.2	3	2.8	2.6
chloroform	0.248	0.003143	0.081946	0.266733	0.557504	0.954259	1.456998	2.06572
Methyl Acetate	0.397	0.019416	0.105627	0.260781	0.484876	0.777914	1.139893	1.570815
Butanol	0.478	0.030824	0.119289	0.265429	0.469242	0.73073	1.049891	1.426727
Methanol Ethyl Ketene	0.496	0.033468	0.122336	0.266864	0.467051	0.722898	1.034405	1.401571
Ethanol	0.526	0.037775	0.127233	0.2694	0.464275	0.711859	1.012152	1.365153

**Table 5: The charge transfer rate of indoline dye in contact to ZnSe at driving energy = 0.99eV.**

Solvent	$\Lambda_{SD}$ (eV)	The driving force energy $G^0$ (eV)						
		$2 \times 10^{-3}$	$4 \times 10^{-3}$	$6 \times 10^{-3}$	$8 \times 10^{-3}$	$10 \times 10^{-3}$	$12 \times 10^{-3}$	$14 \times 10^{-3}$
chloroform	0.248946	1.4277E-10	2.8553E-10	4.2830E-10	5.7106E-10	7.1383E-10	8.5659E-10	9.9936E-10
Methyl Acetate	0.397170	6.1727E-05	1.2345E-04	1.8518E-04	2.4691E-04	3.0863E-04	3.7036E-04	4.3209E-04
Butanol	0.478561	1.6566E-03	3.3133E-03	4.9699E-03	6.6265E-03	8.2831E-03	9.9398E-03	1.1596E-02
Methanol Ethyl K.	0.496887	2.8808E-03	5.7617E-03	8.6425E-03	1.1523E-02	1.4404E-02	1.7285E-02	2.0166E-02
Ethanol	0.526165	6.2604E-03	1.2521E-02	1.8781E-02	2.5042E-02	3.1302E-02	3.7562E-02	4.3823E-02

**Table 6: The charge transfer rate of indoline dye in contact to ZnSe at driving energy = 1.19eV.**

Solvent		The charge transfer rate $\beta_{et}(\frac{1}{\text{Sec}})$						
		$\langle K_{SD}(\epsilon) \rangle \text{eV/ state}$						
$\Lambda_{SD}(\text{eV})$		$2 \times 10^{-3}$	$4 \times 10^{-3}$	$6 \times 10^{-3}$	$8 \times 10^{-3}$	$10 \times 10^{-3}$	$12 \times 10^{-3}$	$14 \times 10^{-3}$
chloroform	0.248946	6.4758E-20	1.2952E-19	1.9427E-19	2.5903E-19	3.2379E-19	3.8855E-19	4.5330E-19
Methyl Acetate	0.397170	1.9309E-11	3.8617E-11	5.7926E-11	7.7235E-11	9.6544E-11	1.1585E-10	1.3516E-10
Butanol	0.478561	3.3523E-09	6.7046E-09	1.0057E-08	1.3409E-08	1.6761E-08	2.0114E-08	2.3466E-08
Methanol Ethyl K.	0.496887	8.1576E-09	1.6315E-08	2.4473E-08	3.2630E-08	4.0788E-08	4.8946E-08	5.7103E-08
Ethanol	0.526165	2.8887E-08	5.7773E-08	8.6660E-08	1.1555E-07	1.4443E-07	1.7332E-07	2.0221E-07

### Discussion

The rate of the charge transfer in Eq. (14) is related to orientation energy and it is influenced by the polarity of solvents media of the indoline dye in contact with the ZnSe cell. The orientation energy in the table (2) increases with the increase of the dielectric constant of solvents because of the increased polarity of the system. It is seen that orientation energy increases alternatively with the increased dielectric constant from 4.81, 7.3, 17.51, 18.8 and 23.40 in Table (2). The orientation energy increases from 0.248946, 0.397170, 0.478561, 0.496887 and 0.526165eV for chloroform, Methyl Acetate, Butanol, Methanol Ethyl Ketene and Ethanol respectively. It is the indoline dye exactly matched with the ZnSe semiconductor. More importantly, the increased orientation energy means that the system takes more energy to reorientation system in order to begin transferring the charge from excited energy levels of indoline dye to the conduction band in the ZnSe semiconductor. In fact, the optical properties limit the orientation energy due to refractive index with dielectric constant and charge transfer rate increase when the orientation energy decreases in the entire system as it is shown in both Tables (5) and (6). Furthermore, the orientation energy increases with decreasing reflective index and increasing the dielectric constant of solvents.

In turn, the activation energy  $G_C$  (eV) for indoline dye in contact with the ZnSe system increases with decreasing the orientation energy and wavelength of the absorption spectrum of indoline dye. It will be increased by decreasing the orientation energy parameters for each solvent media. On the other hand, the potential energy  $U_C$  (eV) in table (4) increase with decreasing the driving force energy  $G^0$  (eV) from 3.8 eV to 2.6 eV. Increasing the orientation energy effects on potential forcefully. It increases potential with the increase of the orientation energy and vice versa. The increased potential at the interface and the decrease of charge transfer and lower photocurrents. However, the charge transfer for indoline dye in contact to ZnSe system is high with Ethanol solvent and low with chloroform solvent and this aspect refers to the charge transfer rate for indoline dye in contact to ZnSe system with Ethanol as well as the larger comparison between other solvents. Since similarity in the behaviour of charge transfer density of indoline dye contact to ZnSe with solvents states and it is indicated when increasing the orientation energy the result is that the rate of the charge transfer is decreased. Tables (5) and (6) show the charge transfer rate in the system is decreased with the increase of the driving energy force. The charge transfer rate is summarised in Table (5) and table (6). As expected, the increase of the orientation energy has been achieved by the increase of polarity for the system and decreasing the charge transfer rate and increasing the potential. Table (6) of the charge transfer rate indicates the decrease and increase of the driving energy compared to the results in a table (5)

However, the charge transfer can be found in both tables (5) and (6) and it can be increased with increasing of the coupling strength largely. It is noteworthy to mention that the charge transfer is very suitable with ethanol solvents and this indicates that ethanol is a significant media solvent for the system.

### Conclusions

It has been concluded that due to the charge transfer rate in indoline dye in contact with the ZnSe device, the orientation energy largely influences the activation energy, potential and charge transfer rate for the indoline dye in contact with the ZnSe device interface. The increase of the orientation energy limits the charge transfer rate crosses the indoline dye in contact with the ZnSe device and it affects all characteristics of cell through the activation of energy and potential. The solvent media influences forcefully to charge transfer rate of cell devices by depending on the effect of the transfer parameters. The rate of the charge transfer performs when changing orientation energy with solvents, so that the activation energy, driving force and potential are evaluated theoretically. For increased transition, the potential energy increases and the charge transfer rate decreases. It is seen that the rate of the charge transfer decreases and potential increases with the increase of orientation energy and the driving force energy.

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