Theoretical Study of the Electronic Transition Rate Production in Alq$_3$ molecule With Au Metal Interface

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Abstract: The electronic transition rate between a Alq$_3$ molecular and Au metal in different coupling coefficient has examined using simple theoretical picture through Marcus theory for electronic transfer and quantum postulate. The electronic transfer rate contribution is discussion the transfer mechanism, its induced by the transition energy for molecule - metal system. The Alq$_3$ molecule is named ( tris(8-hydroxyquinoline)aluminum ) and has chemical structure (C$_{27}$H$_{18}$AlN$_3$O$_3$). The rate of electron transfer for Alq$_3$-Au system studies with 2-methylpyridin, Hexanone, Acetone, Bezonitrile, Propanonitrile, Nitrobenzene and 1,2-ethanediol solvents. It has been shown that electron transition across the Alq$_3$-Au interface associated with solvent increases with decreases the transition energy and potential at interface.

Key Word: Electronic Transition Rate, Alq$_3$ molecule, Au Metal.

1. Introduction

Electron transfer is one of the most reaction in applied material and advance technology, electron is a mobile particle from state vector called donor to another state vector called acceptor[1]. The charge transfer was one of the important ubiquitous and a basically phenomenon in physics, biology and chemistry It has key elementary step in much more fields processes involved supermolecules, molecules, ions in solution, electrochemical systems condensed phase and solar cells system in radiative or nonradiative processes. [2–4]. The molecule used in many system as single molecule with metal electrodes, molecule with semiconductor, it has very important for advanced future electronic and in technology of conversion energy[5]. Charge transfer systematic has been studied of photoinduced reactions in donor acceptor molecules, it has leding to discussion the mechanism of transfer and significant insights factors controlling on the transfer process [6]. The molecular electronics has used in different goals such that resistors, molecular films, diodes and transistors. The challenge of the most devices used electrode–molecule interface has relied on the chemisorption phenomena of molecule contact on metal surfaces[7]. Charge transfer in metal–molecule devices is a major studies in a rapidly growing interdisciplinary research area, it study the fundamental and applied of charge transfer at nanoscale to controlling the electronic conductance at energy level of molecule and nanotechnology[8]. The heterojunction devices are play wide increases scientific attention as results to using different material in photovoltaic and solar cell as well as
model contained molecule as donor and solid as acceptor [9]. The molecule - metal interface is central components in technology devices. These interface is often strongly effected on the optical and electrical characteristics of device[10]. In the present paper, the electron transfer rate has study and computed for Alq3 molecule has chemical structure in figure (1) contact with Au metal and study the effect of transition energy, driving force and potential on the transfer rate.

![Figure 1: chemical structure of dye molecule Alq3](image)

2. Theoretical

The flow rate probable of transfer from electronic donor state to another acceptor state is given by:

\[ \Gamma_{\alpha_i \rightarrow \beta_i} = \frac{2\pi}{\hbar} \sum_i \mathbb{F}(E) \left| \langle \hat{H}_{\alpha_i \beta_i} \rangle \right|^2 \delta(E_{\beta_i} - E_{\alpha_i}) \]  

(1)

Where \( \hbar \) is Dirac constant, \( \mathbb{F}(E) \) is Fermi Dirac function, \( \langle \hat{H}_{\alpha_i \beta_i} \rangle \) is the coupling of transition and \( \delta(E_{\beta_i} - E_{\alpha_i}) \) is Dirac function. The Fermi of electronic occupancy for the total electrons transfer through molecule metal interface is given by [11].

\[ \mathbb{F}(\epsilon) = \left[ e^{-\frac{\epsilon}{k_BT}} + 1 \right]^{-1} = \frac{e^{-\frac{\epsilon}{2k_BT}}}{e^{-\frac{\epsilon}{2k_BT}} + e^{\frac{\epsilon}{2k_BT}}} \]  

(2)

Inserting Eq.(2) in Eq.(1)

\[ \Gamma_{\alpha_i \rightarrow \beta_i} = \frac{2\pi}{\hbar} \sum_i \frac{e^{-\frac{\epsilon}{2k_BT}}}{(e^{-\frac{\epsilon}{2k_BT}} + e^{\frac{\epsilon}{2k_BT}})} \left| \langle \hat{H}_{\alpha_i \beta_i} \rangle \right|^2 \delta(E_{\beta_i} - E_{\alpha_i}) \]  

(3)

For all electronic state in molecule metal system, we integral Eq.(3) for total density \( \rho_{(E)} \).

\[ \Gamma_{\alpha_i \rightarrow \beta_i} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \frac{e^{-\frac{\epsilon}{2k_BT}}}{(e^{-\frac{\epsilon}{2k_BT}} + e^{\frac{\epsilon}{2k_BT}})} \left| \langle \hat{H}_{\alpha_i \beta_i} \rangle \right|^2 \rho_{(E)} \delta(E_{\beta_i} - E_{\alpha_i}) \ dE \]  

(4)

However, the activity density of metal \( D_{act(M)}(E) \) can be written as [12].

\[ D_{act(M)}(E) = \sum_i \delta(E_{\beta_i} - E_{\alpha_i}) \]  

(5)

Substituting Eq.(5) in Eq.(4) to obtained.

\[ \Gamma_{\alpha_i \rightarrow \beta_i} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \frac{e^{-\frac{\epsilon}{2k_BT}}}{(e^{-\frac{\epsilon}{2k_BT}} + e^{\frac{\epsilon}{2k_BT}})} \left| \langle \hat{H}_{\alpha_i \beta_i} \rangle \right|^2 \rho_{(E)} D_{act(M)}(E) \ dE \]  

(6)
So as activation density of states transfer process is \[13\].

\[
D_{\alpha \beta (M)}(E) = D_M(E) \frac{l_M}{r_M^{2/3}(\frac{\pi}{2})^{3/2}}
\]  

(7)

Where \(D_M(E)\) is density of metal states, \(l_M\) is effective coupling length and \(r_M\) is average diameter of an atom in the metal lattice in \(\frac{cm}{atom}\). Eq.(6) with Eq.(7) for effective is given.

\[
\Gamma_{\alpha i \to \beta_i} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \frac{E}{e^{E/2k_BT} + e^{E+2k_BT}} |\langle \hat{H}_{\alpha \beta} \rangle|^2 \rho(E) D_M(E) \frac{l_M}{r_M^{2/3}(\frac{\pi}{2})^{3/2}} dE
\]

(8)

However, we insert the density of electronic states \(\rho(E_i)\) for all system.

\[
\hat{\rho}(E_i) = \frac{1}{4\pi T M k_B T} \frac{e^{-(T_M+i\Delta E)^2}}{m} \frac{D_M(E) l_M}{r_M^{2/3}(\frac{\pi}{2})^{3/2}} dE
\]

(9)

Inserting Eq.(9) in Eq.(8) to results

\[
\Gamma_{\alpha i \to \beta_i} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \frac{1}{4\pi T M k_B T} \frac{e^{-(T_M+i\Delta E)^2}}{m} \frac{D_M(E) l_M}{r_M^{2/3}(\frac{\pi}{2})^{3/2}} dE
\]

(10)

The density \(D_M(E)\) of metal is obtained from Droid model \[14\] and given by

\[
D_M(E) = \frac{3}{2} \left( \frac{N_M(E_F)}{E_F} \right)
\]

(11)

Inserting Eq.(11) in Eq.(10) to obtained

\[
\Gamma_{\alpha i \to \beta_i} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \left( \frac{1}{4\pi T M k_B T} \frac{e^{-(T_M+i\Delta E)^2}}{m} \frac{3 N_M(E_F)}{E_F} \frac{l_M}{r_M^{2/3}(\frac{\pi}{2})^{3/2}} \right) dE
\]

(12)

However, the potential for system is given by

\[
\Delta U = \frac{(E_F - 1E + T_M)^2}{4 T M}\n\]

(13)

Where \(E_F\) is the Fermi energy at metal, \(1E\) is the ionized energy of molecule and \(T_M\) is the transition energy We can remove the independent term on \(E\) out integral to results.

\[
\Gamma_{\alpha i \to \beta_i} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \frac{1}{4\pi T M k_B T} \frac{3 N_M(E_F)}{E_F} \frac{l_M}{r_M^{2/3}(\frac{\pi}{2})^{3/2}} dE
\]

(14)

The exponential factors \(e^{-E/2k_BT}\) in Eq.(14) can be expand to.

\[
e^{-E/2k_BT} = 1 - \frac{E}{2k_BT} + \frac{1}{2!} \left( \frac{E}{2k_BT} \right)^2 - \frac{1}{3!} \left( \frac{E}{2k_BT} \right)^3 + \frac{1}{4!} \left( \frac{E}{2k_BT} \right)^4 \ldots + \frac{1}{n!} \left( \frac{E}{2k_BT} \right)^n
\]

(15)

Inserting Eq.(15) in Eq.(14) to obtained.
\[
\Gamma_{\alpha_i-\beta_i} = \frac{2\pi}{h^3} \sqrt{\frac{1}{4\pi T_Mk_BT^2}} \left( \frac{N_M(E_F)}{E_F} \right) \left( \frac{l_M}{r_M} \right) e^{-\frac{T_M+\Delta E}{m}} \int_{-\infty}^{\infty} \left( \langle \hat{H}_{\alpha_i\beta_i} \rangle \right)^2 \left( \frac{1}{e^{\frac{E}{2k_BT}} + e^{\frac{E}{2k_BT}}} \right) \left[ 1 - \left( \frac{E}{2k_BT} \right) \right] + \\
\frac{1}{2!} \left( \frac{E}{2k_BT} \right)^2 + \frac{1}{3!} \left( \frac{E}{2k_BT} \right)^3 + \frac{1}{4!} \left( \frac{E}{2k_BT} \right)^4 + \ldots + \frac{1}{n!} \left( \frac{E}{2k_BT} \right)^n dE
\] (16)

Under assume

\[
I(E) = \frac{E^2 dE}{(e^{\frac{E}{2k_BT}} + e^{\frac{-E}{2k_BT}})} - \frac{E^2 dE}{(e^{\frac{E}{2k_BT}} + e^{\frac{-E}{2k_BT}})} + \frac{1}{2!} \left( \frac{E}{2k_BT} \right)^2 \int_{-\infty}^{\infty} \frac{E^2 dE}{(e^{\frac{E}{2k_BT}} + e^{\frac{-E}{2k_BT}})} + \ldots + \frac{1}{n!} \left( \frac{E}{2k_BT} \right)^n \int_{-\infty}^{\infty} \frac{E^2 dE}{(e^{\frac{E}{2k_BT}} + e^{\frac{-E}{2k_BT}})} \] (17)

We can solved integral to results

\[
I = \left[ \pi k_BT + \frac{1}{2!} \left( \frac{1}{2k_BT} \right)^2 (\frac{\pi k_BT}{4})^3 + \frac{1}{4!} \left( \frac{1}{2k_BT} \right)^4 \frac{5(\pi k_BT)^5}{16} + \ldots + \frac{1}{n!} \left( \frac{1}{2k_BT} \right)^n \beta (\pi k_BT)^{n+1} \right] \] (18)

On the other hand the potential upon interface is written as

\[
U = \frac{(E_F-\Delta E+T_M)^2}{4T_M} \] (19)

Inserting Eq.(18) and Eq.(19) in Eq.(16) and divided per number of electron concentration to obtained the total rate .

\[
\Gamma_{\alpha_i/\beta_i} = \frac{\Gamma_{\alpha_i-\beta_i}}{N_M(E_F)} = \frac{2\pi}{h^3} \sqrt{\frac{1}{4\pi T_Mk_BT^2}} \left( \frac{1}{E_F} \right) \left( \frac{l_M}{r_M} \right) e^{-\frac{T_M+\Delta E}{m}} \left( \langle \hat{H}_{\alpha_i\beta_i} \rangle \right)^2 \left[ \pi k_BT + \frac{1}{2!} \left( \frac{1}{2k_BT} \right)^2 (\frac{\pi k_BT}{4})^3 + \frac{1}{4!} \left( \frac{1}{2k_BT} \right)^4 \frac{5(\pi k_BT)^5}{16} + \ldots + \frac{1}{n!} \left( \frac{1}{2k_BT} \right)^n \beta (\pi k_BT)^{n+1} \right] \] (20)

The driving force energy for electronic transfer is given by [15].

\[
\Delta E = E_{abs} - T_M = \hbar \frac{c}{\lambda} - T_M \] (21)

Where \( E_{abs} = \hbar \frac{c}{\lambda} \) is the absorption energy by electron , \( \hbar \) is Planck constant, \( f \) is the frequency, \( f = \frac{c}{\lambda} \) where \( c \) is the velocity of light and \( \lambda \) is the wave length. The transition energy \( T_M \) due to electronic transfer reaction for a molecule- metal interface is [16].

\[
T_M(eV) = \frac{e^2}{8\pi \varepsilon_o} \left( \frac{1}{n^2} - \frac{1}{R} - \frac{1}{2D} \right) \] (22)

Where \( e \) is the electronic charge , \( \varepsilon_o \) is the vacuum permittivity, \( n \) is the refractive index , \( \varepsilon \) is the static dielectric constant , \( D \) is the distance between the complex and electrode , \( R \) is the radius of the molecule .The calculated radius of material be estimated using forma [17].

\[
R = \frac{3M}{4\pi N \rho} \] (23)

where \( M \) is the molecular weight, \( N \) is Avogadro's number, and \( \rho \) is the mass density.
3. Results

The electronic transfer rate has play important role in study and analysis the electronic properties in molecule–metal system. This studies introduce much more information about charge transport through different systems of molecule–metal depends on the characters of two different material and electrons behaviour cross interface. Firstly, we can estimation the transition energy $T_{M/m}(eV)$ from Eq.(22) using the properties of Au metal and Alq3 molecule in table (1) and general properties of solvent from table (2). The radii of Au metal and Alq3 are calculated from Eq.(23) with insertion molecular weight and mass density from table (1), the results are $R = 5.181$ for Alq3 and $1.46$ for Au metal respectively.

Table1. General properties of dye molecules[18].

| Properties                  | Alq3     | Au       |
|-----------------------------|----------|----------|
| Molecular weight g/mol      | 459.43   | 196.9665 |
| Crystal structure           | $\text{C}_{27}\text{H}_{18}\text{AlN}_{3}\text{O}_{3}$ | Au       |
| Mass Density (g/cm3)        | 1.31     | 19.3     |
| Radius(Å)                  | 5.181    | 1.46     |
| HOMO eV                    | 5.62     |          |
| LUMO eV                    |          | 2.85     |

Table2. General properties of solvents[19]

| Solvent type               | Refraction index (n) | Dielectric constant (ε) |
|---------------------------|----------------------|-------------------------|
| 2-methylpyridin           | 1.4984               | 9.9533                  |
| Hexanone                  | 1.4007               | 14.136                  |
| Acetone                   | 1.3559               | 20.493                  |
| Bezonitrile               | 1.5257               | 25.592                  |
| Propanonitrile            | 1.3633               | 29.324                  |
| Nitrobenzene              | 1.5030               | 34.809                  |
| 1,2-ethanediol            | 1.4306               | 40.245                  |

Next, we can evaluated the transition energy using Eq.(22) with refractive index and dielectric constant of solvent from table (2) and radi of molecule with $D \approx R_{\text{Au}} + R_{\text{Alq3}}$ and taken $\frac{e^2}{8\pi\varepsilon_0} \approx 7.2$ eV. The results are shown in table (3).

Table3. Calculated Transition Energy $T_{M/m}$ for Au/Alq3 system

| Solvent type               | Refractive index (n) | Dielectric constant (ε) | Polarity function $F(n,e)$ | Transition Energy $T_{M/m}$ eV |
|---------------------------|----------------------|-------------------------|-----------------------------|--------------------------------|
| 2-methylpyridin           | 1.4984               | 9.9533                  | 0.344                       | 0.292                          |
| Hexanone                  | 1.4007               | 14.136                  | 0.439                       | 0.372                          |
| Acetone                   | 1.3559               | 20.493                  | 0.495                       | 0.419                          |
| Bezonitrile               | 1.5257               | 25.592                  | 0.390                       | 0.331                          |
| Propanonitrile            | 1.3633               | 29.324                  | 0.503                       | 0.427                          |
| Nitrobenzene              | 1.5030               | 34.809                  | 0.413                       | 0.350                          |
| 1,2-ethanediol            | 1.4306               | 40.245                  | 0.463                       | 0.393                          |

Since, the driving force energy can be calculated using Eq.(21) with transition energy from table(3) and absorption energy from spectrum of Alq3 molecule have wave length ranging (300 to 800)nm, results are listed in table(4) and figure (2).
Table 4. Calculated Driving Force $\Delta E$ \text{Au/Alq}_3

| $\lambda$ (nm) | Energy | 2-Methylpyridine | Hexanone | Acetone | Bezonitri le | Propanonitrile | Nitrobenzene | 1,2-ethanediol |
|---------------|--------|------------------|----------|---------|-------------|----------------|--------------|----------------|
| 300           | 4.133  | 3.840            | 3.761    | 3.713   | 3.802       | 3.706          | 3.782        | 3.740          |
| 350           | 3.542  | 3.250            | 3.170    | 3.123   | 3.211       | 3.115          | 3.191        | 3.149          |
| 400           | 3.099  | 2.807            | 2.727    | 2.680   | 2.768       | 2.672          | 2.749        | 2.706          |
| 450           | 2.755  | 2.463            | 2.383    | 2.335   | 2.424       | 2.328          | 2.404        | 2.362          |
| 500           | 2.479  | 2.187            | 2.107    | 2.060   | 2.148       | 2.052          | 2.129        | 2.086          |
| 550           | 2.254  | 1.962            | 1.882    | 1.834   | 1.923       | 1.827          | 1.903        | 1.861          |
| 600           | 2.066  | 1.774            | 1.694    | 1.646   | 1.735       | 1.639          | 1.715        | 1.673          |
| 650           | 1.907  | 1.615            | 1.535    | 1.487   | 1.576       | 1.480          | 1.556        | 1.514          |
| 700           | 1.771  | 1.479            | 1.399    | 1.351   | 1.440       | 1.344          | 1.420        | 1.378          |
| 750           | 1.653  | 1.360            | 1.281    | 1.233   | 1.322       | 1.226          | 1.302        | 1.260          |
| 800           | 1.549  | 1.257            | 1.177    | 1.130   | 1.218       | 1.122          | 1.199        | 1.156          |

Figure 2. the driving force energy with transition energy absorption energy from spectrum of Alq$_3$ molecule have wave length

We can noted the potential at interface of Au –Alq$_3$ is effected on charge transfer between Alq$_3$ molecule and Au electrodes. It can be estimated using Eq. (19) upon contact using $E_F = 5.53 \text{ eV}$, $\text{IE}= 5.8\text{ eV}$ [18] and taken transition energy from table (3), results are formulated in table (5).
The rate of electronic transfer at Alq$_3$-Au contact can also be calculated using Eq.(20) using results of transition energy from table (2) and potential at contact from table(5) and using effective coupling length $l_M = 1 \times 10^{-8}$cm [20] with using typicaly value of $\langle H_{\alpha\beta} \rangle = 2.25 \times 10^{-2}$,2.5 $\times 10^{-2}$,2.75 $\times 10^{-2}$,3 $\times 10^{-2}$,3.25 $\times 10^{-2}$,3.5 $\times 10^{-2}$,3.75 $\times 10^{-2}$ eV/state ,the results are shown in table (6) and figure(3).

**Table 5.** Calculated potential at Alq$_3$-Au contact

| Solvent type    | $T_{M/m}$ eV | $U_1 \times 10^{-3}$eV | Exp-$(U/0.025)$ |
|-----------------|--------------|------------------------|-----------------|
| 2-methylpyridin | 0.292        | 0.4273                 | 0.983           |
| Hexanone        | 0.372        | 7.005                  | 0.755           |
| Acetone         | 0.419        | 13.344                 | 0.586           |
| Benzonitrile    | 0.331        | 2.810                  | 0.893           |
| Propanonitrile  | 0.427        | 14.451                 | 0.560           |
| Nitrobenzene    | 0.350        | 4.658                  | 0.830           |
| 1,2-ethanediol  | 0.393        | 9.634                  | 0.680           |

**Table 6.** results of rate of electron transfer at Alq3-Au interface.

| Solvent          | The rate of electron transfer $\Gamma_{\alpha/\beta} \times 10^{-14}$ |
|------------------|----------------------------------------------------------|
|                  | Coupling strength $\langle H_{\alpha\beta} \rangle \times 10^2$ |
|                  | 2.25 | 2.5 | 2.75 | 3 | 3.25 | 3.5 |
| 2-methylpyridin  | 2.942 | 3.632 | 4.394 | 5.230 | 6.138 | 7.118 |
| Hexanone         | 2.004 | 2.474 | 2.994 | 3.563 | 4.182 | 4.850 |
| Acetone          | 1.464 | 1.808 | 2.188 | 2.603 | 3.055 | 3.544 |
| Benzonitrile     | 2.513 | 3.103 | 3.754 | 4.468 | 5.244 | 6.082 |
| Propanonitrile   | 1.388 | 1.714 | 2.074 | 2.469 | 2.897 | 3.360 |
| Nitrobenzene     | 2.267 | 2.799 | 3.387 | 4.031 | 4.730 | 5.486 |
| 1,2-ethanediol   | 1.755 | 2.167 | 2.622 | 3.120 | 3.662 | 4.247 |

**Figure 3.** The rate of electronic transfer at Alq3-Au contact with coupling coefficent $\langle H_{\alpha\beta} \rangle$
4. Discussion

Based on the simple model of electron transfer for Alq3-Au interface, we can discuss the charge transfer mechanism in terms of transition energy, driving force, potential over contact and rate of electron transfer. Table (3) shows the transition energy is a function of both refractive index and dielectric constant or polarity function beside the structure of two materials. The transition energy increases with increases polarity function and vice versa. In fact, the potential over contact Alq3 with Al metal dependent on the Fermi energy and ionization energy and transition energy, it has invoked this model to investigated the effect of potential quantity on transition cross interface of Alq3 organic molecular and Al metal electrodes in the context photovoltaic devices. Since the driving force energy in table (4) and figure (2), show that increasing with decreasing wave length and decreasing with increasing with transition energy. This because the transition energy is energy taken from absorption to reforming to transfer. Furthermore, the potential at interface is hard effected on transition rate also relate to Fermi energy of metal and ionization energy with transition energy. We can find the Alq3-Au devices has high potential with Propanonitrile solvent that’s has upper potential 14.451 mV while methylypyridin has lower potential 0.4273 mV.

In table (6) we can find the transfer rate results, evaluated with Eq. (20) for Alq3 molecule contact with Au metal, its show increases with increases the coupling strength between Alq3 and Au metal. The figure (3), show the transition rate is found to be increases with decreases the transition energy and vice versa. The Alq3-Au with methylypyridin solvent give good and large rate compare with the other solvent this show the agreement with the methylypyridin is good solvent and suitable media to devices and it supply good media to energy level alignment for Alq3 molecule –Au metal systems. Interestingly, the transfer rate increases for the lower potential cases (methylpyridin) and the rate decreases for the upper potential cases (Propanonitrile). These because upper potential embedded the electron transfer cross interface while low potential is permitted more electron to transfer cross interface.

5. Conclusion

In summary, the electron transfer rate evaluations demonstrated a relationship between the transition energy, the resultant polarity solvent media, driving force, material structure, potential at interface and the coupling coefficient of electronic transport. It has been used quantum theory with applied the transition theory to derived an expression for electronic rate with assume alignment energy levels for two different materials in molecule-metal interfaces. In the rate calculation, both terms of transition energy and coupling coefficient with potential term exponential are force dependent on rate quantity of Alq3 molecule and Au metal. In particular, the rate increases with decreases transition energy and potential at interface while the rate increases with increases coupling coefficient of the Alq3 relative to Au electrode. Furthermore, this paper has demonstrated a simple model to discussion relationship between the rate of electron transfer and the transition energy, driving force and it has the potential at interface.

6. References

[1] Al-Agealy HJ, Hassoni MA, Ahmad MS, Noori RI, Jheil SS 2014. A Theoretical Study of Charge Transport at Au/ZnSe and Au/ZnS Interfaces Devices. Ibn AL-Haitham Journal for Pure and Applied Science. 27(1) 176-87.
[2] Bixon M, Jortner J 1999 Electron transfer from isolated molecules to biomolecules. Advances in Chemical Physics. Part 1.106 35-202.
[3] Würfel, P. Würfel U 2009 Physics of solar cells: from basic principles to advanced concepts. 2nd edition (John Wiley & Sons)
[4] Khudyakov I, Zharkov A.A, and Burshtein A I 2010 J. Chem. Phys 132 (1) 014104/1–014104/6.
[5] Balachandran J, Reddy P, Dunietz B D and Gavini V 2012 End-group-induced charge transfer in molecular junctions: effect on electronic-structure and thermopower. The Journal of Physical Chemistry Letters 3(15) 1962-1967.

[6] Buck J T, Wilson R W , Mani T 2019 Intramolecular Long-Range Charge-Transfer Emission in Donor–Bridge–Acceptor Systems. journal of physical chemistry letters, 10(1)3080-3086.

[7] Peiris C R, Vogel YB, Le Brun A P, Aragonès A C, Coote M L, Diez-Pérez I, Ciampi S, Darwish, N 2019 Metal–Single-Molecule–Semiconductor Junctions Formed by a Radical Reaction Bridging Gold and Silicon Electrodes. Journal of the American Chemical Society 141(37) 14788-14797.

[8] Lucia V, Robin O, Klaus K 2010 Surveying Molecular Vibrations during the Formation of Metal–Molecule Nanocontacts . Nano letters 10 657-660.

[9] Al-Agealy Hadi J M, Taif S AlMaadhede, Mohsin A. Hassooni, Abbas K. Sadoon, Ahmed M. Ashweik, Hind Abdlmajeed Mahdi, Rawnaq Qays Ghadhban. 2018 Theoretical study of electronic transfer current rate at dye-sensitized solar cells In AIP Conference Proceedings, vol. 1968, no. 1, 030055. (AIP Publishing LLC).

[10] Egger D.A, Liu Z.F, Neaton J.B, Kronik, L 2015 Reliable energy level alignment at physisorbed molecule–metal interfaces from density functional theory. Nano letters 15(4) 2448-2455.

[11] Al-Agealy H J, Hassoni M A, Ahmad M S, Noori R I, Jheil S S 2014. A Theoretical Study of Charge Transport at Au/ZnSe and Au/ZnS Interfaces Devices. Ibn AL-Haitham Journal for Pure and Applied Science. 27(1) 176-87.

[12] Vasko F.T and Raichev O E 2006 Quantum Kinetic Theory and Applications: Electrons, Photons, Phonons. (Springer Science & Business Media).

[13] William J. Royea, Arnel M. Fajardo, and Nathan S. Lewis 1997 Fermi Golden Rule Approach to Evaluating Outer-Sphere Electron-Transfer Rate Constants at Semiconductor/Liquid Interfaces J. Phys. Chem. B 101 11152-11159.

[14] Kittel C 1999 Introduction to Solid State Physics, 6th edition (Wiley: New York).

[15] Al-agealy, Hadi JM, Mohsin A. Hassooni, Abbas K. Sadoon, and Ahmed M. Ashwiekh 2016 Study and Investigation of Electric Properties of Dye Sensitized Solar Cell Mesopotamia Environmental Journal Special Issue A (2016) 93-105.

[16] Al-Agealy, H.J. and Fadhil, M.Z 2017 Electron Transfer At Metal/Molecule Interface. Ibn AL-Haitham Journal For Pure and Applied Science 26(3)86-93.

[17] Al-Agealy, Hadi JM, and Hazim Hadi Dhaif Al Janeri 2019 Investigation the flow charge rate at InAs/D149 and ZnO/D149 system using theoretical quantum model. In AIP Conference Proceedings, vol. 2123, no. 1, 020055. (AIP Publishing LLC, 2019).

[18] Kahn A, Koch N, Gao W 2003 Electronic structure and electrical properties of interfaces between metals and π-conjugated molecular films. Journal of Polymer Science Part B: Polymer Physics 41(21) 2529-2548.

[19] Winget, Paul, Derek M. Dolney, David J. Giesen, Christopher J. Cramer, and Donald G. Truhlar.1999 Minnesota solvent descriptor database. Dept. of Chemistry and Supercomputer Inst., University of Minnesota, Minneapolis, MN 55455.

[20] Chidsey C.E, 1991 Free energy and temperature dependence of electron transfer at the metal-electrolyte interface. Science 251(4996) 919-922.