



# Study of Charge Flow Coefficient Au Metal with $\alpha$ – NPD Molecule Dye

Mohsin A. Hassooni<sup>1\*</sup>, Hadi J.M, Al-agealy<sup>2</sup>, Rawnaq Qays Ghadhban<sup>3</sup>

## Abstract

The coefficient of charge transfer at heterogeneous devices of Au metal with a well-known  $\alpha$  – NPD dye is investigated using quantum model. Four different solvents are used to estimate the effective transition energy. The potential barrier at the interface of Au and  $\alpha$  – NPD dye has been determined using effective transition energy and the difference between the Fermi energy of Au metal and the ionization energy of  $\alpha$  – NPD dye. A possible transfer mechanism across the potential barrier of Au/ $\alpha$  – NPD dye and the coupling strength interaction between the electronic levels in systems of Au and  $\alpha$  – NPD is discussed. Different data of effective transition energy and potential barrier calculations suggest that the solvent is more suitable to bind Au with  $\alpha$  – NPD dye.

**Key Words:** Charge Flow, Au Metal,  $\alpha$ -NPD Molecule Dye.

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## Introduction

The transfer of an electron is part of many more physical chemistry processes, biophysics and technology; it occurs in a variety of molecules from small ion pairs up to large biological systems [1]. The electron transfer has involved molecular electronics, its attractive increased interest, because molecules may be able to control electronic transition and it promises exploring the different molecular functions for electronic devices [2]. The electron transition through an adsorbate and a solid surface substrate are involved in the rearrangement of atoms as well as changes in the electronic charge distribution [3]. In the recent years, the charge transfer mechanisms are investigated through many more systems such as molecule/solid system at molecule/metal interfaces and metal/semiconductors interfaces [4]. The charge transfer has happened due to three types of transfer. There are Brownian transfer from donor to acceptor, thermal agitation of polar media and transfer by tunneling from

donor to acceptor. The standard theory of transfer introduced in many papers of Marcus in 1956 [5]. The interface between different materials plays an important role in organic and solid devices such as organic solar cells, field effect transistors, and light emitting diodes. Potential at a heterojunction is determined by the chemical bonding at the interface of the two materials. The potential at the interface of two materials isn't simply equal to the difference between the electron affinity of the acceptor and the ionization potential of the donor [6]. We proposed a simple quantum model for donor-acceptor to Au metals and  $\alpha$  – NPD molecule to describe the charge transfer and evaluate the charge flow coefficient for the system, it's taken into account the continuum energy levels in two materials by assuming Au metal and  $\alpha$  – NPD molecules possess closely spaced occupied electronic states. The chemical structure of  $\alpha$ -NPD is the N, N'-diphenyl-N, N'-bis(1-naphthyl)-1,10-biphenyl-4,4'-diamine ( $\alpha$ -NPD) molecule.

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**Corresponding author:** Mohsin A. Hassooni

**Address:** <sup>1,2,3</sup>Department of Physics – College of Education – Ibn Al-Haitham – University of Baghdad.

<sup>1\*</sup>E-mail: mohsin.a@ihcoedu.uobaghdad.edu.iq

<sup>2</sup>E-mail: alagealyhadi@yahoo.com

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### Theory

The charge flow coefficient of transfer at interface of Au/  $\alpha NPD$  is given by [7].

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \int |T_{\alpha NPD}^{Au}(\epsilon)|^2 \wp_{\alpha NPD}^{Au}(\epsilon) \delta(\epsilon_{Au} - \epsilon_{\alpha NPD}) d\epsilon \quad (1)$$

Where  $\hbar$  is the Dirac constant,  $|T_{\alpha NPD}^{Au}(\epsilon)|^2$  is square coupling constant,  $\wp_{\alpha NPD}^{Au}$  is the density of state at Au/  $\alpha NPD$  system and  $\delta(\epsilon_{Au} - \epsilon_{\alpha NPD})$  is the dirac function energy of Au/  $\alpha NPD$  system. The density of state  $\wp_{\alpha NPD}^{Au}(\epsilon)$  depends on the effective transition energy  $\Delta_{\alpha NPD}^{Au}$  and driving force energy and given by [8].

$$\wp_{\alpha NPD}^{Au}(\epsilon) = (4\pi k_B T \Delta_{\alpha NPD}^{Au})^{-\frac{1}{2}} e^{-\frac{(E_{\alpha NPD}^{Au} + \Delta_{\alpha NPD}^{Au})^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} \quad (2)$$

For charge transfer in Au/  $\alpha - NPD$  system, the difference in energy  $E_{\alpha NPD}^{Au}$  is the driving force

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \int |T_{\alpha NPD}^{Au}(\epsilon)|^2 (4\pi k_B T \Delta_{\alpha NPD}^{Au})^{-\frac{1}{2}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} \delta(\epsilon_{Au} - \epsilon_{\alpha NPD}) d\epsilon \quad (6)$$

where  $k_B$  is Boltzman constant,  $T$  is a room temperature ( $T=25^\circ c$ ). The charge flow coefficient

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \int |T_{\alpha NPD}^{Au}(\epsilon)|^2 (4\pi k_B T \Delta_{\alpha NPD}^{Au})^{-\frac{1}{2}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} F(\epsilon) \delta(\epsilon_{Au} - \epsilon_{\alpha NPD}) d\epsilon \quad (7)$$

For charge transfer, the effective density of state for metal-dye system  $D_{eff}(Au)$  can be form by [7].

$$D_{eff}(Au) = \delta(\epsilon_{Au} - \epsilon_{\alpha NPD}) \quad (8)$$

Thus, the effective density of states for the charge-transfer process is [9].

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \int |T_{\alpha NPD}^{Au}(\epsilon)|^2 (4\pi k_B T \Delta_{\alpha NPD}^{Au})^{-\frac{1}{2}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} F(\epsilon) D_{Au} \frac{l_{Au}}{\rho_{Au} \left(\frac{\epsilon}{\pi}\right)^{2/3}} d\epsilon \quad (10)$$

However, the nuclear terms is constant over integrate space and can remove out integral in

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \frac{l_{Au}}{\rho_{Au} \left(\frac{\epsilon}{\pi}\right)^{2/3}} \frac{|T_{\alpha NPD}^{Au}(\epsilon)|^2}{(4\pi k_B T \Delta_{\alpha NPD}^{Au})^{\frac{1}{2}}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} \int F(\epsilon) D_{Au} d\epsilon \quad (11)$$

The integral in Eq.(10) is estimated due to statistics of Boltzmann to describe Fermi function at an metal electrode, and the integral reduces to electrons concentration at the surface of Au metal [9].

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \frac{l_{Au}}{\rho_{Au} \left(\frac{\epsilon}{\pi}\right)^{2/3}} \frac{|T_{\alpha NPD}^{Au}(\epsilon)|^2}{(4\pi k_B T \Delta_{\alpha NPD}^{Au})^{\frac{1}{2}}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} n_F(\epsilon_F) \quad (13)$$

However the charge flow coefficient per concentration of metal  $n_F(\epsilon_F)$  in Eq. (13) become

$$\Gamma_{\alpha NPD}^{Au}(\epsilon) = \frac{2\pi}{\hbar} \frac{l_{Au}}{\rho_{Au} \left(\frac{\epsilon}{\pi}\right)^{2/3}} \frac{|T_{\alpha NPD}^{Au}(\epsilon)|^2}{(4\pi k_B T \Delta_{\alpha NPD}^{Au})^{\frac{1}{2}}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} \quad (13)$$

The effective transition energy of the system with solvents around the equilibrium of system is [10].

energy given by.

$$E_{\alpha NPD}^{Au} = (E_F(Au) - IE_{\alpha NPD}) \quad (3)$$

Where  $E_F(Au)$  is the Fermi energy of Au metal and  $IE_{\alpha NPD}$  is the Ionization energy of  $\alpha - NPD$  molecule. Since, the potential barrier at interface of Au/  $\alpha - NPD$  system can be written in form.

$$\mathbb{U} = \frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4\Delta_{\alpha NPD}^{Au}} \quad (4)$$

Substituting Eq.(3) in Eq.(2) to obtained.

$$\wp_{\alpha NPD}^{Au}(\epsilon) = (4\pi k_B T \Delta_{\alpha NPD}^{Au})^{-\frac{1}{2}} e^{-\frac{[\Delta_{\alpha NPD}^{Au} + (E_F(Au) - IE_{\alpha NPD})]^2}{4k_B T \Delta_{\alpha NPD}^{Au}}} \quad (5)$$

The charge flow coefficient of transfer in Eq. (1) with Eq. (5) becomes.

in Eq.(6) would be changed with Fermi occupancy function for Au/  $\alpha NPD$  system to.

$$D_{eff}(Au) = D_{Au} \frac{l_{Au}}{\rho_{Au} \left(\frac{\epsilon}{\pi}\right)^{2/3}} \quad (9)$$

Where  $D_{Au}$  is the density of electronic states in Au metal at room temperature,  $l_{Au}$  is the effective coupling length and  $\rho_{Au}$  is the atomic density of Au metal. Substituting Eq.(8) and Eq.(9) in Eq.(7) to result.

Eq.(10) to obtains

$$\int_{-\infty}^{\epsilon_F} F(\epsilon) D_{Au} d\epsilon = n_F(\epsilon_F) \quad (12)$$

The charge flow coefficient transition in Eq. (11) with Eq. (12) reduce to.

$$\Delta_{\alpha NPD}^{Au} (eV) = \frac{e^2}{8\pi\epsilon_0} \left(\frac{1}{n^2} - \frac{1}{\epsilon}\right) \left(\frac{1}{R} - \frac{1}{2D}\right) \quad (14)$$

where  $e$  is the electron charge,  $\epsilon_0$  is the vacuum



permittivity,  $\epsilon$  is the static dielectric constant of the solvent,  $n$  is the refractive index of the solvent,  $D$  is the distance between the complex and electrode,  $R$  is the radius of the molecule. The radius of the molecule can be estimated from the apparent molar volume using spherical approach [11].

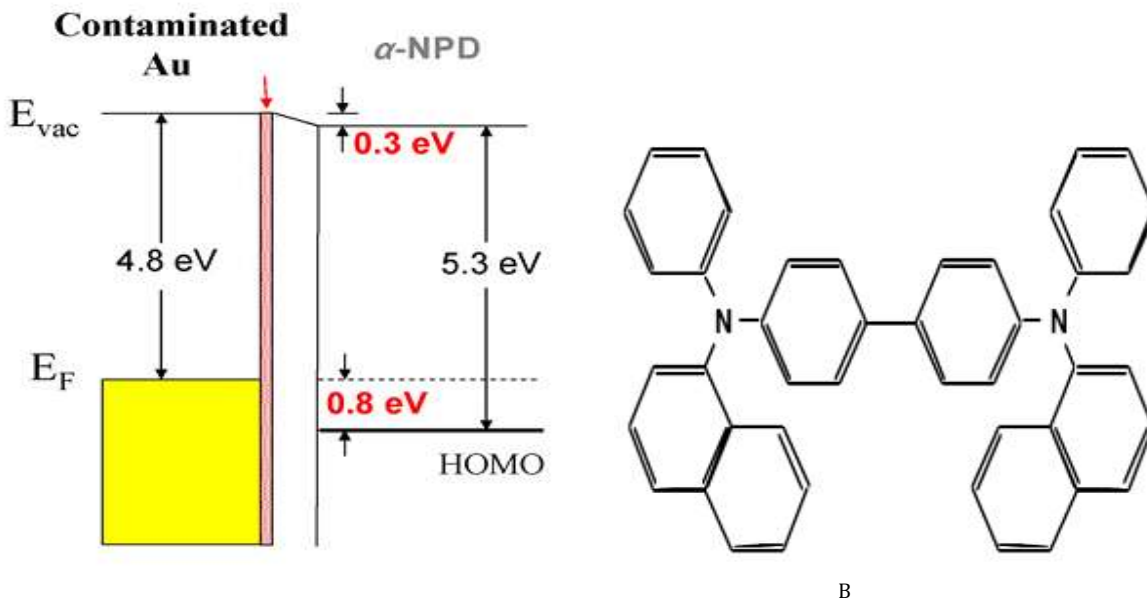
$$R = \left(\frac{3M}{4\pi N\rho}\right)^{\frac{1}{3}} \quad (15)$$

Where  $M$  is the molecular weight,  $N$  is Avogadro

number, and  $\rho$  is the density.

### Results

Interestingly, the schematic of flow charge transfer from energy levels of  $\alpha$  – NPD molecule dye is relatively to energy level of Au metal and chemical structure relisted in figure (1)[12].



**Figure 1.** A- Schematic energy level for Au contact with  $\alpha$  – NPD and B- Chemical structure of ( $\alpha$ -NPD) molecule[12].

Where ionization energy  $IE = 5.3$  eV and Fermi energy  $4.8$  eV [13]. The alignment of energy levels are the first important condition to perform to the investigation and discussion the flow charge transfer from donor ( $\alpha$  – NPD) to acceptor (Au metal), the alignment of energy is corporation to facility of transfer. Here, the potential at interface

has compelled evidence that Au can also be incorporated with  $\alpha$  – NPD donor dye. Importantly, this potential created at interface is limited the quantity of flow charge will transfer from molecule to Au metal. The characteristic of Au and  $\alpha$  – NPD molecule are listed in table (1).

**Table 1.** Main properties of  $\alpha$  – NPD molecule and Au metal.

Properties	$\alpha$ – NPD	Au[16]
Molecular weight g/mol	588.74	196.97
Crystal structure	triclinic crystal	face centered cubic
Mass Density (g/cm <sup>3</sup> )	1.35[14]	19.3
Lattice constant(Å)	a = 10.3077Å, b = 11.3545Å, c = 14.4778Å[15]	4.086
Radius(Å)	5.57078	1.59344
IE(eV)	5.2[ 13]	

The main properties of solvents Ethanol, Aceton, table (2).

DMF, 1-Butanol and Chloro from are tabulated in

**Table 2.** Common properties of some solvents

Solvent	Chemical Formula[17]	Dielectric Constant [17]	Optical Dielectric Constant[17]	$\Delta_{\alpha NPD}^{Au}$ (eV)
Ethanol	CH <sub>4</sub> O	24.5	1.3614	0.393976
Aceton	C <sub>3</sub> H <sub>6</sub> O	21.01	1.356	0.392021
DMF	C <sub>3</sub> H <sub>7</sub> NO	38.25	1.430	0.365654
1-Butanol	C <sub>4</sub> H <sub>10</sub> O	17.84	1.397	0.360493
Chloroform	C <sub>1</sub> H <sub>1</sub> Cl <sub>3</sub>	4.7113	1.4459	0.210184



The transition energy for Au Metal with  $\alpha - NPD$  Dye with Ethanol, Aceton, DMF, 1-Butanol and Chlorofrom are calculated used Eq. (14) taken into account the refractive index  $n$  and dielectric constant  $\epsilon$  for solvent from table(2) and estimated the radius of  $\alpha - NPD$  from Eq.(15) and taken  $D = R_{NPD} + R_{Au}$ . The radii of  $\alpha - NPD$  and Au metal are evaluated from Eq.(15) with inserting molecular weight are 588.74 [16] and 196.9665 [16] for  $\alpha - NPD$  and Au alternatively, the mass density for  $\alpha - NPD$  and Au are 1.35(g/cm<sup>3</sup>) [14] and 19.3 (g/cm<sup>3</sup>) [16], results of radii are 1.46 Å  $\alpha - NPD$  and Au respectively. With radii of  $\alpha - NPD$  and Au and refractive index and dielectric constant from table(2), it leads to calculate the transition energy  $\Delta_{\alpha NPD}^{Au}$  using Eq.(14). Results are listed in table(3), it lies in range 0.210184 to 0.393976 eV.

**Table 3.** Results calculation of transition energy  $\Delta_{\alpha NPD}^{Au}$ (eV).

Solvent	Chemical Formula[17]	$\Delta_{\alpha NPD}^{Au}$ (eV)
Ethanol	CH <sub>4</sub> O	0.393976
Aceton	C <sub>3</sub> H <sub>6</sub> O	0.392021
DMF	C <sub>3</sub> H <sub>7</sub> NO	0.365654
1-Butanol	C <sub>4</sub> H <sub>10</sub> O	0.360493
Chloro from	C <sub>1</sub> H <sub>1</sub> Cl <sub>3</sub>	0.210184

However, the strength coupling may be taken about  $|T_{\alpha NPD}^{Au}(\epsilon)|^2 = 2 \times 10^{-4}, 4 \times 10^{-4}, 6 \times 10^{-4}, 8 \times 10^{-4}, 1 \times 10^{-3} eV^2 state^{-1}$  [18]. The Fermi energy taken be close to  $E_F(Au) = eV$  and ionization energy is  $E_{\alpha NPD} = 5.2 - 5.5 eV$  [13]. The concentration of electrons in metal (Au) is  $0.590 \times 10^{29} m^{-3}$  [19]. The charge flow coefficient  $\Gamma_{\alpha NPD}^{Au}(\epsilon)$  for Au/ $\alpha - NPD$  system can be evaluated using Eq. (13) by inserting values of  $|T_{\alpha NPD}^{Au}(\epsilon)|^2, E_F(Au)IE_{\alpha NPD}$  with taken three values of effective length parameters  $l_{Au} = 1 \times 10^{-8} cm, 1.5 \times 10^{-8} cm$  and  $2 \times 10^{-8} cm$  [18,20]. The results of the calculations containing the charge flow rate of the three cases of **effective length** completely are shown in table (4) for  $1 \times 10^{-8} cm$ , table (5) for  $1.5 \times 10^{-8} cm$  and table(6) for  $2 \times 10^{-8} cm$ .

**Table 4.** The calculation of flow charge coefficient transition  $\Gamma_{\alpha NPD}^{Au}(\epsilon)$  with  $l_{Au} = 1 \times 10^{-8} cm$ .

$\Delta_{\alpha NPD}^{Au}$	$\Gamma_{\alpha NPD}^{Au}(\epsilon)$				
	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 2 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 4 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 6 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 8 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 10 \times 10^{-4}$
0.393976	7.898E+24	1.5796E+25	2.3694E+25	3.1592E+25	3.9490E+25
0.392021	7.8729E+24	1.5746E+25	2.3619E+25	3.1492E+25	3.9365E+25
0.365654	7.3741E+24	1.4748E+25	2.2122E+25	2.9496E+25	3.6871E+25
0.360493	7.2415E+24	1.4483E+25	2.1725E+25	2.8966E+25	3.6208E+25
0.210184	1.0400E+24	2.0799E+24	3.1199E+24	4.1598E+24	5.1998E+24

**Table 5.** The calculation of flow charge coefficient transition  $\Gamma_{\alpha NPD}^{Au}(\epsilon)$  with  $l_{Au} = 1.5 \times 10^{-8} cm$ .

$\Delta_{\alpha NPD}^{Au}$	$\Gamma_{\alpha NPD}^{Au}(\epsilon)$				
	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 2 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 4 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 6 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 8 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 10 \times 10^{-4}$
0.392021	1.1809E+25	2.3619E+25	3.5428E+25	4.7237E+25	5.9047E+25
0.393976	1.1847E+25	2.3694E+25	3.5541E+25	4.7388E+25	5.9235E+25
0.365654	1.1061E+25	2.2122E+25	3.3184E+25	4.4245E+25	5.5306E+25
0.360493	1.0862E+25	2.1725E+25	3.2587E+25	4.3449E+25	5.4311E+25
0.210184	1.5599E+24	3.1199E+24	4.6798E+24	6.2397E+24	7.7996E+24

**Table 6.** The calculation of flow charge coefficient transition  $\Gamma_{\alpha NPD}^{Au}(\epsilon)$  with  $l_{Au} = 2 \times 10^{-8} cm$ .

$\Delta_{\alpha NPD}^{Au}$	$\Gamma_{\alpha NPD}^{Au}(\epsilon)$				
	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 2 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 4 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 6 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 8 \times 10^{-4}$	$ T_{\alpha NPD}^{Au}(\epsilon) ^2 = 10 \times 10^{-4}$
0.393976	1.5796E+25	3.1592E+25	4.7388E+25	6.3184E+25	7.8981E+25
0.392021	1.5746E+25	3.1492E+25	4.7237E+25	6.2983E+25	7.8729E+25
0.365654	1.4748E+25	2.9496E+25	4.4245E+25	5.8993E+25	7.3741E+25
0.360493	1.4483E+25	2.8966E+25	4.3449E+25	5.7932E+25	7.2415E+25
0.210184	2.0799E+24	4.1598E+24	6.2397E+24	8.3196E+24	1.0400E+25



## Discussion

Various solvents are giving the polar media for charge transfer through interface of molecular the metal-molecular junction. In table (2), we list the common solvents are selected with  $\alpha$ NPD – Au system the selected polar media (solvent) is effected for celly on quantity of flow charge coefficient. From table(3) we observed that solvent has large refractive index 1.4459 for Chloro from lead to lower values of transition energy 0.210184eV compare solvent has lower refractive index 1.356 for Aceton lead to large transition energy 0.392021eV. The effect of dielectric constant on transition energy for system was viewing from result of polarity effect that means polarity effect produce from corporation between refractive index and dielectric constant. The potential at interface was played general basic role in determining the flow charge transfer. Detailed examination of molecule contact metal systems, showed increase in the flow charge for increase in the strength transmission energy with an increase in the effective length indicating enhancement transmitted processes. However, for system of  $\alpha$ NPD molecule interface with Au metal, we suggestion a localization potential at interface play an important role to transfer process along with interface, the flow charge transfer decrease in the height potential, it is controlling the transmission over larger distance.

Furthermore, the strength coupling coefficients are effect on charge transfer from combine or overlapping the closer levels energies with each other to able more electrons cross over potential delocalized at interface using easily pathway to reach acceptor state. Tables (4),(5) and (6) indicate the flow charge coefficient increased with increased the strength coupling, this because increased strength coupling lead to more electrons to transfer over potential and the increase strength coupling indicate the levels energetically close to each other and electrons can transport from one levels of donor to another level in acceptor. On the other hand, the behavior of flow charge coefficient with transition energy becomes more significant as decreasing with increasing the transition energy (0.393976). The increased transition energy for system with solvent lead to limit the electrons to transfer. The large transition energy means the system has more energy to reformation before transfer; it results to decreased energy for

electrons to transfer. The shifts of flow charge coefficient in three tables (4),(5) and (6) reduced to effect of effective length that incorporated with transition energy and strength coupling of system, the flow charge coefficient increased with increased the effective length and vice versa.

## Conclusion

We have been summarized that flow charge transfer cross metal-molecular junctions relative to the alignment energetically of Au and  $\alpha$  – NPD using and it must be closed to each other approximations. An increased the strength coupling corresponding to increase the flow charge as result to overlapping energy levels of molecule and metal and leads to more facilitate to transport. A decrease in refractive index lead to increases the transition energy and decreased the flow charge transfer coefficient is observed due to use different solvent media of the metal contact with molecule junctions.

Size of the effective length played a significant role on the flow charge coefficient, the increased of effective length as well as increased effect on the flow charge transport.

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