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Theoretical Study of Heterogeneous Electronic Transition Rate at the Metal/ Ionic Liquid Interface Using Quantum Theory

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ABSTRACT

The purpose of this research is study the heterogeneous electronic transition through metal/liquid interface using simple model. The kinetic of electron transfer phenomenon discussion using postulate of quantum transition theory. The energy levels for metal and liquid assume to be alignment depending on continuum model theory. The behaviour of electron transfer at metal-liquid interface affected by barrier height. The transition of negative charge on the interface of metal /liquid which suffering much more impediment to transfer cross the potential barrier .The net of electron that transfer give the average rate of electronic transfer and it indicate the electrical properties of metal/liquid devices.

Keywords:

Heterogeneous electronic transfer

Metal /liquid

Potential barrier

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دراسة نظرية لمعدل الانتقال الالتروني لسطح معدن سائل بأستعمال النظرية الكمية

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الخُلاصة

ان غرض البحث هو دراسة الانتقال الالكتروني لوصلة غير متجانسة من خلال سطح صلب – سائل باستعمال انموذج بسيط. ظهاهرة ميكانيكيةالانتقال الالكتروني توقشت بأستعمال مباديء النظرية الكمية للانتقال. ان مستويات الطاقة للمعدن والسائل افترضت لتكون متوائمة اعتماداً على انموذج نظرية الاستمرارية. ان سلوك الانتقلل الالكتروني بين سطحي معدن – سائل يتأثر بحاجز الجهد.

ان انتقال الشحنة السالبة عبر سطح معدن-سائل يعاني مزيداً من الممانعة للانتقال عبر بئر الجهد. ان الحاصل للانتقال الالكتروني تعطي معدل الانتقال الالكتروني و هذا يشير الى

الكلمات المفتاحية:

الانتقال الالكتروني غير المتجانس

معدن-سائل

بئر الجهد

الخصائص الكهربائية لنبيطة معدن-سائل.

1. INTRODUCTION

The transport of electron through interface of two or more material has been occurred in many variety biological and chemical system. The liquid- liquid interface is one of simple system that is using to control of charge transfer reaction pathways in different an oxide – reduce reaction system [1]. The investigation of reaction at liquid/liquid interface that take f major interesting in sciences beside technology [2]. The process of electron transfer is a principle important of scientific and technological. Charge transfer reaction was one a primary process in different photochemical and photophysical process that supplied new ways for energy degradation at different excited state of molecules produce an excited state of charge transfer in dielectric environments [3]. The kinetics of charge-transfer and mass has been electrochemical investigations for different redox using second-generation [4].

However, many practical problems remain when its performing electrochemical estimation in room temperature ionic liquids, its included electing a suitable electrode for references [5]. In recent years, the room temperature ionic liquids became increasing attention research area due to many unique chemical and physical properties [6]. Including negligible vapour pressure, higher conductivity, higher chemical and thermal stability and their dissolve ability in wide scale of organic compounds and inorganic compounds. However, in the room temperature ionic liquids has been employed in many area field at chemical extraction [7], organic synthesis [8], and enzymatic catalysis [9] and chemical extraction [10].

2. Theory

The rate of electronic transition between electronic in molecule liquid acceptor state and an electrode donor state in room temperature could be further as [11].

$$\kappa^{m-L} = \frac{4\pi^2}{h}|C_{KD}(E)|^2 \int \mathrm{D(E)}\boldsymbol{\delta}(E_k - E_{\mathrm{D}})dE \qquad (1)$$

Where h is the Planck constant , $C_{KD}(E)$ is the overlapping constant , $\mathrm{D(E)}$ is the density of state ,`$E_k$and $E_{\mathrm{D}}$are the electronic state at electrode and molecule donor state respectively . The density of electronic state is given by [12].

$$\mathrm{D(E)} = \quad (4\pi\mu^{\mathrm{m-L}}\mathrm{k_B T})^{\frac{-1}{2}} exp\frac{-(\mu^{\mathrm{m-L}}+\Delta\mathbb{V})^2}{4\mu^{\mathrm{m-L}}\mathrm{k_B T}} \qquad (2)$$

Where$\mu^{\mathrm{m-L}}$ is the transition energy, $\mathrm{k_B}$ is the Boltzman constant, $\Delta\mathbb{V}$ is the potential of electron transfer reaction at the interface .Inserting Eq.(2) in Eq. (1), results .

$$\kappa^{m-L} = \frac{4\pi^2}{h}|C_{KD}(E)|^2 \int (4\pi\mu^{\mathrm{m-L}}\mathrm{k_B T})^{\frac{-1}{2}} exp\frac{-(\mu^{\mathrm{m-L}}+\Delta\mathbb{V})^2}{4\mu^{\mathrm{m-L}}\mathrm{k_B T}}\boldsymbol{\delta}(E_k - E_{\mathrm{D}})dE \qquad (3)$$

Under the room temperature T, the potential difference and environment for metal–liquid interface $\Delta\mathbb{V}$ is related to (E) to [13].

$$\Delta\mathbb{V} = \Delta\mathbb{V}^o - E \qquad (4)$$

Here $\mathbb{V}^o$is the driving energy of electron transfer reaction then related to absorption spectrum and given from [14].

$$\Delta\mathbb{V}^o = hc/\lambda - \mu^{\mathrm{m-L}} \qquad (5)$$

Here c is the velocity of light and λ is the wave length. Then the rate equation due to Eq. (4)

$$\kappa^{m-L} = \frac{4\pi^2}{h}\left(4\pi\mu^{\mathrm{m-L}}\mathrm{k_B T}\right)^{\frac{-1}{2}} \times \iint_{-\infty}^{\infty} |C_{KD}(E)|^2 \quad exp\frac{-(\mu^{\mathrm{m-L}}+\Delta\mathbb{V}^o-E)^2}{4\mu^{\mathrm{m-L}}\mathrm{k_B T}} f_{(E)}\boldsymbol{\delta}\left(E_k - E_{\mathrm{D}}\right) d^3K dE \qquad (6)$$

Where $\left|\overline{C_{KD}(E)}\right|^2$ is the overlapping coupling matrix for electronic state of the metal and liquid state, it may be written as.

Where

$$\left|\overline{C_{KD}(E)}\right|^2 = \int_{-\infty}^{\infty} |C_{KD}(E)|^2 \boldsymbol{\delta}(E_k - E_\mathrm{D}) d^3K \tag{7}$$

$f_{(E)}$ is probability of the Fermi-Dirac distribution of the electrons in the at interface that given by [15].

$$f_{(E)} = \frac{1}{1+exp^{\frac{E}{\mathrm{k_B T}}}} \tag{8}$$

Then, we substituting Eqs. (7) and (8)in Eq.(6) we gate.

$$\kappa^{m-L} = \frac{4\pi^2}{h}(4\pi\mu^{\mathrm{m-L}}\mathrm{k_B T})^{\frac{-1}{2}} \times \int_{-\infty}^{\infty} \left|\overline{C_{KD}(E)}\right|^2 exp\,\frac{-(\mu^{\mathrm{m-L}}+\Delta\mathbb{V}^o - E)^2}{4\mu^{\mathrm{m-L}}\mathrm{k_B T}} \frac{1}{1+exp^{\frac{E}{\mathrm{k_B T}}}} dE \tag{9}$$

The equation of rate constant for electron transfer can be solved using mathematical physics to results.

$$\kappa^{m-L} \approx \frac{4\pi^2}{h}(4\pi\mu^{\mathrm{m-L}}\mathrm{k_B T})^{\frac{-1}{2}} \exp - \frac{\mu^{\mathrm{m-L}}}{4\mathrm{k_B T}} \left|\overline{C_{KD}(E)}\right|^2 \left[[1 - \frac{\pi^2 \mathrm{k_B T}}{16\mu^{\mathrm{m-L}}}\right] \tag{10}$$

The transition energy $\mu^{\mathrm{m-L}}$ for system redox active at metal electrode interface is [16].

$$\mu^{\mathrm{m-L}} = \frac{q^2}{8\pi\varepsilon_o} f(\mathrm{n},\varepsilon)\left(\frac{1}{r} - \frac{1}{2d}\right) \tag{11}$$

where q^2 is the square of electronic charge ,ε_o is permittivity of vacuum, d is the distance from complex to electrode , r is the molecule radius and $f(\mathrm{n},\varepsilon)$ is the polarity must be written as..

$$f(\mathrm{n},\varepsilon) = \left(\frac{1}{n^2} - \frac{1}{\varepsilon}\right) \tag{12}$$

Where n and ε are optical and static dielectric constant. The radii of the molecule can be estimation using an expression [17].

$$r = \left(\frac{3M}{4\pi N\rho}\right)^{\frac{1}{3}} \tag{13}$$

Here M is the molecular weight, N is Avogadro's number, and ρ is the density.

3. Results

In order to investigation and study the electronic properties at Mg/ PTCDA and Al/ PTCDA interface, we can evaluation theoretically an important electronic rate of transition factor that indicate the electronic fature at electronic devices. The electronic rate determined using a simple model of transition due to the density of the distribution of electronic states D(E) , transition energy$\mu^{\mathrm{m-L}}$, $\Delta\mathbb{V}$ is the potential of electron transfer reaction, the driving energy $\mathbb{V}^o$, the overlapping coupling matrix $|C_{KD}(E)|^2$and room temperature T. The electronic rate is results as the solving an Eq.(10) with MATLAB program The transition energy $\mu^{\mathrm{m-L}}$ could be calculation using Eq.(10) by estimation the radii of Mg and Al metal and PTCDA dye using Eq.(13) .Due to the radii of Mg,Al and PTCDA material . The radii of metal Mg, Al and PTCDA may be estimation using Eq.(13) by inserting the density mass of ρ_{Mg} , ρ_{Al}, and molecular weight of M_{Mg} , $M_{\mathrm{Al}}$from table(1) and $\rho_{\mathrm{PTCDA}} = 1.764 g/cm^3$[22]and $M_{\mathrm{PTCDA}} = 392.316711\, g.mol^{-1}$ [23],the results are $r_{\mathrm{Mg}} = 1.76\ \mathrm{A^o}$,$r_{\mathrm{Al}} = 1.43\mathrm{A^o}$and $r_{\mathrm{PTCDA}} = 4.45A^o$ alternativelly .

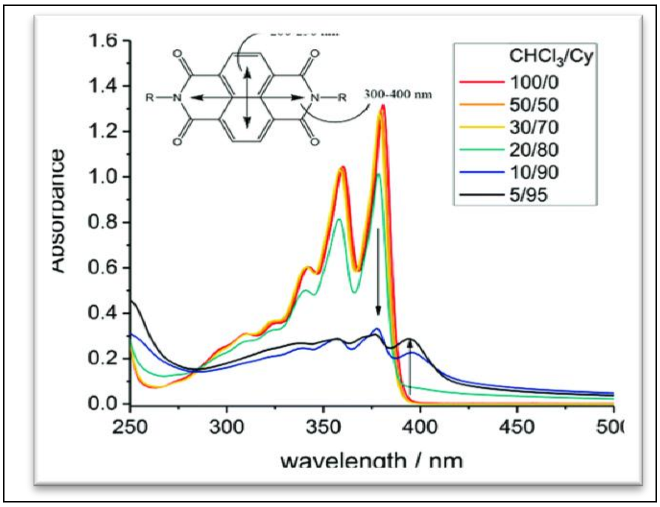

Figure 1. The UV/V absorbance spectral of the PTCDA –dye.

Table 1. Common properties of Metals.

Properties	**Mg**	**Al**
Atomic weight	24.305[18]	26.982 [18]
Lattice constant	320.94, 320.94, 521.08 pm[19]	0.405[20]
Density (g/cm^3)	1.74[18]	2.70 [18]
Melting point (ºC)	650[18]	660[18]
Radius calculated	1.76 Å	1.43 Å
Work function	4.1[20]	4.05 [21]

The exact transition energy of electrons transition is evaluation from Simple Eq.(10) , as inserting many of the constants such that refractive index and dielectric constant for solvent from table (2) in Eqs.(11-12) and treatment mathematically to solving using MATLAB program , results has been shown in table(2) for Mg / PTCDA and Al / PTCDA respectively.

Additionally, the driving force energy that drive more electrons to transfer cross interface of Mg/PTCDA and Al/PTCDA system was calculation from Eq.(5) due to absorption energy for PTCDA dye as supporting from figure (1) and results of transition energies from table (2),results are shown in table (3) and (4) for Al/PTCDA and Mg/PTCDA.

Table 2. Data calculation of transition energies at Mg/ PTCDA and Al/ PTCDA at Water, Formed, Formic acid, Acetontrile and Ethanol solvents.

Solvent	n**[23-24]**	ϵ **[23-24]**	$\mu^{\mathrm{m-L}}$**for Mg/ PTCDA**	$\mu^{\mathrm{m-L}}$**for Al/ PTCDA**
Water	1.3329	78.54	0.571106	0.526641
Formmid	1.4475	109	0.485939	0.448105
Formicacid	1.3694	58.5	0.535844	0.494124
Actontrial	1.3682	3.8	0.288574	0.266106
Ethanol	1.3594	24.55	0.516023	0.475846

Table3. Theoretical calculated of driving energy $\Delta\mathbb{V}^{o}$(eV) at Al/ PTCDA devices with solvents.

Solvent	**The driving force energy $\Delta\mathbb{V}^{o}$(eV) at PTCDA /Al interfaces**									
	350nm	400nm	450nm	500nm	550nm	600nm	650nm	700nm	750nm	800nm
Water	3.0186	2.5754	2.2307	1.9550	1.7294	1.5414	1.3823	1.2460	1.1278	1.0244
Formmid	3.0971	2.6540	2.3093	2.0335	1.8079	1.6199	1.4609	1.3245	1.2063	1.1029
Formic acid	3.0511	2.6079	2.2633	1.9875	1.7619	1.5739	1.4148	1.2785	1.1603	1.0569
Actel	3.2791	2.8360	2.4913	2.2155	1.9899	1.8019	1.6429	1.5065	1.3883	1.2849
Ethanol	3.0694	2.6262	2.2815	2.0058	1.7802	1.5922	1.4331	1.2968	1.1786	1.0752

Table 4. Theoretical calculated of driving energy $\Delta\mathbb{V}^{o}$(eV) at **Mg** / PTCDA devices with solvents.

Solvent	**The active driving force energy $\Delta\mathbb{V}^{o}$(eV) at PTCDA /Mg interfaces**									
	350nm	400nm	450nm	500nm	550nm	600nm	650nm	700nm	750nm	800nm
Water	2.9741	2.5310	2.1863	1.9105	1.6849	1.4969	1.3379	1.2015	1.0833	0.9799
Formmid	3.0593	2.6161	2.2714	1.9957	1.7701	1.5821	1.4230	1.2867	1.1685	1.0651
Formicaci	3.0094	2.5662	2.2215	1.9458	1.7202	1.5322	1.3731	1.2368	1.1186	1.0152

d										
Actel	3.2566	2.8135	2.4688	2.1931	1.9675	1.7795	1.6204	1.4840	1.3659	1.2625
Ethanol	3.0292	2.5860	2.2414	1.9656	1.7400	1.5520	1.3929	1.2566	1.1384	1.0350

The electrons rate constant expression in Eq.(10) must be solving using MATLAB program and substituting all parameters of transition energy ,and the overlapping coupling matrix are taking $\left|\overline{C_{KD}(E)}\right|$ =0.01115cm-1,0.01177cm^{-1}, 0.01239cm^{-1}, 0.01363cm^{-1} and 0.01425cm^{-1}[25] and the results are listed in tables (5)and (6) for Mg/PTCDA and Al/ PTCDA system respectively.

Table 5. Results calculation of electrons transition rate $\kappa^{m-L}$for Mg/ PTCDA devices at Water, Formamid, Formic acid, Acetontrile, and Ethanol solvents.

Solvent	**Rate of electrons transition at Mg/ PTCDA**				
	The overlapping coupling matrix $\left|\overline{C_{KD}(E)}\right|(cm^{-1})$				
	$0.01115cm^{-1}$	$0.01177cm^{-1}$	$0.01239cm^{-1}$	$0.01363cm^{-1}$	$0.01425\ cm^{-1}$
Water	1.6184E+09	1.8034E+09	1.9984E+09	2.4184E+09	2.6434E+09
Formamid	3.4816E+09	3.8795E+09	4.2990E+09	5.2025E+09	5.6866E+09
Formic acid	2.2263E+09	2.4808E+09	2.7491E+09	3.3269E+09	3.6364E+09
Acetontrile	1.8876E+10	2.1034E+10	2.3308E+10	2.8207E+10	3.0831E+10
Ethanol	2.6607E+09	2.9648E+09	3.2854E+09	3.9759E+09	4.3458E+09

Table 6. Results calculation of electrons transition rate $\kappa^{m-L}$for Al/ PTCDA devices at Water, Formamid, Formic acid, Acetonitrile, and Ethanol solvents

Solvent	**Rate of electrons transition at Al/ PTCDA**				
	The overlapping coupling matrix $\left|\overline{C_{KD}(E)}\right|(cm^{-1})$				
	$0.01115cm^{-1}$	$0.01177cm^{-1}$	$0.01239cm^{-1}$	$0.01363cm^{-1}$	$0.01425cm^{-1}$
Water	2.4186E+09	2.6951E+09	2.9865E+09	3.6142E+09	3.9505E+09
Formamid	4.8672E+09	5.4235E+09	6.0100E+09	7.2731E+09	7.9499E+09
Formic acid	3.2366E+09	3.6065E+09	3.9965E+09	4.8365E+09	5.2865E+09
Acetontrile	2.2584E+10	2.5166E+10	2.7887E+10	3.3748E+10	3.6888E+10
Ethanol	3.8084E+09	4.2437E+09	4.7026E+09	5.6910E+09	6.2205E+09

4. Discussion

The determination of the electronic properties at interface energetic using charge transition measurements techniques was much more difficulties at metal because different nature for two materials and much delocalized the electronic state for PTCDA liquid along the chains molecule structure. Its greatly the polarity was effected on the electronic and optical properties of these metal/liquid devices materials. Electric characteristic at metal/liquid system depending on the calculation of electrons transition rate $\kappa^{m-L}$and the transition energy $\mu^{\mathrm{m-L}}(eV)$ and overlapping of electronic coupling $|C_{KD}(E)|$ at room temperature T(K) . Firstly, the more important aspects at interface is potential barriers that depending on the nature of metal and molecule of liquid through the electronic density of state. For the study electronic feature at metal/liquid devices, one assume a continuum energy levels state for PTCDA molecule and Mg and Al levels energy. However, the position of energy levels of molecule respect to Fermi energy levels at metal must be alignment. Table(2) show that Mg/PTCDA needed more energy to reformation before transfer than Al/PTCDA with different solvent and that's results to increases the transfer of electrons at Al/PTCDA than Mg/PTCDA in limit range 0.88 to 1.14 .This indicate that Mg/PTCDA have more polarity and have more energy to reformation and that's lead to decreasing the total energy of flow electrons .On the other hand ,the rate with solvent Formamid ,Formic acid and Ethanol solvent larger than rate with Acetontrile and Water solvent for both system ,this indicate the effect of potential barrier that cooperation with transition energy to impedance transfer of electrons .Data in tables(5)and (6) for both system indicate that the electronic transfer due interface of two systems dependent on quantity of electrons energies to transition the potential barrier.. The transfer of electrons is limited by the quantity of driving force energy .It drive much more electrons to transfer a potential at interface. The driving force of flow electrons depending on the absorption spectrum in figure (1) that's refers how can the electrons transfer to crossing interface potential from Fermi energy state at Mg or Al metal to state at PTCDA molecule that are showing at table (5) and table(6) . The driving force results at tables (3-4) are good useful parameter to Investigated the potential dependence of transfer of electrons at interface. As long as the overlapping coupling between metal and molecule energy levels should be effected on rate that showing from results at tables (5) and (6). Understandably, the overlapping between two wave function of electronic state would be deformation the Potential at interface and do to decreasing this potential and lead to cross more electrons and leading to transfer large electrons from Mg or Al metal to the organic PTCDA molecule.

5. Conclusion

In conclusion, it's clear that the electrons transfer are limited the electrical properties at metal/liquid interface system. It's clearing controllably the transition energy and potential at interface cooperation with the overlapping coefficient. The electrons transfer rate show that increases with decrease the transition energy and increases driving force energy and overlapping coupling coefficient. In summary, conclusion that Al metal was more alignment levels with PTCDA than Mg and leading to increases the transfer at Al/PTCDA more Mg/PTCDA devices increases the transfer at Al/PTCDA more Mg/PTCDA devices.

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