

Theoretical Investigation of the Flow Charge Transfer Rate Through Cu/NTCDA molecule Interface

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Article Info

Volume 83

Page Number: 8821 - 8829

Publication Issue:

May - June 2020

Abstract:

We investigated and studied the flow charge transfer rate at NTCDA molecule contact to Cu metal through seven different solvents groups. It can be understood the effect of transition energy on the electronic properties of NTCDA/Cu junctions depending on results of flow charge transition rate. Our investigation suggests that solvents type effect on the flow charge transfer between the NTCDA molecule and Cu metal, it plays an important role in the limits of the electric properties. We find that the transition energy of charge transfer, which is governed by the polarity of media, is strongly limited to the values of flow charge rate through NTCDA/Cu devices. In particular, Propanonitrile solvent with NTCDA/Cu system exhibit a strong transfer and large flow rate overall coupling strength, whereas 2-methylpyridin solvent with NTCDA/Cu system shows exhibited a smaller transfer and flow charge rate overall coupling strength. Finally, the electronic energy levels of Cu is closely related to the HOMO–LUMO energies of NTCDA molecule energies in NTCDA/Cu devices.

Article History

Article Received: 19 November 2019

Revised: 27 January 2020

Accepted: 24 February 2020

Publication: 18 May 2020

Keywords: NTCDA molecule, optical properties, flow charge transition rate, coupling strength.

INTRODUCTION

The electron transfer processes is one of the basic reaction in different fields of science, it's abounding in organicmolecular systems physics, physical chemistry and biophysics [1]. Metal–molecule devices has the promised that by changed the builds blocks of organic ligands with metal material and an increasing applications for many different fields of life[2]. The electron transfer through Molecule – metal has attracted increasable continuous in due to their basically importance for different fields such that: electrochemistry, irradiation-induced of thin

organic film, molecular photovoltaic and molecular electronics[3]. Theory of electronic transition processes is an important field of persistent interesting in physics and technology. The electron transfer cross molecule - solid interface has investigated by many researchers in the past several decades[4]. Due to theoretical point of view, hadi etal theory are employed to investigated electron transfer through charge localized on donor and acceptor states of electrons. The alignment of energy levels for different material interfaces is the most parameter important in this theory between the two localized states[5-7]. In this contribution, the flow

charge transfer through NTCDA molecule has chemical formula 1,4,5,8-Naphthalenetetracarboxylic dianhydride that's illustrated in figure(1) contact with Cu metal will be studied and calculated using quantum scenario for transition from donor NTCDA to an acceptor Cu system under tunneling potential at interface. Within a quantum picture, the use of continuum energy levels for two material within polarity media solvent for system.

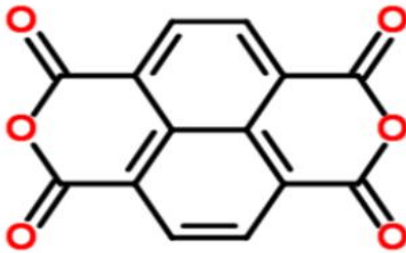


FIGURE 1 . Illustrated of chemical structure for NTCDA molecule dye.

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \int_{-\infty}^{\infty} F(E) |\langle \hat{H}_{\alpha\beta} \rangle|^2 \delta(E_{\beta} - E_{\alpha}) dE \quad (1)$$

Where h is Planck constant, $F(E)$ is the occupation Fermi Dirac, $\langle \hat{H}_{\alpha\beta} \rangle$ is the strength coupling and $\delta(E_{\beta} - E_{\alpha})$ is Dirac potential. The occupancy Fermi function for flow electrons transfer from molecule to metal is written as [9].

$$F(E) = \frac{e^{-\frac{E}{2k_B T}}}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} \quad (2)$$

Furthermore, we introduce the density of electronic state $\rho(E)$ in Cu-NTCDA molecule system [10].

$$\hat{\rho}(E) = \sqrt{\frac{1}{4\pi T_M \frac{m}{k_B T}}} e^{\frac{-(T_M + \Delta E^0)^2}{4T_M \frac{m}{k_B T}}} \quad (3)$$

Inserting Eq.(3) and Eq.(2) in Eq.(1) to obtained.

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M \frac{m}{k_B T}}} \int_{-\infty}^{\infty} \frac{e^{-\frac{E}{2k_B T}}}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} |\langle \hat{H}_{\alpha\beta} \rangle|^2 e^{\frac{-(T_M + \Delta E^0)^2}{4T_M \frac{m}{k_B T}}} \delta(E_{\beta} - E_{\alpha}) dE \quad (4)$$

Since, the activity density of metal $D_M(E)$ will be given by [11].

$$D_M(E) = \sum \delta(E_{\beta} - E_{\alpha}) \quad (5)$$

Then Eq.(4) with Eq.(5) lead to .

THEORY

Firstly, the fundamental assumptions of the charge transfer theory in metal-molecule interface is that continuum energy levels of localized electronic state at donor and acceptor state in two material metal and molecule. This assumption has been enabled us to discussion the transfer through homogenous devices. Generally, it has been supposed that an electron transfer over potential at interface of two materials. In order to investigate and calculated the flow charge transfer rate theoretically, it has been achieved via approximately solved the probability of N electrons have flow from donor state to an acceptor state by reaction rate given by [8].

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \int_{-\infty}^{\infty} \frac{e^{-\frac{E}{2k_B T}}}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} |\langle \hat{H}_{\alpha\beta} \rangle|^2 e^{\frac{-(T_M + \Delta E^0)^2}{4T_M k_B T}} D_M(E) dE \quad (6)$$

While the activation density of states related with atomic density of metal ρ_M by [12].

$$D_M(E) = \rho_M \frac{l_M}{r_M^{2/3} \left(\frac{6}{\pi}\right)^{1/3}} \quad (7)$$

Where l_M is coupling length and r_M is average diameter of an atom in the metal lattice in $\left(\frac{cm}{atom}\right)$.

Inserting Eq.(7) with Eq.(6) to results .

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \int_{-\infty}^{\infty} \frac{e^{-\frac{E}{2k_B T}}}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} |\langle \hat{H}_{\alpha\beta} \rangle|^2 e^{\frac{-(T_M + \Delta E^0)^2}{4T_M k_B T}} \rho_M \frac{l_M}{r_M^{2/3} \left(\frac{6}{\pi}\right)^{1/3}} dE \quad (8)$$

The atomic density of metal reduced to [13].

$$\rho_M = \frac{3N(E_F)}{2E_F} \quad (9)$$

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

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \int_{-\infty}^{\infty} \frac{e^{-\frac{E}{2k_B T}}}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} |\langle \hat{H}_{\alpha\beta} \rangle|^2 e^{\frac{-(T_M + \Delta E^0)^2}{4T_M k_B T}} \frac{3N(E_F)}{2E_F} \frac{l_M}{r_M^{2/3} \left(\frac{6}{\pi}\right)^{1/3}} dE \quad (10)$$

So , the driving force is given by

$$\Delta E^0 = E_F - IE \quad (11)$$

Where E_F is the Fermi energy at metal , IE is the ionized energy of molecule.

We must remove the constant term out integral expression and inserting Eq.(11) in Eq.(10) to obtained .

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \frac{3N(E_F)}{2E_F} \frac{l_M}{r_M^{2/3} \left(\frac{6}{\pi}\right)^{1/3}} e^{\frac{-(T_M + E_F - IE)^2}{4T_M k_B T}} \int_{-\infty}^{\infty} \frac{e^{-\frac{E}{2k_B T}}}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} |\langle \hat{H}_{\alpha\beta} \rangle|^2 dE \quad (11)$$

On the other hand ,the Eq.(11) can be rewrite with expand of exponential to.

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \frac{3N(E_F)}{2E_F} \frac{l_M}{r_M^{2/3} (\frac{6}{\pi})^{1/3}} e^{\frac{-(T_M + E_F - IE)^2}{\frac{4T_M k_B T}{m}}} \int_{-\infty}^{\infty} \frac{|\langle \hat{H}_{\alpha\beta} \rangle|^2}{(e^{-\frac{E}{2k_B T}} + e^{\frac{E}{2k_B T}})} \left[1 - \left(\frac{E}{2k_B T} \right) + \frac{1}{2!} \left(\frac{E}{2k_B T} \right)^2 - \frac{1}{3!} \left(\frac{E}{2k_B T} \right)^3 + \dots + \frac{1}{n!} \left(\frac{E}{2k_B T} \right)^n \right] dE \quad (12)$$

The integral in Eq.(12) must be solving mathematically .

$$\Gamma_{\alpha}^{\beta}(E) = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \frac{3N(E_F)}{2E_F} \frac{l_M}{r_M^{2/3} (\frac{6}{\pi})^{1/3}} e^{\frac{-(T_M + E_F - IE)^2}{\frac{4T_M k_B T}{m}}} |\langle \hat{H}_{\alpha\beta} \rangle|^2 \left[\pi k_B T + \frac{1}{2!} \left(\frac{1}{2k_B T} \right)^2 \frac{(\pi k_B T)^3}{4} + \frac{1}{4!} \left(\frac{1}{2k_B T} \right)^4 \frac{5(\pi k_B T)^5}{16} + \dots \dots \frac{1}{n!} \left(\frac{1}{2k_B T} \right)^n \beta(\pi k_B T)^{n+1} \right] \quad (13)$$

However , the approximation of flow rate per electrons concentration is .

$$\Gamma_{\alpha \rightarrow \beta} = \frac{\Gamma_{\alpha}^{\beta}(E)}{N(E_F)} \approx \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi T_M k_B T}} \frac{3}{2E_F} \frac{l_M}{r_M^{2/3} (\frac{6}{\pi})^{1/3}} e^{\frac{-(T_M + E_F - IE)^2}{\frac{4T_M k_B T}{m}}} |\langle \hat{H}_{\alpha\beta} \rangle|^2 \left[\pi k_B T + \frac{1}{2!} \left(\frac{1}{2k_B T} \right)^2 \frac{(\pi k_B T)^3}{4} + \frac{1}{4!} \left(\frac{1}{2k_B T} \right)^4 \frac{5(\pi k_B T)^5}{16} \right] \quad (14)$$

The theoretical driving energy for electrons to transfer cross interface of two material is [14].

$$\Delta E^0 = E_{\lambda} - T_M \quad (15)$$

Where $E_{\lambda} = h \frac{c}{\lambda}$ is the absorption energy by electron , c is the velocity of light and λ is the wave length.

The transition energy T_M for electrons transfer has charge e from molecule to metal is [15].

$$T_M(eV) = \frac{e^2}{8\pi\epsilon_0} \left(\frac{1}{n^2} - \frac{1}{\epsilon} \right) \left(\frac{1}{R} - \frac{1}{2D} \right) \quad (16)$$

where ϵ_0 is vacuum permittivity, n and ϵ are the optical and the static dielectric constant ,

R is the radius of the molecule and D is the distance between the complex and electrode.

The radii of materials are calculated by [16].

$$R = \left(\frac{3M}{4\pi N\rho} \right)^{1/3} \quad (17)$$

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

RESULTS

The flow rate of electron transfer is showing in Eq. (14) that produced due to transfer from NTCDA molecule to Cu metal is determined by the relationship between the transition energy $T_{\frac{M}{m}}(eV)$, Fermi energy of Cu metal, effective length l_M , mass density r_M , ionization energy of molecule IE and coupling strength $\langle \hat{H}_{\alpha\beta} \rangle$ parameters. One of the most important parameter in Eq.(14) is the transition energy $T_{\frac{M}{m}}(eV)$ in Eq.(16). The transition energy $T_{\frac{M}{m}}(eV)$ dependent on individual parameters such as radius of molecule R and separation distance between Cu metal and NTCDA molecule D and optical and dielectric constant. The radii of both Cu and NTCDA are calculated by the relationship in Eq.(17) between the molecular weight $M = 63.546$ for Cu and 268.178 for NTCDA molecule in unit g/mol and density of mass $\rho = 8.96$ for Cu and 1.8 for NTCDA molecule in unit g/cm³ from table(1) with Avogadro's constant to results $R=1.28 \text{ \AA}$ for Cu metal and $R=1.28 \text{ \AA}$ for NTCDA molecule.

TABLE 1. Characteristic of NTCDA dye molecule and Cu metal [17].

Properties	NTCDA	Cu
Molecular weight	268.178	63.546
g/mol		
Crystal structure	C ₁₄ H ₄ O ₆	Cu
Mass Density (g/cm ³)	1.8	8.96
Lattice constant(Å)		3.61
Radius(Å)	3.8948	1.28
Ionization energy eV	8	
HOMO eV	5.6	
LUMO eV	4	

TABLE 2. The main properties of solvents[18]

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

Furthermore, the transition energy can be estimation using Eq. (16) with inserting radius of molecule $R=1.28 \text{ \AA}$ and distant between Cu and NTCDA $D \approx R_{Cu} + R_{NTCDA}$ and taken account the refractive index and dielectric of solvents from table (2) and $\frac{e^2}{8\pi\epsilon_0} \approx 7.2 \text{ eV}$, results are shown in table(3)

TABLE 3. Evaluated data transition energy $T_{M/m}(eV)$ for Cu/ NTCDA system.

Solvent type	Refractive index (n) [18]	Dielectric constant (ε)[18]	Calculation Polarityfunction F(n,ε)	Calculation transition energy $T_{M/m} (eV)$
2-methylpyridin	1.4984	9.9533	0.344	0.397
Hexanone	1.4007	14.136	0.439	0.506
Acetone	1.3559	20.493	0.495	0.570
Bezonitrile	1.5257	25.592	0.390	0.450
Propanonitrile	1.3633	29.324	0.503	0.581
Nitrobenzene	1.5030	34.809	0.413	0.477
1,2-ethanediol	1.4306	40.245	0.463	0.534

The driving force energy is deduced numerically according to Eq.(15) depending to transition energy

from table(3) and spectrums energy of NTCDA molecule with wave length limited (300 to 400)nm ,results

are shown in table(4) and figure (2).

TABLE 4. Data results of driving force ΔE for Cu/ ADCTN interface system

Wave length λ nm	Energy(e V)	2-Methy lp-yrudin	Hexanon e	Acetone	Bezonitril e	Propan-onitrile	Nitrobe-nzene	1,2-etha-nediol
300	4.133	3.735	3.627	3.562	3.683	3.552	3.656	3.598
350	3.542	3.145	3.036	2.971	3.092	2.961	3.065	3.008
400	3.099	2.702	2.593	2.529	2.649	2.518	2.622	2.565
450	2.755	2.357	2.249	2.184	2.305	2.174	2.278	2.220
500	2.479	2.082	1.973	1.909	2.029	1.898	2.002	1.945
550	2.254	1.856	1.748	1.683	1.804	1.673	1.777	1.719
600	2.066	1.668	1.560	1.495	1.616	1.485	1.589	1.531
650	1.907	1.509	1.401	1.336	1.457	1.326	1.430	1.372
700	1.771	1.373	1.265	1.200	1.321	1.190	1.294	1.236
750	1.653	1.255	1.147	1.082	1.203	1.072	1.176	1.118
800	1.549	1.152	1.043	0.979	1.099	0.968	1.072	1.015

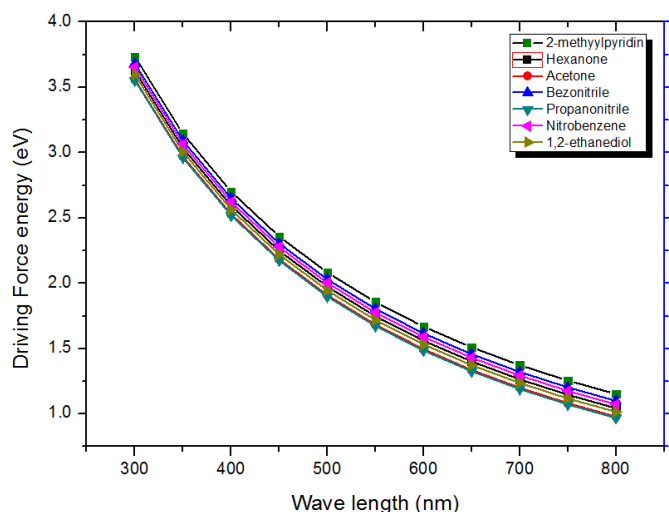


FIGURE 2.Driving force energy verse wave length of spectrum for NTCDA molecule in NTCDA/Cu system.

Furthermore, the coupling strength in Eq.(14) for molecule-metal is taken $\langle \hat{H}_{\alpha\beta} \rangle = 2.25 \times 10^{-2}, 2.5 \times 10^{-2}, 2.75 \times 10^{-2}, 3 \times 10^{-2}, 3.25 \times 10^{-2}, 3.5 \times 10^{-2}, 3.75 \times 10^{-2} \text{ eV/state}$

for the contact surfaces of two material. The coupling strength indicated the kinds of transfer non adiabatic electron transfer. In this situation, electrons with $\langle \hat{H}_{\alpha\beta} \rangle \ll 1$ is called non adiabatic reaction while $\langle \hat{H}_{\alpha\beta} \rangle \gg 1$ is called adiabatic reaction. According to this, the transfer of electron in NTCDA/Cu system is non-adiabatic transfer.

The interface of NTCDA-Cu is effected on charge transfer between NTCDA molecule and Cu electrodes. It can be estimated using Eq.(19) upon contact and taken transition energy from table (3), results are formulated in table(5).

In order to obtain the flow electronic rate for NTCDA/Cu interface theoretically, it can be applied Eq.(14) and taking data of transition energy from table (3) and using $E_F = eV$ for Cu metal, $IE = 8 \text{ eV}$ for NTCDA molecule [17], effective coupling length $l_M = 1 \times 10^{-8} \text{ cm}$ [19] with strength coupling $\langle \hat{H}_{\alpha\beta} \rangle$ and atomic density from table(1), results are listed in table (5) and figure(3).

TABLE 5. The calculated of flow electronic rate at NTCDA/Cu interface system.

Solvent	The flow electronic rate $\Gamma_{\alpha}^{\beta}(E) \times 10^{-16}$					
	Coupling strength $\langle \hat{H}_{\alpha\beta} \rangle \times 10^{-2}$					
	2.25	2.5	2.75	3	3.25	3.5
2-methylpyridin	0.0116	0.0144	0.0174	0.0207	0.0243	0.0282
Bezonitrile	0.1219	0.1505	0.1821	0.2167	0.2544	0.2950
Nitrobenzene	0.3176	0.3921	0.4744	0.5646	0.6626	0.7685
2-Hexanone	0.7627	0.9417	1.1394	1.356	1.5914	1.8457
1,2-ethanediol	1.6044	1.9807	2.3967	2.8522	3.3474	3.8822
Acetone	3.5371	4.3668	5.2838	6.2881	7.3798	8.5589
Propanonitrile	4.302	5.3111	6.4264	7.648	8.9758	10.4098

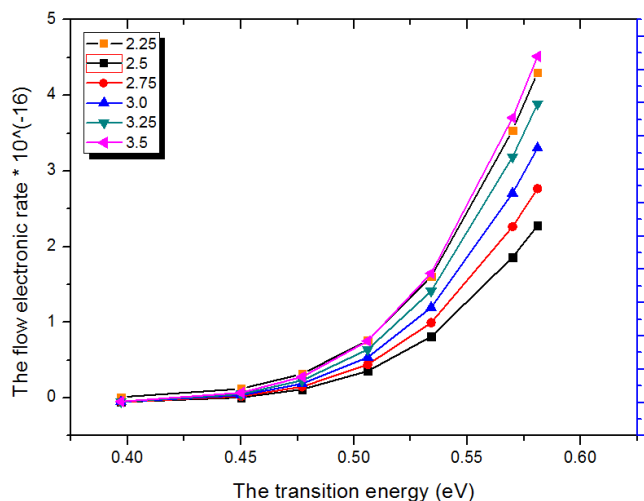


FIGURE 3. Results of flow electronic rate at NTCDA/Cu interface with variety strength coupling $\langle \hat{H}_{\alpha\beta} \rangle$.

DISCUSSION

Due to theoretical analytical expression for the flow electronic rates given in Eq.(14), we note that transition energy and strength coupling with driving force energy are the key parameters that limited the flow rate of electrons. The transition energy of different solvents of NTCDA molecule contact with Cu metal are displayed in table (3). The lower transition energy has been done on 0.397 eV with 2-methylpyridin solvent and the upper transition energy has been recorded at 0.581 eV with

Propanonitrile solvent. The table(3) shows that the transition energy increases with increases the Polarity function and decreases with increases refractive index (n), and that the transition energy of these solvents showed moderate shift with increased dielectric constant, it indicates that with the addition of solvent has large polarity, the transition energy will be extended more for solvents have increased dielectric constant compare with solvent has decreased refractive index. The results of transition energy for NTCDA/Cu system will be support that good knowledge for media of electrons transfer between NTCDA molecule and Cu metal in solution and gold coupling interaction between energy levels for Cu and NTCDA molecule.

The NTCDA-CU devices binding forcedly was determined by strength coupling that limited of transfer reaction types, there is an adiabatic of interaction between Cu with NTCDA molecules complexes. However, the driving force energy in table(4) and figure(2), show the electrons move forcedly cross interface with increasing energy for decreased wave length and increased absorption energy. This because the electron has more energy to transfer cross potential at interface. Furthermore, the driving force and transition energy are large effected on the limited of flow charge rate. Table(5) show the flow charge transition rate is increases with

increased the strength coupling and vice versa, these indicate the alignment of energy levels for two material is best to transfer over potential at interface. On the other hand, the flow charge rate increased with increased the transition energy, that's means the transition energy supplied good rearrangement levels to transfer. Repeated to table(3) and table (5), we can the system NTCDA /Cu with solvent Propanonitrile has large flow charge rate and large transition rate compare with same system with 2-methylpyridin solvent has low flow charge rate and low transition rate. This indicate the flow charge rate is strongly function of transition energy. The flow chsrge rate for NTCDA/Cu with other Bezonitrile, Nitrobenzene, Hexanone, 1,2-ethanediol and Acetone solvents were done in table (5) showing alternative results between 2-methylpyridin solvent and Propanonitrile Solvent observed. In summary the flow charge transfer rate increases with increase the transition energy, driving force and coupling strength. These three parameters has supplied the electrons by more energies to transfer the interface from donor state to an acceptor state in NTCDA/Cu system.

CONCLUSION

Theory of the electron transfer mechanism has been described and investigated in this paper based on the concept of transition theory and quantum postulate for mobile electrons in a NTCDA/Cu metal. To summarize, the flow charge rate calculations is limited the relationship between the transition energy, driving force and coupling strength with Fermi energy and ionization energy of the Cu and NTCDA respectively. In particular, the transition energy of the NTCDA molecule relative to Cu metal could be determined the flow charge transfer between the NTCDA and the Cu. Furthermore, this study has demonstrated a simple quantum relationship between the charge transfer and the rearrangement of the

electronic states for two material NTCDA and Cu, which in turn limited the electronic properties of NTCDA/Cu devices. That's lead to expect the transition energy and driving force energy have determine the nature of the potential at interface and it can be guide the electrons to transfer cross interface between NTCDA and Cu materials.

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