# Effect of traps' adjacency on the electric field dependence of mobility in organic systems*

He Yun(何 鋆), Chen Xiao-Qing(陈小青), and Hou Xiao-Yuan(侯晓远)†

*Key Laboratory of Micro and Nano Photonic Structures (Ministry of Education) and State Key Laboratory of Surface Physics, Fudan University, Shanghai* 200433, *China*

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In some organic materials, varying the finite distance between adjacent carrier traps modifies the Coulomb potential around each trap, resulting in a more complex field-dependence of mobility, differing from (but not incompatible with) the usually considered relationship of $\ln\mu \propto \sqrt{E}$, a relationship which has been successfully explained by the Poole–Frenkel effect. To investigate the influence of the adjacency of traps, a model system is proposed, which consists of two traps separated by distance $\alpha$. Our numerical calculation shows that with increasing $\alpha$, the dependence of mobility on the electric field changes from linear to exponential. Moreover, beyond a certain large $\alpha$, i.e., as the distance to the nearest trap approaches infinity, the proposed model is essentially the same as the Poole–Frenkel effect. The proposed model accounts for the effect of the energy barrier shape, especially the effect of the location of the potential-energy maximum, a phenomenon which is not accommodated in the Poole–Frenkel model. Because the model assumes the Coulomb interaction between the adjacent traps, it applies to those charged traps which may exist in organic materials for various reasons.

**Keywords:** electric field-dependent mobility, trap, organic semiconductor

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## 1. Introduction

Ever since the conductivity of organic materials was discovered, tremendous efforts have been made to explore the conduction mechanism. Due to the complexity, no single theory exists that can explain all the transport phenomena observed in organic materials. The investigations of mobility in organic single crystals such as pentacene indicate that their conduction is band-like transport.[1,2] However, in disordered small-molecule materials such as NPB, TPD, and AlQ, because of the intermolecular weak van der Waals force, no energy band exists, and under an applied electric field, the carriers are believed to hop from site to site. Many experimental researchers have shown that the electric field dependence of the mobility in these highly disordered systems is described by $\ln\mu \propto \sqrt{E}$, where $\mu$ is the carrier mobility and $E$ is the electric field.[3–7] Meanwhile, lots of theoretical research has been carried out. Bässler investigated the carrier transport in organic disordered materials by using the Miller–Abraham model combined with the Gaussian distribution of density of states; his Monte Carlo simulation verified the above $\mu$–$E$ relationship.[8] In fact, this $\ln\mu \propto \sqrt{E}$ dependence can be explained by using a simple physical model: the Poole–Frenkel effect.[9] However, for some molecularly doped polymers, many reports show more complex behaviors.[10–17] Borsenberger *et al.* found that the mobility follows a linear relationship with the electric field in a triphenylamine-doped bisphenol-A-polycarbonate system,[18] and Stolka *et al.* observed that in films of solid solution of N,N'-diphenyl-N,N'-bis(3-methylphenyl)-[1, 1'-biphenyl]-4,4'-diamine in bisphenol-A-polycarbonate, the electric field dependence of the mobility is $\ln\mu \propto E$.[19] Obviously, these two relationships cannot be explained by the Poole–Frenkel effect, and the investigation of the physics beneath these different relationships is still missing so far. The Poole–Frenkel effect reveals the main physical picture of the carrier hopping process, i.e., an electric field lowers the energy barrier by $\beta_{\rm PF}\sqrt{E}$, and it can be applied to explain many experimental results about the electric field dependency of mobility;[11] however, it considers only the influence of the electric field on the Coulomb potential of a single trap while ignoring the effect of the adjacent traps. In fact, the Poole–Frenkel effect applies to the interface cases. For the carriers in other cases, e.g., in bulk, the potential around each trap is quite different from that around a single isolated trap, and sometimes the Poole–Frenkel effect is too simple to fully account for the carrier transport. In the present work, in order to take account of the effect of adjacent traps, a model system consisting of two traps is established. The electric field dependence of the mobility is investigated via numerical calculation of the tunneling probability. It is found that the relationship between electric field $E$ and mobility $\mu$ depends on the distance between the adjacent traps. When the distance $\alpha$ is short, the relationship is linear, $\mu \propto E$. With increasing $\alpha$, the relationship gradually changes to exponential, $\mu \propto \exp(E)$. Moreover, for very large distance $\alpha$, the model presented in this work reduces to

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†Corresponding author. E-mail: xyhou@fudan.edu.cn

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the Poole–Frenkel effect, which means that the effect of the adjacent traps becomes negligible.

## 2. Theory and discussion

Consider the electron transport as an example. If the electron trap is regarded as a positively charged center at a fixed position, the Coulomb potential energy of the electron is

$$V(r) = -\frac{e^2}{4\pi\varepsilon r}, \tag{1}$$

where $\varepsilon$ is the dielectric constant of the material, with a given value of $2.66\times10^{-11}$ F/m in the calculations below, $e$ is the elementary charge, and $r$ is the distance from the center. The maximum value of $V(r)$ is zero and the corresponding distance is infinite.

When uniform electric field $E$ is applied, the potential energy of the electron becomes

$$V_1(r) = -\frac{e^2}{4\pi\varepsilon|r|} - eEr. \tag{2}$$

As Fig. 1(a) shows, $V_1(r)$ is reduced on the right side of the trap and has a maximum at

$$r_1 = \sqrt{e/(4\pi\varepsilon E)} \tag{3}$$

from the center. The height of the potential barrier is lowered in the field by the amount

$$\Delta U = V(\infty) - V_1(r_1) = \beta_{\rm PF}\sqrt{E}, \tag{4}$$

where $\beta_{\rm PF}$ is the Poole–Frenkel factor and equals $\sqrt{e^3/\pi\varepsilon}$. This is the well-known Poole–Frenkel effect.[9]

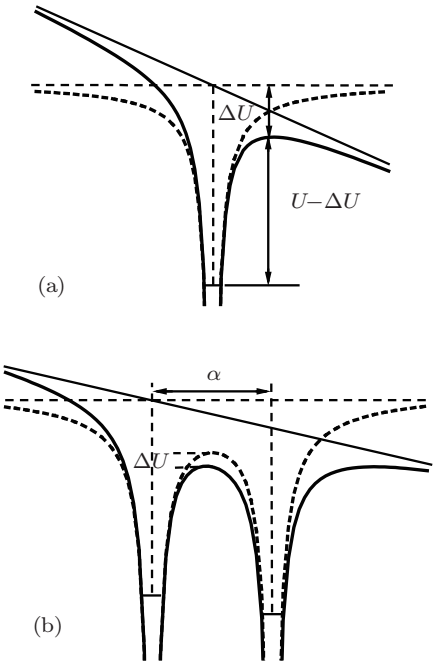



**Fig. 1.** (a) Poole–Frenkel effect, and (b) the proposed model system. The dashed and solid lines show the potentials in the absence and the presence of an electric field, respectively; and $\Delta U$ represents the reduction of the energy barrier.

Obviously, the Poole–Frenkel effect accounts for the influence of an electric field on the mobility with respect to only a single isolated trap, while disregarding the effect of neighboring traps which exist in any real material. Here a model system is proposed to investigate the neighbors' effects. As shown in Fig. 1(b), the system consists of two traps, the distance between them is $\alpha$, i.e., only the effect of the nearest neighbor is taken into account. The potential energy of the electron in the proposed system is

$$\mathrm{V}_2(r) = -\frac{e^2}{4\pi\varepsilon|r|} - \frac{e^2}{4\pi\varepsilon|(\alpha-r)|} = -\frac{\theta}{|r|} - \frac{\theta}{|\alpha-r|}, \tag{5}$$

where $\theta = \sqrt{e^2/4\pi\varepsilon}$. When electric field $E$ is applied, the potential energy becomes

$$\begin{aligned}\mathrm{V}_3(r) &= -\frac{e^2}{4\pi\varepsilon|r|} - \frac{e^2}{4\pi\varepsilon|(\alpha-r)|} - eEr \\ &= -\frac{\theta}{|r|} - \frac{\theta}{|\alpha-r|} - eEr.\end{aligned} \tag{6}$$

As Fig. 1(b) shows, in the absence of the externally applied field, $V_2(r)$ has a maximum just at the middle between the two adjacent traps. In the presence of the field, the height of the energy barrier is lowered, like the case of the Poole–Frenkel effect, while the location of the potential maximum, $r_2$, shifts to the left side

$$r_2 = \frac{\alpha}{2} - \frac{1}{2\sqrt{3}}\sqrt{B} + \frac{1}{2}\sqrt{\alpha^2 - \frac{B}{3} + \frac{4\sqrt{3}\alpha\theta}{Eq\sqrt{B}}}, \tag{7}$$

where

$$\begin{aligned}A &= \alpha^6E^3q^3 + 54\alpha^2Eq\theta^2 \\ &\quad -6\sqrt{3}\sqrt{\alpha^8E^4q^4\theta^2 + 27\alpha^4E^2q^2\theta^4},\end{aligned}$$

and

$$B = \alpha^2 + \frac{\alpha^4Eq}{\sqrt[3]{A}} + \frac{\sqrt[3]{A}}{Eq}.$$

The variation of the location of the potential energy maximum with the electric field for different values of $\alpha$ is shown in Fig. 2. It can be seen that for any $\alpha$, $r_2$ decreases with increasing field, while for a given electric field, $r_2$ increases with increasing $\alpha$. Moreover, the larger $\alpha$ is, the greater the influence of the field is. Meanwhile, when $\alpha$ increases from 0.7 nm to 3 nm, the relationship between $r_2$ and the electric field is basically linear, while it is not linear if $\alpha$ exceeds 3 nm. If $\alpha$ approaches infinity, the relationship appropriately looks like the single isolated trap case (the Poole–Frenkel effect).

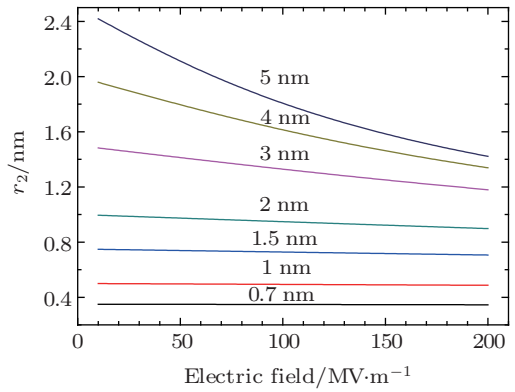



**Fig. 2.** (color online) Location of the maximum of $V_3(r)$ versus electric field for different $\alpha$.

The variation of the maximum potential energy with the electric field according to Eqs. (6) and (7) is shown in Fig. 3. The maximum potential energy increases with increasing $\alpha$ for a given electric field; and it decreases with increasing field for a given $\alpha$. As shown in Fig. 2, the larger $\alpha$ is, the greater the influence of the field is. When $\alpha$ is between 0.7 nm and 3 nm, the relationship between the maximum potential energy and the electric field looks linear. The relationship begins to deviate from linearity if $\alpha$ exceeds 3 nm, similar to the relationship between the location of the potential maximum and the electric field.

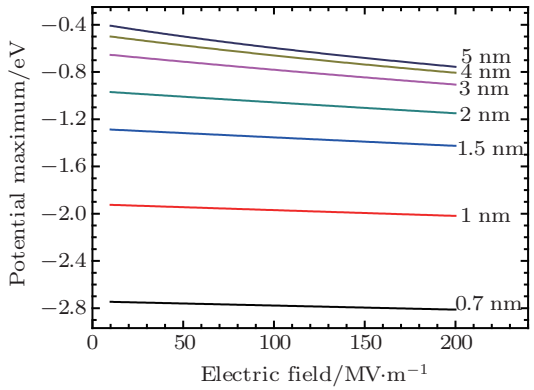



**Fig. 3.** (color online) Maximum of $V_3(r)$ versus electric field for different $\alpha$.

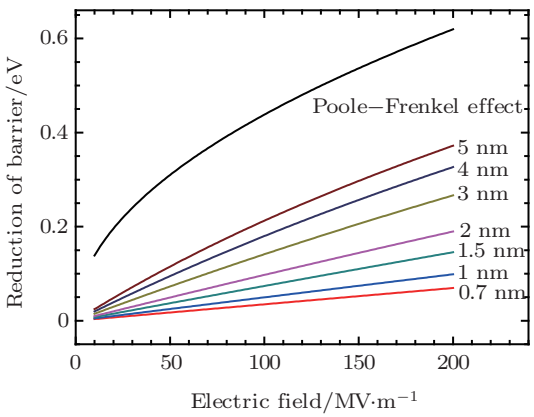



**Fig. 4.** (color online) Reduction of energy barrier versus electric field for different $\alpha$.

The height of the energy barrier is lowered by an amount of $\Delta U = V_2(\alpha/2) - V_3(r_2)$ in the electric field, and the relationship between $\Delta U$ and $E$ is shown in Fig. 4. For any given $\alpha$, $\Delta U$ increases with increasing field, and for a given field, $\Delta U$ increases with increasing $\alpha$. When $\alpha$ approaches infinity, it is as if the trap was the only trap in existence (the Poole–Frenkel effect). As Fig. 4 shows, the reduction of the energy barrier in the case of the Poole–Frenkel effect is the largest, this means that the electron tunneling probability is much higher for an isolated trap than for a trap with neighbors. However, the tunneling probability depends not only on the height but also on the shape of the energy barrier.

For simplicity of calculation, the energy barrier is approximated to be a triangular one with three ends. According to the results shown in Figs. 2 and 3, the relationships of location of potential energy maximum-to-electric field and that of maximum potential energy-to-electric field are both linear when distance $\alpha$ between the adjacent traps is less than 3 nm; in such a case, the three vertices of the triangular barrier can be set as $(0, -\Delta)$, $(C–\lambda E, -D–\eta E)$, and $(\alpha, -\Delta)$, where $\Delta$ is the trap energy of electrons, $C-\lambda E$ is the location of the potential maximum, $-D-\eta E$ is the value of the potential maximum, and $C$, $D$, $\lambda$, and $\eta$ can be obtained by fitting the lines shown in Figs. 2 and 3 for different $\alpha$ less than 3 nm. The triangular barrier $U(x)$ is

$$\frac{\Delta - D - \eta E}{C - \lambda E} x - \Delta, \quad (0 \le x \le C - \lambda E), \tag{8}$$

$$\frac{D + \eta E - \Delta}{\alpha - C + \lambda E}(x - C + \lambda E) - D - \eta E, \quad (C - \lambda E < x \le \alpha), \tag{9}$$

where $x$ is the distance from the trap. Figure 5 shows the schematic diagram of the proposed approximately triangular energy barrier.

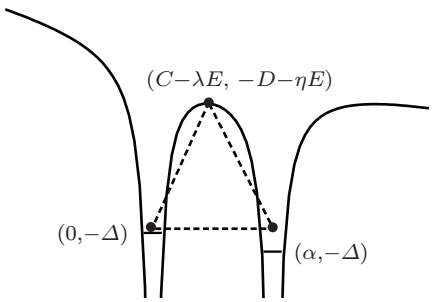



**Fig. 5.** Schematic diagram of approximately triangular energy barrier with three corners $(0, -\Delta)$, $(C–\lambda E, -D–\eta E)$, and $(\alpha, -\Delta)$.

According to the WKB approximation, the electron tunneling probability through this linear barrier is

$$T = \exp\left[-\frac{2}{\hbar}\sqrt{2m}\int_{x_1}^{x_2}\sqrt{U(x)-(-\Delta)}\,\mathrm{d}x\right]$$
$$= \exp\left[-\frac{2}{\hbar}\sqrt{2m}\left(\int_0^{C-\lambda E}\sqrt{\frac{\Delta-D-\eta E}{C-\lambda E}}x\,\mathrm{d}x+\int_{C-\lambda E}^{\alpha}\sqrt{\frac{D+\eta E-\Delta}{\alpha-C+\lambda E}(x-C+\lambda E)-D-\eta E+\Delta}\,\mathrm{d}x\right)\right]$$
$$= \exp\left(-\frac{4}{3\hbar}\sqrt{2m}\alpha\sqrt{\Delta-D-\eta E}\right) = \exp\left(-\frac{4}{3\hbar}\sqrt{2m}\alpha\sqrt{E_\mathrm{t}-\eta E}\right), \quad (10)$$

where $\hbar$ is the reduced Planck constant, $m$ is the electron mass, $E_\mathrm{t}$ is the depth of the trap and equals $\Delta$–$D$. When $E_\mathrm{t} = 0.4$ eV and $\alpha$ increases from 0.7 nm to 3 nm, the variation of the tunneling probability with the electric field is as shown in Fig. 6.

As Fig. 6 shows, the tunneling probability increases with increasing electric field for any given $\alpha$. Moreover, the larger $\alpha$ is, the greater the influence of the field on the tunneling probability is. When the field increases from 10 MV/m to 200 MV/m, the tunneling probability of electrons increases only from $4.94\times10^{-2}$ to $6.42\times10^{-2}$ for $\alpha = 0.7$ nm, while it increases about 2 orders of magnitude from $2.96\times10^{-6}$ to $5.36\times10^{-4}$ for $\alpha = 3$ nm. For a given electric field, the tunneling probability decreases with increasing $\alpha$, e.g., it decreases from $4.94\times10^{-2}$ to $2.96\times10^{-6}$ with $\alpha$ increasing from 0.7 nm to 3 nm when the field is 10 MV/m, a reduction of about 4 orders of magnitude.

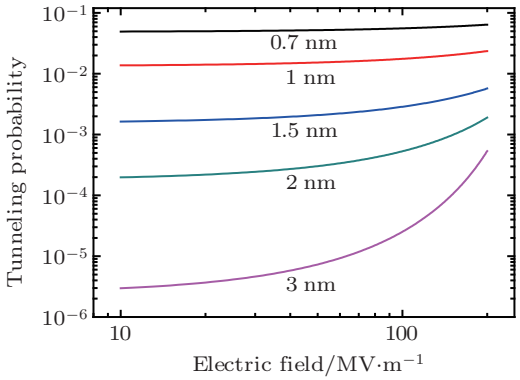



**Fig. 6.** (color online) Tunneling probability versus electric field for different $\alpha$.

To clearly show the variation of the relationship between tunneling probability and electric field for different $\alpha$, a plot of linear scale is shown in Fig. 7. When $\alpha = 0.7$ nm, the fitted line indicates that the relationship between tunneling probability and electric field is linear, and with an increase of $\alpha$, the relationship begins to deviate from linearity. When $\alpha$ equals 3 nm, the curves in Fig. 7 indicate that the tunneling probability changes with the electric field exponentially. In the present case, the mobility of the carriers is proportional to the tunneling probability, i.e., $\mu \propto T(E)$. Combining this insight with the relationship between tunneling probability and electric field, it can be concluded that when $\alpha$ increases from 0.7 nm to 3 nm, the electric field dependence of mobility changes from $\mu \propto E$ to $\ln\mu \propto E$.

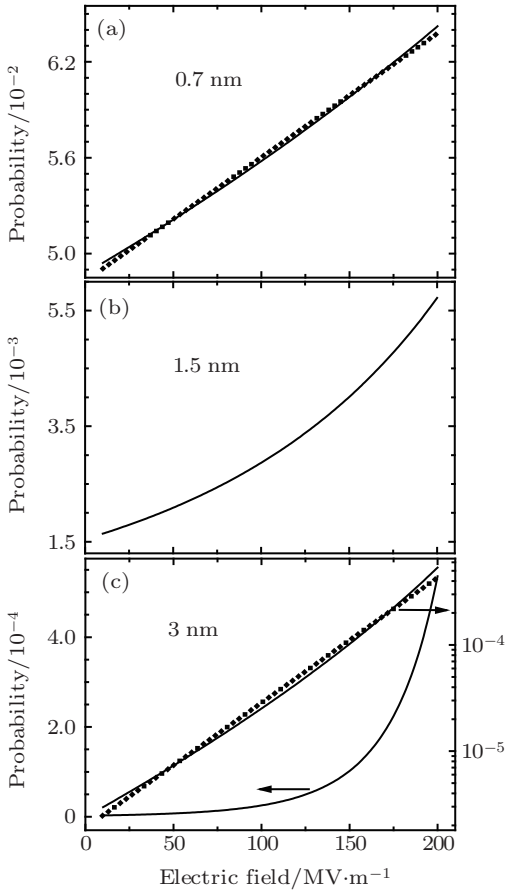



**Fig. 7.** Tunneling probability versus electric field for different $\alpha$: (a) $a = 0.7$ nm, (b) $a = 1.5$ nm, (c) $a = 3$ nm. For $\alpha = 3$ nm, the results are shown with both linear (left side) and logarithmic (right side) scales. The dashed lines are linear fits to $\mu$ versus $E$ and $\mu$ versus $\exp(E)$, respectively.

Many investigations about the organic small-molecule materials, polymers, and molecularly doped polymers have shown that the carrier mobility satisfies an empirical expression[3–7,11,14,20]

$$\mu(E,T) = \mu_{00}\exp\left[-(\Delta-\beta_\mathrm{PF}\sqrt{E})\left(\frac{1}{kT}-\frac{1}{kT_0}\right)\right],$$

where $\mu_{00}$ is a constant, $\Delta$ is the activation energy at zero electric field, $E$ is the electric field, $T$ is the temperature, $T_0$ is an empirical parameter, $k$ is the Boltzmann constant, and $\beta_\mathrm{PF}$ is the Poole–Frenkel factor. The electric field dependence of mobility is $\ln\mu \propto \sqrt{E}$, this relationship can be explained by the Poole–Frenkel effect. The energy barrier of the carriers is lowered from $\Delta$ to $\Delta-\beta_\mathrm{PF}\sqrt{E}$ by applying the field. The hopping probability is proportional to $\exp[-(\Delta-\beta_\mathrm{PF}\sqrt{E})/kT]$, result-

ing in $\ln\mu \propto \sqrt{E}$.[11,13–17,21,22] However, two other $\mu$–$E$ relationships, $\mu \propto E$ and $\mu \propto \exp(E/E_0)$, were also observed and cannot be explained by the Poole–Frenkel effect.[18,19]

The Poole–Frenkel effect only accounts for the influence of the electric field on a single trap, while no accommodation is made for the effect of adjacent traps, which will affect the hopping process of the carriers. Figure 4 shows that in the presence of the electric field, the reduction of the energy barrier when adjacent traps exist is much smaller than that in the single trap case, which means that the Poole–Frenkel effect overvalues the reduction of the energy barrier and might be not suitable in some cases. Besides, figure 2 shows that the barrier shape, especially the location of the potential energy maximum, is also affected by the field, a phenomenon which is not accommodated in the Poole–Frenkel effect. With consideration of the adjacent traps, the electric field dependence of mobility depends on the distance $\alpha$ between the traps. As shown in Figs. 6 and 7, with increasing $\alpha$, the relationship between tunneling probability and electric field changes from linear to exponential, indicating that the adjacent traps do influence the field dependence of the tunneling probability, which is proportional to the mobility. Therefore, both the linear and the exponential relationships observed experimentally in molecularly doped polymers[18,19] can be explained by the model proposed in the present work. Meanwhile, for a real material, $\alpha$ will change with the doping ratio, i.e., a low doping ratio leads to a large $\alpha$ between the adjacent traps, while a high doping ratio results in a small $\alpha$. As shown in Fig. 6, the tunneling mobility decreases with increasing $\alpha$. This means that the mobility will decrease with decreasing doping ratio, which is consistent with Stolka's report.[19] It should be noted that the model presented is based on the assumption that the interaction between the adjacent traps is the Coulomb interaction, thus the model applies to those charged traps which may exist in organic materials due to photo-oxidation of the $\pi$-conjugated backbone or the instability of radical-anions with respect to water, hydroxyl groups, or oxygen.[23,24] Besides, in practical organic devices, the $J$–$V$ characteristics would be affected by the field dependence of mobility, thus sometimes, the influence of the adjacent traps cannot be ignored and would be helpful in analyzing the $J$–$V$ characteristics and the related performance of organic devices.

## 3. Conclusion

In conclusion, the effect of adjacency of traps on the mobility is taken into account, and a model system consisting of two traps is established. The calculation shows that the electric field dependence of mobility changes from linear to exponential with the increase of the distance between the adjacent traps. Moreover, the result also shows that the Poole–Frenkel effect is the very-large-$\alpha$ case of the proposed model.

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