The role of acoustic phonon scattering in charge transport in organic semiconductors: a first-principles deformation-potential study

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The electron-acoustic phonon scattering for charge transport in organic semiconductors has been studied by first-principles density functional theory and the Boltzmann transport equation with relaxation time approximation. Within the framework of deformation-potential theory, the electron-longitudinal acoustic phonon scattering probability and the corresponding relaxation time have been obtained for oligoacene single crystals (naphthalene, anthracene, tetracene and pentacene). Previously, the electron-optic phonon scattering mechanism has been investigated through Holstein-Peierls model coupled with DFT calculations for naphthalene. Numerical results indicate that the acoustic phonon scattering intensity is about 3 times as large as that for the optic phonon and the obtained mobility is in much better agreement with the result of the experiment done for ultrapure single crystals. It is thus concluded that for closely packed molecular crystal where the electron is partly delocalized, acoustic phonon scattering mechanism prevails in the charge transport. Moreover, it is found that the intrinsic electron mobility is even larger than hole mobility. A frontier orbital overlap analysis can well rationalize such behavior.

1 Introduction

In recent years, organic semiconducting materials have found a lot of applications in electronic devices such as field effect transistors[1−3], light emitting diodes[4] and solar cells[5]. The major advantages of organic materials include flexibility without loss of performance, low cost for fabrication due to the possibility of using spin coating and inkjet printing method[6,7], and low power consumption in organic-based devices. Charge carrier mobility has crucial influence on the performance of organic electronic devices. Although recently much experimental progress[2,8−10] has been achieved on improving the charge carrier mobility of organic semiconductor, there are still some debates on the theoretical understanding of carrier transport mechanism in organic
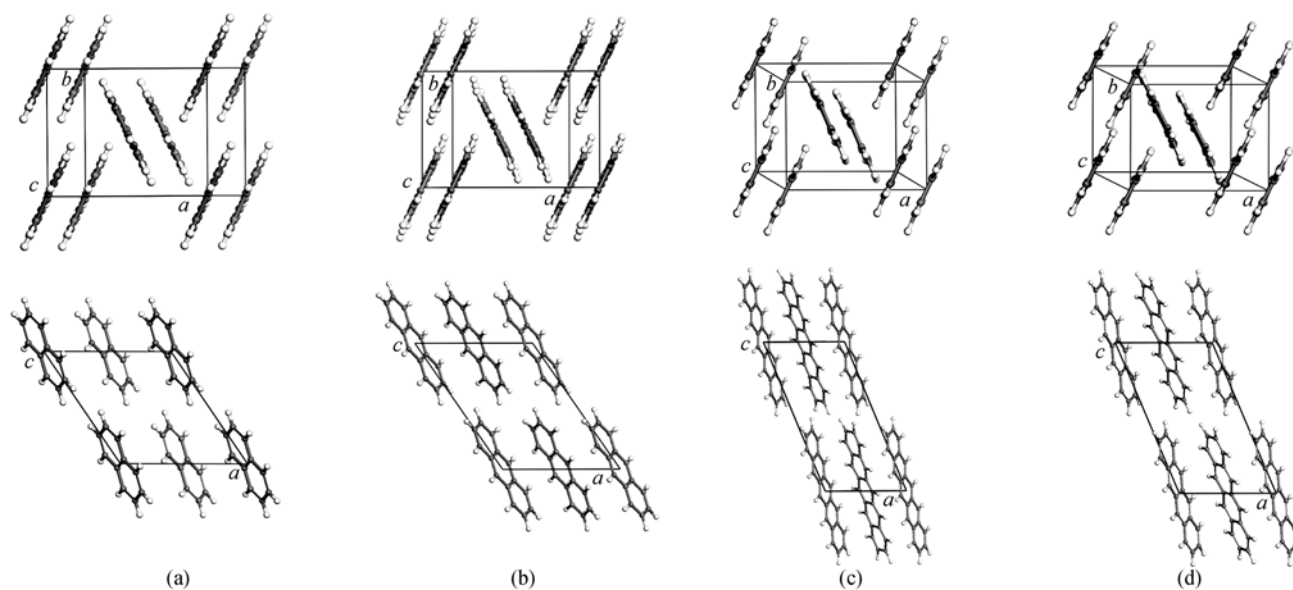
crystal[11].

The oligoacenes including naphthalene, anthracene, tetracene and pentacene (for crystal structures see Figure 1) are widely regarded as the prototypical materials in organic electronic devices and the synthesis of the ultrapure single crystals[8] enables us to study the intrinsic charge transport mechanism in organic molecular crystals. Up to now there exist two mechanisms describing charge transport in organic crystal, the hopping model based on localized electron picture and the small polaron model. For the hopping model it is believed that the car-

Figure 1 Crystal structures of oligoacenes. (a) Naphthalene; (b) anthracene; (c) tetracene; (d) pentacene.

riers would hop between localized states by the assistance of phonons, which can be described by the famous Marcus theory[12]. In the delocalized picture, the electron is dressed by the phonon to form a polaron and the electron-phonon scatterings play a central role. For many organic solids, it has been shown that the hopping model can provide reasonable description[13]. However, since organic materials cover a wide range of crystal packing forms, some closely packed systems, such as oligoacenes, demonstrate remarkable band-width, namely, a few tenth of an eV[14]. Wang et al.[15] have investigated the charge transport in naphthalene using the first-principles projected Holstein-Peierls model, where only electron-optic phonon scatterings have been considered. The charge mobility is proportional to the scattering time and various scattering mechanisms contribute to the total

scattering time as $\dfrac{1}{\tau} = \dfrac{1}{\tau_{op}} + \dfrac{1}{\tau_{ac}} + \dfrac{1}{\tau_{imp}} + \cdots$, where $\tau_{op,\ ac,\ imp}$

is the scattering time from optic phonon, acoustic phonon, impurity, etc. The inverse of the total mobility is a sum of the inverse of mobilities obtained from different scattering channels. It is seen that the shortest relaxation time scattering channel contributes the most to the mobility.

Note that for a delocalized electron, the coherence length can extend over several lattice constants, which match the most with the acoustic phonon wavelength. Thus, the transport behavior of delocalized electron can be dominated by the scattering with acoustic phonon, instead of optic phonon. It is the prime object of this work to evaluate the acoustic phonon scattering in organic crystal through first-principles calculation. The acoustic phonon scattering mechanism has been investigated using deformation-potential theory in evaluating the charge mobility in covalently bonded inorganic semiconductors[16] and polymers[17,18] within the effective mass approximation. In this work, we present for the first time a calculation of mobility based on Boltzmann equation (thus beyond the effective mass approximation) within the deformation-potential theory for non-covalently bonded organic crystal.

2 Methodological approaches

The Boltzmann equation is a very powerful tool for obtaining the transport properties of materials. In general, the mobility of the carriers is defined as $\mu = \sigma/(ne)$ where σ is the conductivity and n is the concentration of carriers. In Boltzmann method, all kinds of scattering processes can be simply introduced by relaxation time approximation. Here, we considered the anisotropic relaxation time $\tau(i, \boldsymbol{k})$ varying over the $\boldsymbol{k}$ states of the ith band in the first Brillouin zone. By means of introducing $\tau(i, \boldsymbol{k})$, the collision term in the Boltzmann equation can be written as $\partial f(i, \boldsymbol{k})/\partial t\big|_{\mathrm{coll}} = -\big[f(i, \boldsymbol{k}) - f_0(i, \boldsymbol{k})\big]\big/\tau(i, \boldsymbol{k})$, where $f_0(i, \boldsymbol{k})$ and $f(i, \boldsymbol{k})$ are the equilibrium and the perturbed distribution functions at $\boldsymbol{k}$ state of the ith band, respectively. Therefore, after evaluating the conductivity and the concentration of carrier, the mobility in relaxation time approximation is[14]

$$\mu_\alpha^{e(h)} = \frac{e}{k_B T} \frac{\sum\limits_{i \in CB(VB)} \int \tau_\alpha(i,\boldsymbol{k}) v_\alpha^2(i,\boldsymbol{k}) \exp\left[\mp \frac{\varepsilon_i(\boldsymbol{k})}{k_B T}\right] d\boldsymbol{k}}{\sum\limits_{i \in CB(VB)} \int \exp\left[\mp \frac{\varepsilon_i(\boldsymbol{k})}{k_B T}\right] d\boldsymbol{k}},$$

(1)

where α denotes the direction of external field and the minus (plus) is for electron (hole) mobility. $\varepsilon_i(\boldsymbol{k})$ and $v_\alpha(i,\boldsymbol{k})$ are band energy and the α component of group velocity at $\boldsymbol{k}$ state of the ith band, respectively. The summation of band was carried out over conduction band (CB) for electron and valence band (VB) for hole. Furthermore, the integral of $\boldsymbol{k}$ states is over the Brillouin zone (BZ).

To obtain the mobility, there are three parameters to be determined as shown in the above formula, namely, $\varepsilon_i(\boldsymbol{k})$, $v_\alpha(i, \boldsymbol{k})$ and $\tau_\alpha(i, \boldsymbol{k})$. First, the energy band $\varepsilon_i(\boldsymbol{k})$ was calculated by the first-principles density functional theory. The *ab initio* software package VASP with LDA exchange-correlation potential[19−21] was used to optimize the lattice structure and to obtain the energy bands. The initial crystal structure of oligoacenes was taken from the Cambridge Structural Database[22−24] and the discrepancy in lattice constants between the LDA results and the experimental values is within 5%. This is a lucky situation because the weak intermolecular interaction poses great challenges in DFT. Probably this is due to some error cancellation. In fact, we have tested some GGA functionals which gave worse results. The gap problem in DFT does not play an essential role here because when transport properties are concerned, the band dispersion is important as we are dealing with the doped situation (by gate electrode).

Second, the group velocity of electron and hole carriers can be obtained from the gradient of the band energy $\varepsilon_i(\boldsymbol{k})$ in $\boldsymbol{k}$-space, namely $v(i,\boldsymbol{k}) = \nabla \varepsilon_i(\boldsymbol{k})/\hbar$. In our self-consistent energy band calculation, the $\boldsymbol{k}$-mesh is 8×8×8 for all the oligoacene crystals. However, this small $\boldsymbol{k}$-mesh is not enough to perform numerical differentiation for obtaining the group velocity. Furthermore, the integration in eq. (1) needs more $\boldsymbol{k}$-point samples to get convergent results. We followed the work of Madsen and Singh[25], which can calculate the group velocity from analytical results by smoothed Fourier interpolation. As a result of the highly densely interpolated $\boldsymbol{k}$-mesh, the obtained group velocity in $\boldsymbol{k}$-space can

give very satisfactory results for transport properties[26]. We first carried out a non self-consistent energy band calculation with $\boldsymbol{k}$-mesh of 8000 $\boldsymbol{k}$ points in BZ. Next, for the group velocity and mobility calculations the $\boldsymbol{k}$ point grid is interpolated ten times as dense as the non self-consistent calculation.

Third, in general, the calculation of anisotropic relaxation time $\tau(i, \boldsymbol{k})$ is a very difficult task. That is why the usual evaluation of transport properties in organic semiconductor adopted the constant isotropic relaxation time approximation[14]. The spherical constant energy surface is assumed in relaxation time calculation, thus the information of anisotropic energy band structure in materials has been completely ignored. In this work, we took the nonspherical band structure of real materials into account and evaluated the relaxation time by the phenomenological definition of collision term in Boltzmann method[27], namely
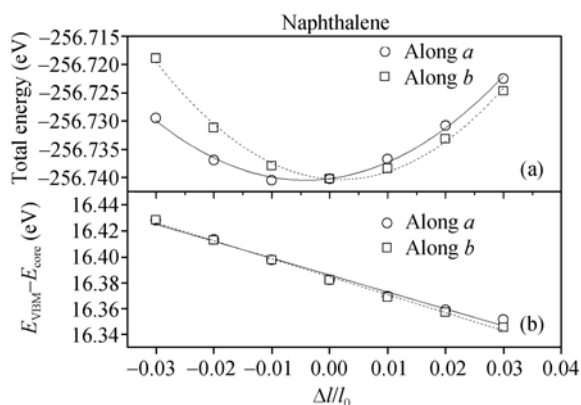
$$\frac{1}{\tau_\alpha(i,\boldsymbol{k})}$$
$$= \sum_{\boldsymbol{k}' \in BZ} \left\{ \frac{2\pi}{\hbar} \left| M_i(\boldsymbol{k},\boldsymbol{k}') \right|^2 \delta\left[\varepsilon_i(\boldsymbol{k}) - \varepsilon_i(\boldsymbol{k}')\right] \left[1 - \frac{v_\alpha(i,\boldsymbol{k}')}{v_\alpha(i,\boldsymbol{k})}\right] \right\}.$$

(2)

Here the delta function denotes that the scattering process is elastic and occurs between the band states with the same band index. It is noticed that once a $\boldsymbol{k}$ state is given, the summation of $\boldsymbol{k}'$ in BZ is on the nonspherical constant energy surface $\varepsilon_i(\boldsymbol{k}) = \varepsilon_i(\boldsymbol{k}')$ obtained from DFT calculation. Therefore, the anisotropic relaxation time in eq. (2) contains the information of energy band structure and can be used to characterize the transport properties of anisotropic materials such as oligoacene single crystals. $M_i(\boldsymbol{k}, \boldsymbol{k}')$ is the scattering probability from state $\boldsymbol{k}$ to state $\boldsymbol{k}'$ in the ith band. In the organic crystal, there are three dominant scatter sources: optic phonons, acoustic phonons, and static impurities. Although all these scatterings can be described by $M_i(\boldsymbol{k},\boldsymbol{k}')$, in this work, we investigated the influence of acoustic phonon scattering on carrier mobility, which can be estimated by deformation-potential theory. Following the work of Bardeen and Shockley[16], the thermal average of electron-longitudinal acoustic phonon scattering probability is $\left\langle \left| M_i(\boldsymbol{k},\boldsymbol{k}') \right|^2 \right\rangle = k_B T \left(E_\beta^i\right)^2 \big/ C_\beta$, where β denotes the Cartesian index of longitudinal acoustic

(LA) wave parallel to $k - k'$, E_β^i is the deformation-potential (DP) constant of the ith band, and C_β is the elastic constant along the direction β. It is noted that the transverse acoustic wave was not included due to its negligible effect on the deformation potential[16]. Moreover, as a first approximation we assumed this probability is independent of state k or k', since we are most interested in the band edge contribution for low carrier concentration. Hence for the charge carrier transport along the α direction we considered only the scattering of parallel LA waves.

To obtain the elastic constant, we dilated the unit cell of oligoacene crystals uniformly along the external field and calculated the total energy of deformed unit cell at different degrees of dilation. By fitting the curve of total energy E to dilation $\Delta l/l_0$ with formula $(E - E_0)/V_0 = C_\alpha (\Delta l/l_0)^2/2$, we can evaluate the elastic constant of the crystal along the transport direction α. Here V_0 and E_0 are volume and total energy of equilibrium cell, respectively. Δl is the change of lattice along the direction α and l_0 is its value at equilibrium geometry. In Figure 2(a) we present the total energy in naphthalene as the function of lattice dilation along a and b directions, which are the transport directions investigated in this work. All the calculated elastic constants of four oligoacene crystals are listed in Table 1.

The DP constant is defined as $E_\alpha^i = V_i / (\Delta l/l_0)$, where V_i is energy change of the ith band with lattice

Table 1 The calculated elastic constants C (10^{10} dyn/cm^2) and deformation potential constants E (eV) of oligoacene crystals

	Naphthalene	Anthracene	Tetracene	Pentacene
C_a	16.24	16.36	13.8	14.45
C_b	21.1	19.93	19.86	19.83
E_a^h	1.31	1.12	1.79	2.1
E_b^h	1.39	1.38	0.47	0.79
E_a^e	0.96	0.42	1.6	1.81
E_b^e	0.56	0.87	0.53	0.38

dilation $\Delta l/l_0$ along the direction of external field. For the sake of simplicity, we took the energy change at conduction band minimum (CBM) for electron part of DP constant and at valence band maximum (VBM) for hole part. Since the absolute energy band position from VASP is based on an unknown constant in bulk crystal, it is difficult to obtain the absolute energy shift from two different calculations with different lattice constants. Here, we adopted an approach proposed by Wei and Zunger[28], which assumes that the localized 1s level is not sensitive to the slight lattice deformation and it can be used as energy reference to obtain the absolute band energy changes for both VBM and CBM. In Figure 2(b) we present the calculated energy difference of naphthalene between the VBM and the closest energy level to core as function of lattice deformation along a and b directions. Around the equilibrium structure, the band energy difference changes linearly with the lattice deformation. Thus we can obtain the DP constant from the slope of fitting lines and all the calculated DP constants of oligoacenes are listed in Table 1.

3 Results and discussion

On the basis of the parameters given in Table 1 and the LDA energy band of oligoacene crystals, we can calculate the temperature dependence of mobility, where all the effects of temperature come from the distribution function. It is believed that the in-plane mobility is more useful to the device applications, so in this work we only studied the mobility along a and b lattice axes. In Figure 3 it can be seen that the electron and hole mobility manifests the typical power law, owing to the bandlike transport mechanism. Furthermore, our calculated temperature dependence can be approximated as $\mu \propto T^{-1.5}$, where the factor -1.5 is the result of carrier transport with parabola band dispersion in deformation potential theory[16]. Hence, any deviation from the power -1.5 comes from

Figure 2 (a) The total energy of unit cell for naphthalene with uniform dilation $\Delta l/l_0$ along the a direction (open circle) and the b direction (open square). The solid line and the dashed line are the corresponding fitting parabola. (b) The band energy of VBM (E_{VBM}) with respect to the closest level to the core level (E_{core}) with uniform lattice deformation along the a direction (open circle) and the b direction (open square). The solid line and the dashed line are the linear fittings.
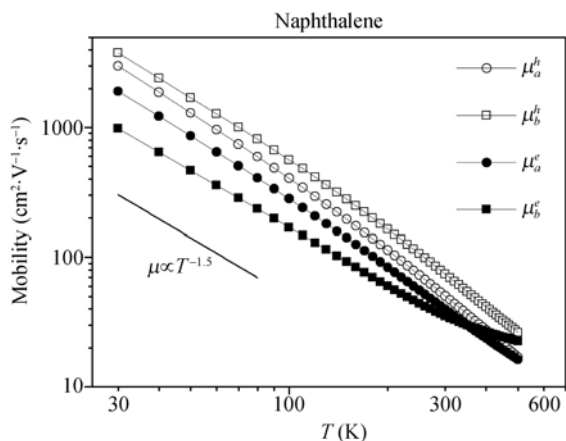
Figure 3 The temperature dependence of carrier mobility for naphthalene. The open circle and square are hole mobility along the *a* and *b* directions, respectively, while the filled circle and square are corresponding to mobility for electrons. The power law with factor −1.5 is also shown in the figure which describes the temperature dependence of carriers with effective mass approximation (parabola band).

the effect beyond the effective mass approximation.

Table 2 shows the calculated electron and hole mobility of oligoacene crystals in the *a-b* plane at room temperature. Here, the results do not show regular molecular length. It is because the transport in organic conjugated crystal is highly sensitive to various parameters of molecular packing[29], such as the relative displacement and orientation among the molecules, which will also change irregularly with the increasing molecular length in oligoacene crystals. As a consequence, the obtained mobility values do not have a regular trend because of the complicated interplay between crystal packing and electron structure.

The hole mobility of all the oligoacenes is calculated to be around a few tens $cm^2 \cdot V^{-1} \cdot s^{-1}$ and the maximum is less than 100 $cm^2 \cdot V^{-1} \cdot s^{-1}$. We have known that for naphthalene the hole transport calculation by only considering optic phonon scattering process gives the mobility values $\mu_a^h \approx 150\ cm^2 \cdot V^{-1} \cdot s^{-1}$ and $\mu_b^h \approx 200\ cm^2 \cdot V^{-1} \cdot s^{-1}$[15], which are about 3 times as great as that obtained from acoustic phonon scattering mechanism in our calculation.

Table 2 The calculated carrier mobility in unit $cm^2 \cdot V^{-1} \cdot s^{-1}$ at $T = 300$ K of oligoacene crystals

	Naphthalene	Anthracene	Tetracene	Pentacene
μ_a^h	50.4	19.2	10.6	15.2
μ_b^h	74.4	42.2	92.5	55.6
μ_a^e	39.8	245	24.5	27.7
μ_b^e	35.3	15.4	87.6	295

In other words, the scattering with the acoustic phonon is about three times as strong as that with the optic phonon in naphthalene. This strongly suggests the important role of acoustic phonon in charge transport. Therefore, it is suggested that in oligoacenes the acoustic phonon is more important to hole carrier transport than the optical phonon. Furthermore, the experimental study of single crystal in naphthalene[8], anthracene[30] and tetracene[9] reported the magnitude of mobility is around 1 $cm^2 \cdot V^{-1} \cdot s^{-1}$, which is much smaller than our result. Such discrepancy could be ascribed to impurities existing in organic crystals. In the case of pentacene, the ultrapurified single crystal exhibits the hole mobility about 35 $cm^2 \cdot V^{-1} \cdot s^{-1}$[31], which agrees much better with our result. It is known that once the impurity concentration and lattice disorder in organic crystal are reduced to be negligible by any method, the charge carrier mobility will approach its intrinsic value where only electron-phonon coupling contributes to the transport. Therefore, it is concluded that the hole carriers in oligoacene single crystals are mainly scattered by acoustic phonons during the transport process.

It is noted that there exists remarkable anisotropic behavior in mobility. de Wijs et al.[32] have found that the anisotropy of pentacene is related to the frustration of molecular orbitals owing to the herringbone structure. Most surprisingly, the electron mobility is calculated to be even larger than the hole mobility, Table 2. In general, the organic semiconductors are of p-type in the field effect transistor device. This is primarily due to two reasons: (i) the electrode work function (gold) is closer to the HOMO level so that the charge injection consists of mostly hole; (ii) organic materials present much more electron trap centers in the bulk than hole traps. Thus, even though the intrinsic mobility for electron could be large, the hole-type transports dominate in organic electronic devices. From theoretical standpoint, there is no reason why organic materials can only transport hole, not electron. Moreover, the unexpected large electron mobility is easily rationalized through the wave function analysis at the CBM and VBM. We depict the typical contour of wave function in a plane parallel to the *a-b* plane for anthracene crystal in Figure 4. For the lowest unoccupied molecule orbital (LUMO) at CBM, which is responsible for electron transport, we found that it presents stronger intermolecular overlap of wave function along the *a*-axis in anthracene and along the *b*-axis in
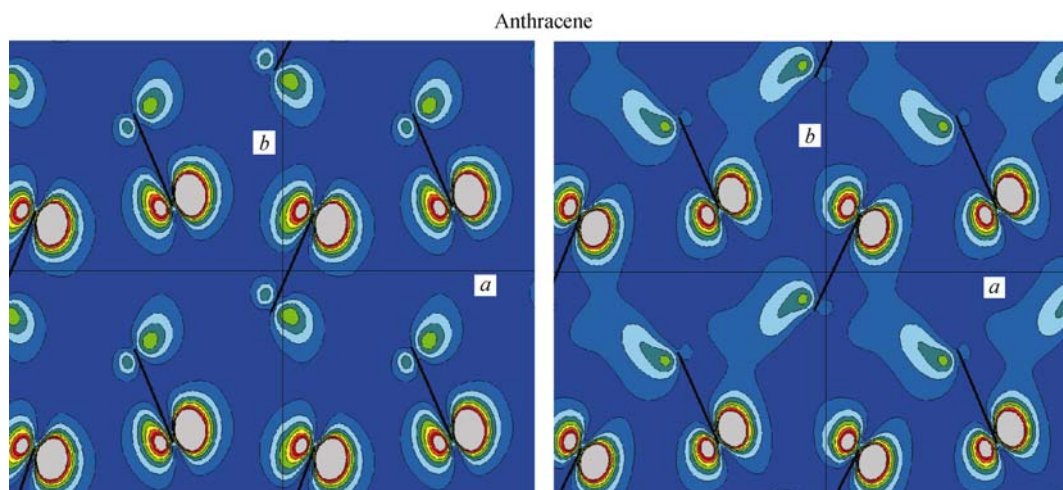
Figure 4 Contour plot of the wave function in a plane parallel to the *a-b* plane at VBM (left) and CBM (right) for anthracene crystal. The herring bone arrangement of the molecules is depicted by the black solid segments.

tetracene and pentacene, while in the other directions the corresponding wave function of the molecule is more localized. However, contrary to the electron case the wave function of the highest occupied molecule orbital (HOMO) at VBM in oligoacenes is all localized, so the hole mobility are relative isotropy with low values.

4 Conclusions

In summary, we have used first-principles density functional theory and the Boltzmann transport equation with relaxation time approximation to investigate the charge transport behavior of non-covalently bonded oligoacene single crystals. We considered only the longitudinal acoustic phonon scattering process in organic crystals and the corresponding relaxation time has been obtained by deformation-potential theory. Our approach has gone beyond the effective mass approximation and the calculated relaxation time is anisotropic which includes the detailed information of energy band structure. We found that the scattering intensity of charge with acoustic phonon is about three times as large as that with optic phonon when compared with our previous work[15]. The obtained temperature dependence of mobility follows the power law. We conclude that the acoustic phonon scattering process is the dominant mechanism for the delocalized charge transport in organic crystals. In addition, the numerical results indicate that potentially the organic crystals are even better for electron transport than for hole transport, which can be easily rationalized by the intermolecular frontier orbital overlap.

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