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Universal description of exciton diffusion length in organic photovoltaic cell

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ABSTRACT

A physical model of exciton diffusion length in organic photovoltaic cell based on percolation theory and Forster resonant transfer rate is presented here. The calculated results show a good agreement with Monte Carlo simulation and experimental data, indicating that the proposed model can well describe the temperature and material disorder dependences of exciton diffusion length. More importantly, the effect of carrier density on the exciton diffusion length can also be discussed based on our model, specifically, more intensive light illumination will lead to larger exciton diffusion length. Furthermore, according to our analysis, the Gaussian distribution density of states (DOS) can be well replaced by an exponential DOS at certain exciton concentration, which would help us get an analytical model for the exciton diffusion length.

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1. Introduction

Organic photovoltaic cell (OPV) is an emerging green energy photovoltaic technology with attractive properties such as low cost, light weight, flexibility, transparency and large area manufacturing compatibility, to meet the need of energy consume [1]. The development for OPV devices has progressed rapidly over recent years. The power conversion efficiencies for state of the art organic photovoltaic cells now exceed 10% [2,3]. Generally, the photo conversion mechanism of OPV can be divided into four main processes including photon absorption, exciton generation, exciton diffusion and exciton dissociation. It is well known that the excitons with large diffusion length can migrate to the junction interface and hence contribute to power conversion, if a coulomb bounded electron–hole pair is not separated within its lifetime [4]. In additional, the exciton diffusion is a crucial procedure which will remarkably affect the efficiencies of OPV.

In organic material, exciton transport is attributed to the exciton diffusion processes from high exciton concentration regions to its surroundings. According to hopping mechanism, the weak interaction in organic semiconductor molecule dominates exciton transport, where the main transfer mechanism between weakly coupled molecule is Forster resonant energy transfer (FRET) [5]. This energy transfer involves Coulombic dipole–dipole coupling of donor and acceptor interactions, and strongly depends on the overlap integral between donor emission and acceptor absorption spectra, as well as the donor–acceptor separation distances.

So far, numerous theories of exciton diffusion in amorphous organic material, such as Monte Carlo simulation, time-integrated photoluminescence quenching model and a numerical analytic theory have been performed to investigate the exciton transport, but still for exciton transport fundamental science questions remain unchanged [6,7]. However, the percolation effect, which is known to be important for charge transport in disordered organic semiconductors [8], has not been addressed in diffusion length model [9,10]. More remarkable, although the influence of temperature, exciton lifetime, and disorder degree on diffusion process have been discussed, however, as far as we know, there is not report on the influence of carrier density on exciton diffusion. It is well known that carrier concentration is one of the most important factors in hopping transport [11], since high carrier density would decrease not only hopping distance but also activation energy. This property should shade light on the role of illumination intensity in the exciton diffusion.

In this work, we propose a unified description of exciton diffusion in OPV based on the percolation theory. The temperature, material disorder, and exaction density dependences of diffusion length can be well described.

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2. Model and method

For disordered organic semiconductors, charge carriers move via incoherent tunneling between spatially and energetically distributed localized states, and the Gaussian density of states is usually assumed to describe the energy distribution of localized states in organic semiconductor as [12]

$$g(E) = \frac{N_t}{\sqrt{2\pi}\sigma} \exp\left(-\frac{E^2}{2\sigma^2}\right), \tag{1}$$

where σ is Gaussian standard deviation, N_t is the number of states per unit volume, E is the energy.

The transport of exciton is attributed to the hopping rate of the exciton jump between localized states, which can be described as Miller–Abrahams transition rate. In Gaussian energetically distributed materials, excitons are scattered by lattice phonons. For intermolecular interaction, especially dipole and dipole interaction, the Forster resonant energy-transfer rate can describe such migration and it is expressed as [7]

$$\Gamma(E_i, E_j, r) = \frac{1}{\tau}\left(\frac{r_F}{r}\right)^6 \times \begin{cases} \exp\left(-\frac{E_j - E_i}{k_B T}\right) & E_j > E_i \\ 1 & E_j < E_i \end{cases}, \tag{2}$$

where the energy transfer from an occupied molecule segment of energy E_i to unoccupied molecule segment with energy E_j, which are separated by distance r, τ is the lifetime of the exciton, r_F is the Forster radius, k_B is the Boltzmann constant, T is the temperature.

The transport of exciton realized by hopping between localized states in the disordered material, should be regarded as a percolation process [13]. Using the percolation theory, one can consider these disordered system as a random resistor network (the network of Miller Abrahams) in order to determine the conductivity [14], thus the conductance between site i and j is described as

$$G_{ij} = G_0 \exp(-S_{ij}), \tag{3}$$

where

$$S_{ij} = -6\ln\left(\frac{r_F}{r}\right) + \frac{|E_j - E_F| + |E_i - E_F| + |E_j - E_i|}{2k_B T}, \tag{4}$$

and E_F is the Fermi energy.

According to Vissenberg's percolation theory [15], the conductivity of the system is given by

$$\delta = \delta_0 \exp(-S_c), \tag{5}$$

where δ_0 is the prefactor, S_c is the exponent of the critical percolation conductance which is related with the onset of percolation when the critical number B_c is reached. For disordered system, this number is given by $B_c \approx 2.8$ [15,16]. The percolation criterion B_c can be defined as

$$B_c = N_b/N_s, \tag{6}$$

where N_b and N_s are the density of bonds and the density of sites in the percolating system, respectively. The density of bonds is given by

$$N_b = \int 4\pi r^2 dr\, dE_i dE_j g(E_i) g(E_j) \theta(S_c - S_{ij}), \tag{7}$$

where θ is the unit step function. The density of sites that can form a bond is written as

$$N_s = \int dE g(E) \theta(S_c k_B T - |E - E_F|). \tag{8}$$

Substituting Eqs. (7) and (8) into Eq. (6), the critical percolation conductance exponent S_c can be obtained. Combining Eq. (5) and the mobility is written as

$$\mu = \frac{\delta}{qn}, \tag{9}$$

where q is the elementary charge, $n = \int dE g(E) f(E, E_F)$ is the density of charge carriers. The energy distribution of the carriers is given by the Fermi Dirac distribution $f(E, E_F)$, where E_F is the quasi Fermi energy determined by the light injection, one can get

$$\mu = \frac{\delta_0 \exp(-S_c)}{q \int dE g(E) f(E, E_F)}. \tag{10}$$

According to the Einstein relation

$$D = \frac{k_B T}{q}\mu. \tag{11}$$

Then, the exciton diffusion length can then be easily calculated as

$$L_D = \sqrt{D\tau} = \sqrt{\tau \frac{k_B T}{q} \frac{\delta_0 \exp(-S_c)}{q \int dE g(E) f(E, E_F)}}. \tag{12}$$

The critical percolation conductance exponent S_c is an intermediate parameter which can be numerical solved by Eqs. (6)–(8), thus, the diffusion length can be obtained.

The exciton diffusion length is compendiously described as Eq. (12). In this equation, intrinsic parameters such as τ, r_F, δ_0 are controlled by the materials, while variable parameters, including disorder degree (induced by chemical defects) and light intensity dependence of carrier density, are reasonable if they are typical for organic semiconductor. At different temperature or disorder degree, the critical percolation conductance can be obtained by solving Eqs. (6)–(8). Then the exciton diffusion length can be acquired according to Eq. (12).

3. Results and discussions

In Fig. 1a, the diffusion length decreases with the increase of Gaussian standard deviation. The increasing of energetic disorder results in the upward shift of thermal level ($E_{th} = \sigma^2/k_B T$) for excitons occupied states, which dissipates the exciton migration, so it is hard for excitons hopping to nearest neighbors. Our physical model agrees with the quantum chemical based Monte Carlo simulations by Athanasopoulos [7]. In Fig. 1b, the calculated Gaussian standard deviation dependences of diffusion length are shown for different Fermi energy, and the relation would be strong at high Fermi energy. In addition, the difference of Fermi energy produces great change of diffusion length and the Fermi energy can be expressed as exciton concentration, thus, the diffusion length relies on the concentration of exciton.

The diffusion length is expected to decrease with the reduction of temperature as thermally activated hopping becomes less frequent. In Fig. 2a, it manifests that the diffusion length relies sensitively on Gaussian width and temperature, showing the behavior of Arrhenius for low Gaussian width and high temperature. However, diffusion length becomes strong dependence on temperature at low Fermi energy. In Fig. 2b, Temperature dependence of exciton diffusion appears to be inferior less than 150 K, which agrees with Mikhnenko's [17], who describes this phenomenon as two steps of exciton diffusion process, including the downhill migration and the thermally activated hopping respectively, and the thermally activated hopping becomes very weak at lower temperatures [17]. Our simulation fits with experimental data well [18].

The generation of exciton is strongly relied on incident light intensity, organic material absorbing rate, voltage, and the morphology of organic cells [19]. The process of exciton diffusion is greatly influenced by exciton concentration, and the large diffusion

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