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Dynamic recombination of triplet excitons in polymer heterojunctions*

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The dynamic recombination of two triplet excitons with opposite spins in the heterojunction structure has been investigated using a nonadiabatic evolution method. We demonstrate that luminous composite states including the excited polaron and the biexciton can be formed efficiently via the triplet exciton–triplet exciton reaction in the heterojunction and therefore this reaction can enhance the electroluminescence efficiency considerably, which is consistent qualitatively with experimental observations. Meanwhile, we find that, although the heterojunctions are beneficial to the generation of luminescent particles, large band offset caused by the heterojunction structure is not helpful to improve the electroluminescence efficiency. In addition, the mechanism of the triplet exciton–triplet exciton reaction in heterojunction is different from that of two similar coupling chains. Our results may deepen the understanding of the electroluminescence mechanism in polymer light-emitting devices.

Keywords: polymers, electron–lattice interaction, excitons

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1. Introduction

In recent years, considerable amounts of research works, both experimental and theoretical, have been devoted to exploring and optimizing the luminescence mechanism in polymer light-emitting devices (PLEDs).[1–3] These devices are normally fabricated with a luminescent polymer sandwiched between metallic electrodes. When a PLED is in operation, electrons and holes are injected into the polymer layer from the cathode and the anode. Because of the strong electron-lattice interactions and instability, these injected charges induce self-localized excitations that include both charge and lattice distortion, such as polarons.[4] The stability of polarons and the effect of polarons on polarizability have been investigated.[5,6] When polarons with opposite charges meet, they can recombine to form singlet and triplet excitons. The generation of photons is achieved from the radiative recombination of singlet excitons while the relaxation of triplet excitons is quantum mechanically forbidden. According to spin statistics, the branching ratio for formation of singlet and triplet excitons should be 1:3 so the electroluminescence (EL) efficiency of PLEDs is limited to 25%. However, many researchers have pointed out that the EL efficiency in PLEDs greatly breaks through the theoretical limitation predicted by spin statistics.[1,2,7,8]

The above-mentioned results indicate that the EL in PLEDs may involve some additional mechanisms beyond the polaron-polaron recombination. It should be noted that triplet excitons have higher yield, longer lifetime and stronger stability than singlet excitons, and triplet excitons will easily accumulate in working PLEDs and therefore have greater probability to interact with other excitations. Up to date, many researchers have been working on the role of triplet excitons in the electroluminescence.[9] Several methods have been reported to generate singlet excitons from triplet excitons, known as triplet harvesting regimes. More recently, highly efficient organic light-emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) molecules were realized. In TADF emitters, triplet-to-singlet upconversion at room temperature is possible due to a small singlet-triplet energy gap.[10] Another channel to utilize triplet excitons in fluorescent OLEDs is through the generation of singlets by triplet-triplet annihilation (TTA).[11,12]. In addition to the singlet exciton, we found that some other luminous composite states, such as the excited polaron and the biexciton, can also be formed in the recombination processes between two triplet excitons with opposite spins by analyses of their electronic spectra. To clarify this point, we previously investigated the scattering and recombination of two triplet excitons and found that the excited polaron is the main luminous product in such a recombination process.[13]

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Over the past few decades, heterojunctions created from thin films of two dissimilar organic semiconductor materials have been widely used to make high efficient organic light emitting diode displays and lighting systems and small molecules or polymer-based organic photovoltaic technologies.[14] For example, in order to balance the injection of holes and electrons, real PLEDs often have a multi-layer structure with a hole transporting layer (HTL) and an electron transporting layer (ETL) inserted into the PLED.[8,15,16] That is, the electroluminescent polymeric material is fabricated as a multi-layer structure, and the heterojunction is formed between dissimilar organic semiconductors. Frontier orbital energy offsets in heterojunction establish the excessive free energy controlling rates of charge recombination and formation of emissive states in PLEDs. Based on the molecular dynamics approach, Sun and coworker found that the band offset caused by heterojunction can overcome the exciton binding energy, enabling the electron to transfer from the donor polymer to the acceptor polymer[17] and thus improving the possibility of exciton dissociation. In this paper, we investigate the recombination of two triplet excitons with opposite spins using a nonadiabatic evolution method based on an extended Su–Schrieffer–Heeger (SSH) model including interchain interactions and electron–electron interactions. In our numerical simulation, a heterojunction constructed by two coupled polymer chains is introduced. We focus on the effect of the heterojunction on the triplet exciton–triplet exciton reaction by investigating the products and their yields, and we especially consider whether such a mechanism is an efficient way for improving the EL efficiency in PLEDs. The triplet exciton–triplet exciton reaction is a dynamical process accompanied by both charge motion and lattice distortion. It is therefore valuable to study it using a real time dynamical method. In this way, we are able to gain some basic physical pictures of this reaction, which may provide guidance for understanding the luminescence mechanism in polymer-based optoelectronic devices.

The paper is organized as follows. Section 2 describes the model and parameters used. The results are presented in Section 3. A summary is given in Section 4.

2. Model and method

The model Hamiltonian we use is the SSH model[18] with a Brazoskii–Kirova-type symmetry-breaking term,[4] including the effect of the intrachain and electron–electron (e–e) interaction.[19] To mimic the polymer heterojunction, we set different values of the on-site energy on the two chains respectively

$$\begin{aligned} H &= \sum_{j,n,s} \Delta_j c^{\dagger}_{j,n,s} c_{j,n,s} \\ &\quad - \sum_{j,n,s} t_n (c^{\dagger}_{j,n,s} c_{j,n+1,s} + c^{\dagger}_{j,n+1,s} c_{j,n,s}) \\ &\quad + \frac{K}{2} \sum_{j,n} (u_{j,n+1} - u_{j,n})^2 + \frac{M}{2} \sum_{j,n} \dot{u}^2_{j,n} \\ &\quad + U \sum_{j,n} c^{\dagger}_{j,n,\uparrow} c^{\dagger}_{j,n,\downarrow} c_{j,n,\downarrow} c_{j,n,\uparrow} \\ &\quad + V \sum_{j,n,s,s'} c^{\dagger}_{j,n,s} c^{\dagger}_{j,n+1,s'} c_{j,n+1,s'} c_{j,n,s}. \end{aligned} \tag{1}$$

Here $j = 1$ and 2 is the chain index. We set $\Delta_1 = 0$ for all sites of the chain 1 and $\Delta_2 = \Delta E$ for all sites of chain 2. The quantity t_n is given by $t_n = t_0 - \alpha(u_{n+1} - u_n) + (-1)^n t_e$, with t_0 being the transfer integral of π electrons in a regular lattice, α the electron-lattice coupling constant, and $u_{j,n}$ the lattice displacement of the atom at the n-th site along the j-th chain from its equidistant position. The quantity t_e is introduced to lift the ground-state degeneracy for nondegenerate polymers. The operator $c^{\dagger}_{j,n,s}$ ($c_{j,n,s}$) creates (annihilates) a π electron at the n-th site with spin s along the j-th chain; K is the elastic constant due to the σ bonds and M is the mass of a CH group. U gives the strength of the on-site Coulomb interactions and V is the nearest-neighbor interactions. In our calculation, we take the weak electron–electron interaction, i.e. $U = 0.4$ eV and $V = 0.2$ eV.

The two chains are coupled by the interchain interactions H',[20]

$$\begin{aligned} H' &= -\sum_{n,s} t_{\perp} (c^{\dagger}_{1,n,s} c_{2,n,s} + c^{\dagger}_{2,n,s} c_{1,n,s}) \\ &\quad + \sum_{n,s,s'} V_{\perp} c^{\dagger}_{1,n,s} c^{\dagger}_{2,n,s'} c_{2,n,s'} c_{1,n,s}, \end{aligned} \tag{2}$$

where $t_{\perp}$ stands for the transfer integral between sites labeled by the same index n on the two chains and $V_{\perp}$ is the e–e interaction term. In the following calculations, $V_{\perp}$ is fixed at 0.1 eV.

The temporal evolution of the lattice is determined by the equation of motion for the atomic displacements,

$$\begin{aligned} M\ddot{u}_{j,n}(t) &= -K(2u_{j,n}(t) - u_{j,n+1}(t) - u_{j,n-1}(t)) \\ &\quad + 2\alpha \sum_{s} (\rho^{s}_{jn,jn+1}(t) - \rho^{s}_{jn,jn-1}(t)), \end{aligned} \tag{3}$$

where the density matrix ρ is defined as

$$\rho^{s}_{jn,j'n'}(t) = \sum_{k} \Phi^{s}_{j,n,k}(t) f_{k,s} \Phi^{s*}_{j'n',k}(t), \tag{4}$$

with $f_{k,s}$ being the time-independent distribution function determined by the initial electron occupation. The electron wave functions $\Phi^{s}_{j,n,k}(t)$ are solutions of the time dependent Schrödinger equation

$$\mathrm{i}\hbar \dot{\Phi}^{s}_{j,n,k}(t) = \sum_{j'n'} h^{s}_{jn,j'n'}(t) \Phi^{s}_{j',n',k}(t). \tag{5}$$

The coupled differential Eqs. (3) and (5) can be solved with a Runge–Kutta method of order eight with step-size control,[21] which has been proven to be an effective approach

for investigating polaron and soliton dynamics and photoexcitation dynamics in conjugated polymers. Although the parameters used here are taken to be those for polyacetylene,[22] i.e., $t_0 = 2.5$ eV, $\alpha = 4.1$ eV/Å, $t_e = 0.05$ eV, $K = 21.0$ eV/Å^2, $a = 1.22$ Å, and $M = 1349.14$ eV fs^2/Å^2, the results are expected to be qualitatively valid for other conjugated polymers with a nondegenerate ground state.

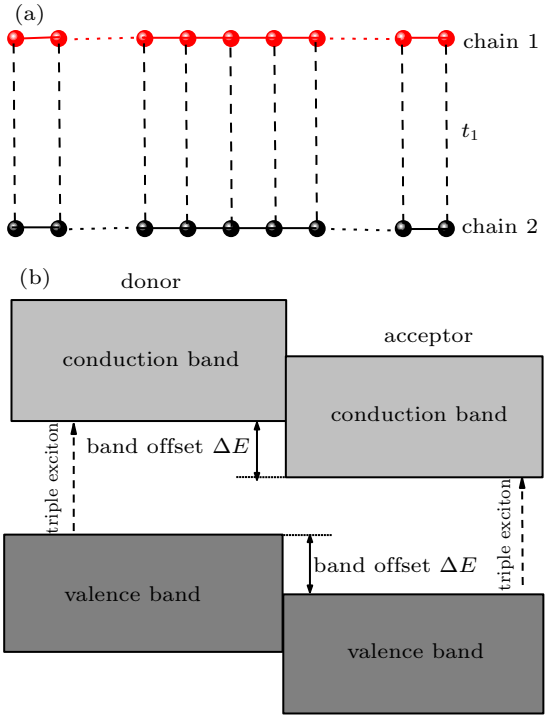


Fig. 1. Schematic diagrams of the polymer heterojunction structure (a) and its energy spectrum (b).

3. Results and discussion

In our numerical simulations, two 100-site parallel polymer chains opposite each other are considered: the CH-units are labeled as 1–100 on chain 1 and 101–200 on chain 2. Initially, a triplet exciton with up spin is located on chain 1 and a triplet exciton with down spin on chain 2. We set different values to the on-site energies of the two chains to mimic the heterojunction constructed by two coupled polymer chains. Figure 1 shows the schematic representation of the heterojunction composed of two polymer chains and its energy spectrum, where ΔE is the band offset. The initial bond configuration and electronic structure can be obtained by minimizing the total static energy of the two-chain system in the absence of the interchain interactions. Then, the interchain interactions are smoothly turned on reaching their full strength within 75 fs, which mimics two triplet excitons approaching each other.

Firstly, we explore the recombination processes between two triplet excitons at different interchain interactions with the band offset being taken as $\Delta E = 0.05$ eV. The results are given in Fig. 2. Here we introduce the bond structure parameter

$$r_n(t) = (-1)^n \left[u_{n-1}(t) + u_{n+1}(t) - 2u_n(t)\right]/4 \qquad (6)$$

to describe the geometry of conjugated polymers. It is easy to see that interchain interactions have significant effects on the recombination processes between two triplet excitons.

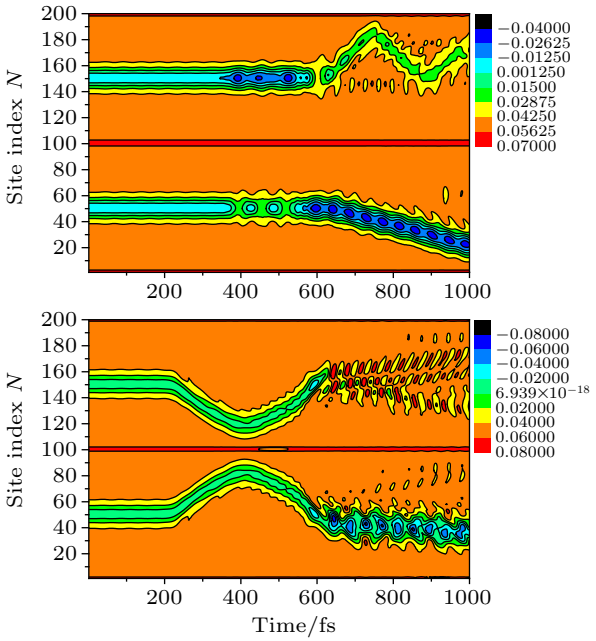


Fig. 2. Temporal evolution of the lattice configuration for the recombination processes between two triplet excitons with different interchain interactions: $t_1 = 0.1$ eV (top panel); $t_1 = 0.18$ eV (bottom panel). The unit of the third axis vertical to the time and site index is 10^{-1} nm.

(1) In the case of $t_1 = 0.1$ eV, we can see from the top panel of Fig. 2 that the recombination processes between two triplet excitons take place at about 350 fs, and two polaron-like states different from the initial triplet excitons have been formed. The one with larger lattice distortion is located on chain 2 and the other with smaller lattice distortion on chain 1. At about 600 fs, two polaron-like states exchange their positions with each other and tend to be stable. Then the state with larger lattice distortion moves toward the end of the chain while the one with smaller lattice distortion oscillates around its initial position, which is apparently due to the Coulomb effect. This fact suggests that states formed have residual charges coupled to their lattice deformations. Alongside this evidence, it can be concluded that these new structures may be mixed with some charged excited states.

To better distinguish the two polaron-like particles we draw the evolutions of the localized electronic energy levels and the occupation numbers with time, as shown in Fig. 3. We use $\varepsilon_1^{\mathrm{u}}$ and $\varepsilon_1^{\mathrm{d}}$ to denote the upper and lower levels corresponding to the triplet exciton with up spin initially located on chain 1, and $\varepsilon_2^{\mathrm{u}}$ and $\varepsilon_2^{\mathrm{d}}$ to denote the upper and lower levels corresponding to the triplet exciton with down spin located on chain 2. Levels $\varepsilon_1^{\mathrm{u}}$ and $\varepsilon_1^{\mathrm{d}}$ are occupied by an electron with up spin while $\varepsilon_2^{\mathrm{u}}$ and $\varepsilon_2^{\mathrm{d}}$ are occupied by an electron with down spin respectively. Due to interchain interactions, the transfer of charges localized in triplet excitons between two chains becomes more and more intense along with time going. After re-

combination, levels $\varepsilon_1^{\mathrm{u}}$ and $\varepsilon_1^{\mathrm{d}}$ get close to each other and form a pair of coupling levels with a smaller energy difference and oscillate violently over a wide range. By analyzing their wave functions, it can be found that levels $\varepsilon_1^{\mathrm{u}}$ and $\varepsilon_1^{\mathrm{d}}$ corresponds to the state with larger lattice distortion shown in Fig. 2. Meanwhile, it can also be seen that the energy difference between $\varepsilon_1^{\mathrm{u}}$ and $\varepsilon_1^{\mathrm{d}}$ is smaller than that of the triplet exciton. That is to say, the polaron-like state formed via two triplet excitons recombination may contain complex particles with larger binding energy than that of the triplet exciton, such as biexciton and excited polaron. However, levels $\varepsilon_2^{\mathrm{u}}$ and $\varepsilon_2^{\mathrm{d}}$ move close to the bottom of conduction band and the top of valence band respectively and form a pair of local levels corresponding to the state with smaller lattice distortion shown in Fig. 2. Following with the formation of two polaron-like states, the occupation numbers of four localized energy levels tend to be stable, as shown in Fig. 3(b). It can be seen that there is a noticeable migration of electrons between different energy levels during the recombination process. For example, the occupation number of level $\varepsilon_1^{\mathrm{u}}$ increases from $1e$ to about $1.5e$ and that of level $\varepsilon_1^{\mathrm{d}}$ decreases from $1e$ to about $0.8e$. Here the occupation number of upper level is larger than that of the lower level, which indicates that the probability of producing luminous particles with reverse polarization,[23] such as excited polaron and biexciton, is very high. Meanwhile, the occupation number of level $\varepsilon_2^{\mathrm{u}}$ decreases from $1e$ to about $0.4e$ and that of level $\varepsilon_2^{\mathrm{d}}$ increases from $1e$ to about $1.3e$.

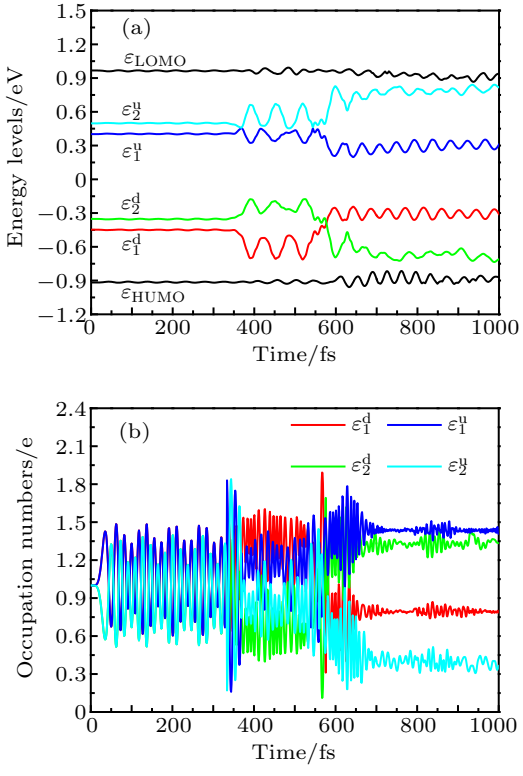


Fig. 3. Evolutions of the localized electronic energy levels (a) and their occupied numbers (b) with time, $t_1 = 0.1$ eV (from the same simulation as the top panel of Fig. 2).

We now analyze the products of the recombination process and determine the branching ratios for the formation of various species in the steady state. Since the two deformations are only weakly coupled to each other by the interchain interactions, we can separately obtain their approximate eigenstates via ignoring the interchain coupling. It is found that such a structure is a mixture of sixteen possible states. For simplicity, we divide these states into four species: state (a) denotes the initial electronic state containing two triplet excitons localized on two coupled chains respectively; state (b) denotes a excited polaron and a polaron with opposite charges; state (c) denotes a biexciton and a ground state; state (d) denotes two singlet excitons with opposite spins, see Fig. 4. We do not show the other possible states as we have found that the yields of other states are very small compared with these four states. Meanwhile, the significant lattice oscillations induced by the triplet exciton–triplet exciton recombination results in the loss of total yield, so the sum of yields for states (a)–(d) may be much less than 100%.

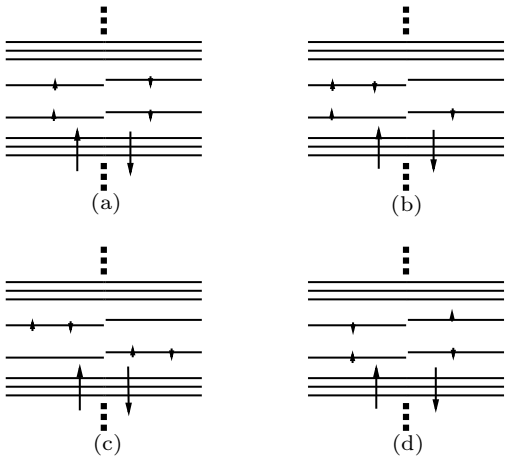


Fig. 4. The schematic diagram of resultant states for the recombination processes between two triplet excitons.

Using a projection method, i.e., after each evolution step, projecting the evolved state $|\Phi(t)\rangle$ onto the space of eigenstates of the system, the relative yield $I_k(t)$ for a given eigenstate $|\Psi_k\rangle$ can be obtained from

$$I_k(t) = |\langle \Psi_k | \Phi(t) \rangle|^2 . \tag{7}$$

Our calculation results show that the average yields of states (a)–(d) within the final stable period are 5%, 40%, 14% and 13%, respectively. Thus we can conclude that the main component contained in the resulting state is the excited polaron in such a reaction. It should be stressed that the products of the triplet excitons recombination, including the excited polaron, the singlet exaction, and the biexciton, are all luminous, and their total yield can be about 67%, which is qualitatively consistent with the experimental results.[10–12] Therefore, this reaction can greatly enhance the quantum EL efficiency. Meanwhile, it can be found that the total yield of emissive species in the heterojunction structure is higher than

that in two similar coupling chains,[13] so the heterojunction structure is beneficial to the generation of luminous composite states via the triplet exciton–triplet exciton reaction and consequently is conducive to improving the efficiency of EL.

(2) In the case of $t_1 = 0.18$ eV, it can be seen from the bottom panel of Fig. 2 that two triplet excitons eventually recombine into one polaron-like state with larger lattice distortion, which is consistent with evolutions of the localized electronic energy levels, as shown in Fig. 5 (a): levels $\varepsilon_1^{\rm u}$ and $\varepsilon_1^{\rm d}$ become closer to each other and form a pair of coupling levels with a smaller energy difference, which corresponds to the generated state. However, levels $\varepsilon_2^{\rm u}$ and $\varepsilon_2^{\rm d}$ enter the conduction band and valence band, respectively, which corresponds to appearance of a ground state on chain 2. From the evolution of the occupation numbers of four localized energy levels we can see that, as the two excitons recombine into a polaron-like state, the occupation numbers of four localized energy levels also tend to be stable. The occupation number of level $\varepsilon_1^{\rm u}$ increases from $1e$ to about $1.6e$ and that of $\varepsilon_1^{\rm d}$ decreases from $1e$ to about $0.3e$, which also means the high probability of producing luminous particles. Our calculation show that the average yields of states (b) and (c) are 8% and 47% while those of states (a) and (d) are very small compared with these two states. Obviously, the main product in this case is the biexciton which can also emit light and therefore the triplet exciton–triplet exciton recombination can improve the luminescence efficiency effectively.

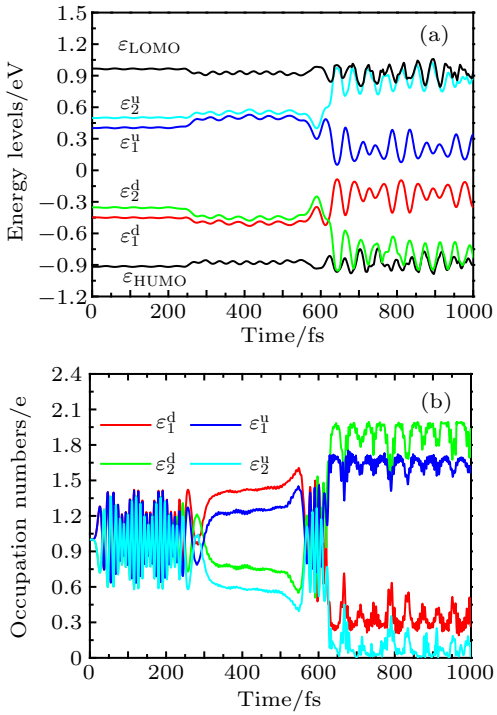


Fig. 5. Evolutions of the localized electronic energy levels (a) and their occupied numbers (b) with time, $t_1 = 0.18$ eV (from the same simulation as the bottom panel of Fig. 2).

The dependences of the yields for states (b), (c) and (d) on the interchain interactions are depicted in Fig. 6. In a real system, it can be estimated by theoretical or experimental work that the interchain coupling is about 0.1 eV for polyacetylene,[24] so we take the interchain interaction in the range from 0.05 to 0.22 eV in this study. We can see that the main product of the triplet exciton–triplet exciton recombination can be the excited polaron or the biexciton, depending on the interchain interaction t_1. The peak corresponding to the high yield of the excited polaron is around $t_1 = 0.1$ eV while the one corresponding to the high yield of biexciton is around $t_1 = 0.18$ eV, which indicates that the mechanism of the triplet exciton–triplet exciton reaction in heterojunction is different from that of two similar coupling chains, and that we can adjust the micro-mechanism of the triplet exciton–triplet exciton reaction by changing the coupling between two chains.

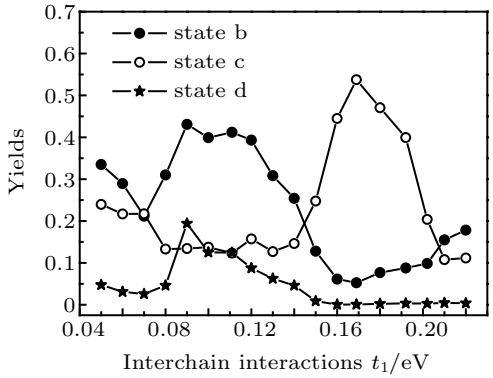


Fig. 6. Dependence of yields for states (b), (c) and (d) on the interchain interactions for the recombination process between two triplet excitons.

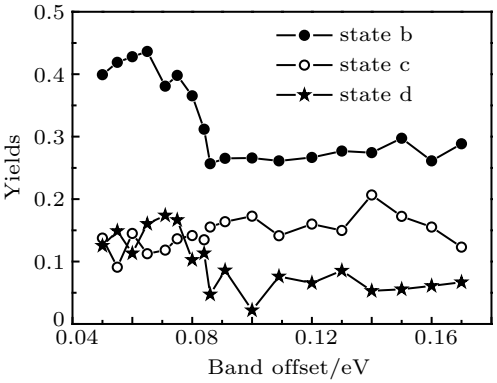


Fig. 7. Dependence of yields for states (b), (c) and (d) on the band offset for the recombination process between two triplet excitons.

Finally, the effect of the band offset caused by the heterojunction structure on the triplet exciton–triplet exciton recombination is discussed. Depicted in Fig. 7 are the yields of excited polaron, biexciton and singlet exciton versus the band offset with $t_1 = 0.1$ eV. It is found that weak band offset ($\Delta E \leq 0.08$ eV) is favorable for the formation of the excited polaron and the singlet exciton. When the band offset is larger than 0.08 eV, it has no obvious effect on the on the triplet exciton–triplet exciton reaction. It should be noted that when the band offset is larger than 0.2 eV, there is almost no interaction between the two triplet excitons, and the initial state is

maintained. Our simulation also shows that large band offset is not conducive to the production of biexciton when the value of t_1 is around 0.18 eV. On the whole, although the heterojunctions are beneficial to the generation of luminescent particles, large band offset in the heterojunction structure is not helpful to improve the electroluminescence efficiency in the triplet exciton–triplet exciton reaction.

4. Conclusions

In summary, we have simulated the scattering and recombination of two triplet excitons with opposite spins in the heterojunction structure using a nonadiabatic evolution method. It is shown that the luminous composite states including the excited polaron, the biexciton and the singlet exciton can be formed efficiently via the triplet exciton–triplet exciton reaction in the heterojunction, and therefore this reaction can enhance the EL efficiency considerably, which is qualitatively consistent with the previous experimental results. Meanwhile, we find that the triplet exciton–triplet exciton reaction is sensitive to the interchain interactions, so we can adjust the micro-mechanism of triplet exciton–triplet exciton reaction by changing the coupling between two chains. Moreover, It is found that the mechanism of the triplet exciton–triplet exciton reaction in heterojunction is different from that of two similar coupling chains, and that the large band offset is not helpful to improve the electroluminescence efficiency in this reaction. Our conclusion may provide a new channel to understand and optimize the mechanism of electroluminescence in light-emitting devices based on conjugated polymers.

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