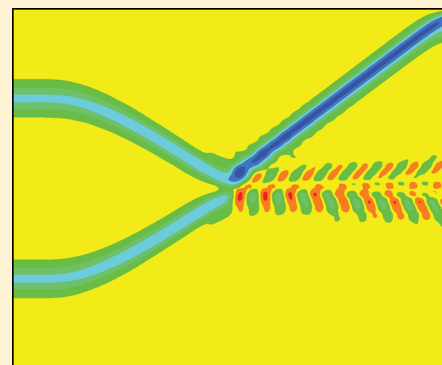


Electroluminescence Enhancement in Polymer Light-Emitting Diodes through Inelastic Scattering of Oppositely Charged Bipolarons

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ABSTRACT: Combining the one-dimensional tight-binding Su–Schrieffer–Heeger (SSH) model and the extended Hubbard model (EHM), the scattering and combination of oppositely charged bipolarons in conjugated polymers are investigated using a nonadiabatic evolution method. On the basis of this physical picture, bipolarons can scatter into a singlet biexcitonic state, in which two electrons and two holes are trapped together by a lattice distortion. This biexcitonic state can emit one photon to an exciton state, which can subsequently decay to the ground state. The results indicate that the scattering and combination of oppositely charged bipolarons may provide guidance for improving the internal quantum efficiency for electroluminescence to as high as 75% in polymer light-emitting diodes.



INTRODUCTION

Generally, the quantum efficiency for electroluminescence in polymer light-emitting diodes (PLEDs) is given by the ratio of the number of emitted photons over the number of emissive singlet excitons (Ex). If exciton combination in PLEDs is a spin-independent process, the maximum quantum efficiency of the PLEDs is limited to 25%.¹ To break the 25% limit, there have been many experiments that have attempted to improve the quantum efficiency for electroluminescence to 22–60% by finding channels.^{2–6} On the theoretical side, there have also been extensive investigations of the physical principles necessary for improving the efficiency of PLEDs. For example, our previous research has shown that the yield of neutral excitons formed by the collision and the combination of oppositely charged polarons depend sensitively on the strength of the external applied fields,⁷ and researchers have shown that the interactions of a bipolaron–exciton pair and/or a polaron–bipolaron pair open channels that enhance the quantum efficiency of electroluminescence.^{8,9} In addition, the scattering and recombination of a polaron and a triplet exciton can induce both the excited polaron and the exciton to emit light, and the maximum quantum efficiency of the PLEDs can reach about 38.2%¹⁰ and even 61.6%.¹¹

To date, the quantum efficiency of the PLEDs has always been related to the yield of singlet excitons. However, there are other luminescent states, such as the singlet biexciton (BE), and there have been extensive studies of biexciton structures in polymer based light-emitting diodes.^{12–18} The singlet biexciton consisting of two electrons and two holes trapped together by lattice distortions can decay to the exciton state with the exciton subsequently decaying to the ground state (GS). The biexcitonic state can therefore provide one more electroluminescence channel, which avoids the triplet exciton, and enhance the quantum efficiency.

In addition to the usual self-localized charge carriers, that is, polarons (spin $1/2$, charge $\pm|e|$),¹⁹ a number of experimental and theoretical studies have also shown the existence of bipolarons (spinless species, charge $\pm 2|e|$) in doped conjugated conducting polymers.^{20–23} The formation, stability, and dynamic evolution of polarons and bipolarons have been simulated by many researchers. For example, bipolarons can be created in organic LEDs when a charge injection results in a large concentration of polarons.²⁴ The charges injected from a metal electrode into a nondegenerate polymer chain can favor the formation of electron (hole) bipolarons, which have better stability than two polarons,²⁵ and, particularly in the case of weak electron–electron interactions, are energetically more stable than a separated pair of polarons.^{26,27} Two acoustic polarons with the same charge and antiparallel spins can also combine with each other to form an acoustic bipolaron.²⁸ Our previous research has also shown that polarons with the same charge and antiparallel spins can scatter into bipolaron states, and the bipolarons can collect in the region where the chains interact and at the interface in polymer/polymer heterojunction materials.²⁹ The conversion of polarons to bipolarons³⁰ and the propagation of a moving charged bipolaron³¹ have also been studied numerically on a single conjugated polymeric chain. The above cited works, therefore, show that the bipolaron, like the polaron, is a common type of self-localized excitation that plays an important role in conjugated polymers, and the participation of bipolarons can open more electroluminescence channels.^{32,33}

Beyond the various species mentioned above, analysis of the electronic spectrum of bipolarons and biexcitons suggests that

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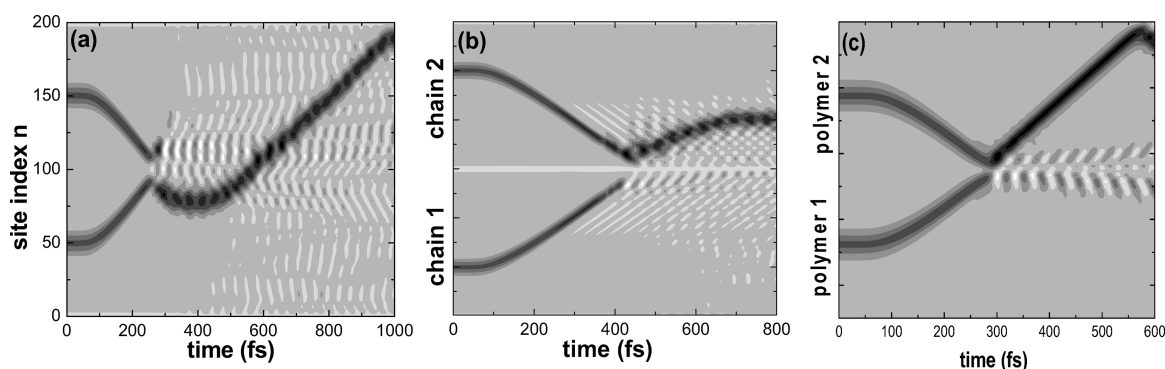


Figure 1. Evolution of the staggered bond order parameter distribution, δ_n , with time under an electric field of strength $E_0 = 1.5 \text{ mV/\AA}$: (a) in a single polymer chain structure; (b) on two coupled polymer chains; and (c) near the heterojunction of a PLED.

biexcitons can be formed by the scattering of oppositely charged bipolarons. To clarify this point, in this paper, the scattering and combination of oppositely charged bipolarons in conjugated polymers are investigated using a nonadiabatic evolution method based on combining the Su–Schrieffer–Heeger (SSH) model and the extended Hubbard model (EHM). In our simulations described below, the lattice is described classically while the electrons are treated by solving the time-dependent Schrödinger equation where transitions between instantaneous eigenstates are allowed.^{34–36} The results show that the formation of biexcitons through the inelastic scattering of oppositely charged bipolarons is of fundamental importance for polymer luminescence and that the inclusion of this channel will provide guidance for improving the internal quantum efficiency of PLEDs.

MODEL AND NUMERICAL METHOD

The Hamiltonian is that of the SSH model with a Brazoskii–Kirova-type symmetry-breaking term,³⁷ including the electron–electron interactions³⁸ and the applied electric field effect, as follows:

$$\begin{aligned}
 H = & - \sum_{n,s} [t_n + (-1)^n t_e] (c_{n+1,s}^\dagger c_{n,s} + hc) \\
 & + \frac{U}{2} \sum_{n,s} \left(c_{n,s}^\dagger c_{n,s} - \frac{1}{2} \right) \left(c_{n,-s}^\dagger c_{n,-s} - \frac{1}{2} \right) \\
 & + V \sum_{n,s,s'} \left(c_{n,s}^\dagger c_{n,s} - \frac{1}{2} \right) \left(c_{n+1,s'}^\dagger c_{n+1,s'} - \frac{1}{2} \right) \\
 & + \frac{K}{2} \sum_n (u_{n+1} - u_n)^2 + \frac{1}{2} m \sum_n \dot{u}_n^2 \\
 & + |e| \sum_{n,s} (na + u_n) \left(c_{n,s}^\dagger c_{n,s} - \frac{1}{2} \right) E(t)
 \end{aligned} \quad (1)$$

where $t_n = t_0 - \alpha(u_{n+1} - u_n)$, in which t_0 is the transfer integral of π -electrons in a regular lattice, α is the electron–lattice coupling constant, and u_n is the lattice displacement of the n -th site from its equidistant position. The quantity t_e is introduced to lift the ground-state degeneracy for nondegenerate polymers. The operator $c_{n,s}^\dagger (c_{n,s})$ creates (annihilates) a π -electron at the n -th site. K is the elastic constant, and m is the mass of a CH group. In this paper, these extended-Hubbard-type interactions are treated within the Hartree–Fock approximation,²⁸ and the applied field

has the form of a half Gaussian constant with an amplitude of E_0 .³⁹ Though the model parameters are those generally chosen for polyacetylene,^{38,40} $t_0 = 2.5 \text{ eV}$, $\alpha = 4.1 \text{ eV/\AA}$, $t_e = 0.05 \text{ eV}$, $K = 21.0 \text{ eV/\AA}^2$, $m = 1349.14 \text{ eVfs}^2/\text{\AA}^2$, and $a = 1.22 \text{ \AA}$, all results given below are also valid for other conjugated polymers with nondegenerate ground states for which the on-site Coulomb interactions, U , and the nearest-neighbor interactions, V , are below the critical values of $U \sim 5.0 \text{ eV}$ and $V \sim 2.0 \text{ eV}$. The values $U = V = 0.5 \text{ eV}$ are used in the present paper.

The initial bond configuration and electron structure can be obtained by solving the self-consistent equations of the bond configuration (u_n) and the electronic wave functions ($\phi_k^s(n)$). Once u_n and $\phi_k^s(n)$ are determined, the temporal evolution of the lattice configuration or charge distribution is determined by the equation of motion for the atom displacements, which can be solved using the Runge–Kutta method of order 8 with step-size control.^{40,41}

RESULTS AND DISCUSSION

A monolayer PLED is normally a sandwich structure; that is, the electroluminescent polymeric materials (EPM) are inserted between the positive electrode and negative electrode. For a given bias, V_0 , applied to the electrodes and for coupling, t' , between the electrodes and EMP, holes and electrons can be injected into the EPM from the positive electrode and negative electrode, respectively. Because of their strong electron–lattice interactions, the lattice structures of conjugated polymers can be distorted easily to form self-trapped elementary excitations (e.g., a hole polaron (P^+), an electron polaron (P^-), a hole bipolaron (BP^+), and an electron bipolaron (BP^-), etc.) on both sides of the EPM.^{25,29} Extending our previous work on the combination of oppositely charged polarons⁹ and the interaction of a polaron–bipolaron pair,⁹ we now focus on the scattering and combination of oppositely charged bipolarons in the EPM electroluminescence layer in the presence of electric fields. For moderate electric fields (e.g., $E_0 = 1.5 \text{ mV/\AA}$) applied along the chain, oppositely charged bipolarons approach each other and collide. Before their collision, the motion of both the electron bipolaron and the hole bipolaron is the same as that reported in ref 30; that is, each independent charged bipolaron moves as one entity consisting of both a charge and lattice defect.

Figure 1a shows the evolution of the staggered bond order parameter $\delta_n \equiv (-1)^n (2u_n - u_{n+1} - u_{n-1})/4$ in a single polymer chain. One can see that the oppositely charged bipolarons in conjugated polymers come close to each other and then

collide, driven by the electric field effect. The wave functions of the two bipolarons begin to overlap strongly when they reach their shortest distance. Eventually, they are close together at the remaining time, and the Coulomb attraction and self-trapped state cooperatively produce a single biexciton deformation with reduced positive charge by transferring two electrons from BP^- to BP^+ . The result of this process is clearly seen in the net charge distributions before and after the collision, as shown in Figure 2. The results show that the net charge of the two bipolarons greatly decreases and simultaneously a slight net charge fluctuation is widely induced on the chain after the collision. The production can also be followed by analyzing the energy levels and occupation numbers, as shown in Figure 3.

Besides the scattering of oppositely charged bipolarons on an isolated single chain in a monolayer PLED, the combination of bipolarons lying on coupled polymer interchains is also common in actual monolayer PLEDs. The interchain coupling Hamiltonian is given by the following equation:^{42–44}

$$H_{\text{int}} = - \sum_{n,s} [t_1 + (-1)^n t_2] (c_{1,n,s}^\dagger c_{2,n,s} + hc) + \sum_{n,s,s'} U_0 \left(c_{1,n,s}^\dagger c_{1,n,s} - \frac{1}{2} \right) \left(c_{2,n,s'}^\dagger c_{2,n,s'} - \frac{1}{2} \right) \quad (2)$$

where $t_1(t_2)$ denotes the transfer integral of the interchain interactions and U_0 is the electron–electron interchain interaction.

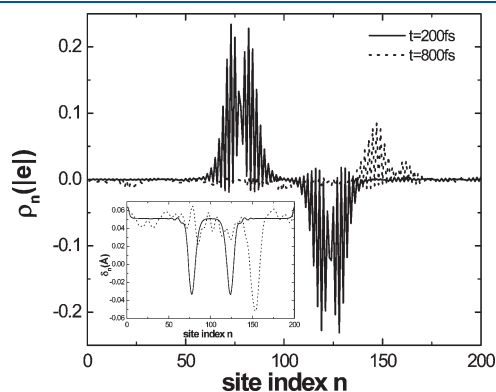


Figure 2. The charge distribution, ρ_n , and the staggered bond order parameter, δ_n (inset) at different times before and after the scattering shown in Figure 1a.

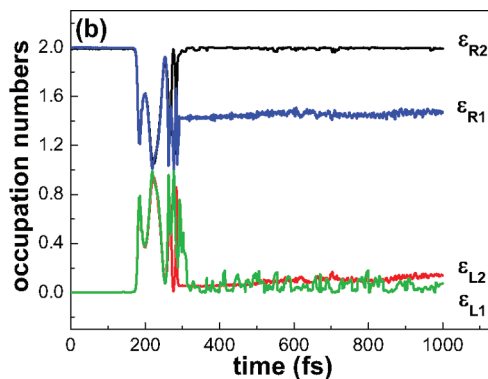
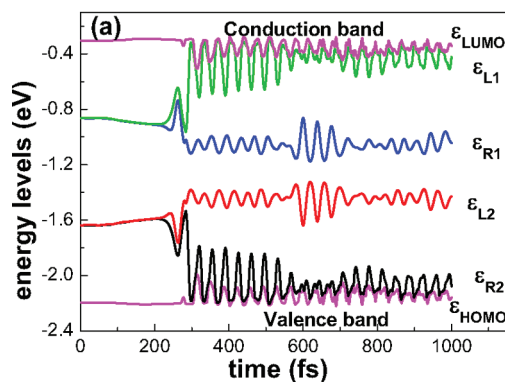


Figure 3. Evolution with time, corresponding to the scattering described in Figure 1a: (a) localized electronic energy levels; and (b) occupation numbers of localized energy levels.

By way of illustration, we consider a system consisting of two 150 site polymer chains placed beside each other and overlapping by 50 sites. A hole bipolaron is introduced near the left end of chain 1, and an electron bipolaron is introduced near the right end of chain 2. The evolution of the staggered bond parameter with time for the case^{42–44} $t_1 = 0.1$ eV, $t_2 = 0.15$ eV, and $U_0 = 0.1$ eV in the presence of an electric field of strength $E_0 = 1.5$ mV/Å is shown in Figure 1b. Similar to the scattering process of the two bipolarons on a single chain, the two bipolarons now also combine to form a lattice deformation (biexciton state) in the overlap area of the two polymer chains. This combination process is also of importance for the formation of biexcitons, because it has a high quantum yield of biexcitons. Similar to the case mentioned above with two bipolarons on the same chain, some charge is excited into higher energy levels during the combination process.

The dependence of the yield of biexcitons on the number of overlapping sites is an interesting issue. We have carefully investigated the dependence of inelastic scattering of oppositely charged bipolarons on the number of overlapping sites in a system consisting of two 200 site polymer chains placed beside each other under the electric field $E_0 = 1.0$ mV/Å. Figure 4 shows that the formation yield of biexcitons increases with increasing the number of overlapping sites to its maximum value of about 30 sites, where the length of overlapping sites is almost the same order of magnitude as the width of the bipolaron, and then decreases as the number of overlapping sites continues to increase. This can be easily understood as the following: the

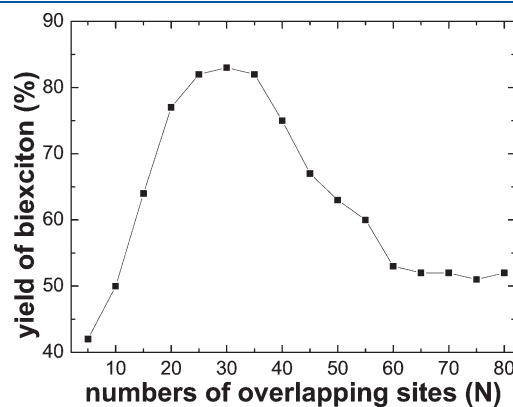


Figure 4. Dependence of the yield of biexcitons on the number of overlapping sites.

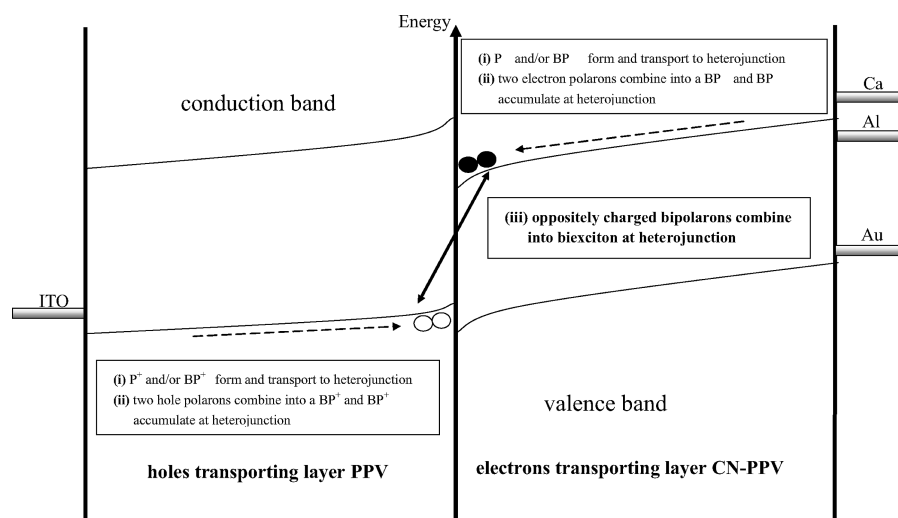


Figure 5. Scheme for forming biexcitons by combination of oppositely charged bipolarons at a HTL/ETL heterojunction (a black dot denotes an electron; a white dot denotes a hole).

number of overlapping sites can affect the overlap of oppositely charged bipolaron wave functions. In turn, the charge transfer between them depends on the overlap of their wave functions and the time they stay close. Therefore, when their wave functions have a larger overlap, making charge transfer more easy, the yield of biexcitons has a larger value.

To balance the injection of holes and electrons, real PLEDs often have a multilayer structure with a hole transporting layer (HTL) and/or an electron transporting layer (ETL) inserted into the PLED.^{3,45,46} That is, the EPM is fabricated as a multilayer structure, and the heterojunction is formed between dissimilar organic semiconductors. In real PPV/CN-PPV PLEDs, as shown in Figure 5, the energy gap of the HTL (PPV layer) is typically larger by 0.2 eV than that of the ETL (CN-PPV layer); that is, the potential barrier is about 0.2 eV, and the hopping integrals at the interface are about 1.0 eV.⁴⁵ For these parameters, most of the bipolarons move toward the heterojunction under the influence of the electric field but are blocked and collect at the heterojunction interface. Thus, the combination of oppositely charged bipolarons to form biexciton states should occur mainly at the heterojunction interface of multiple-layer polymer structures. Figure 1c shows the evolution of the staggered bond parameter with time for the parameters of real PPV/CN-PPV multiple-layer PLEDs under moderate electric field $E_0 = 1.5$ mV/Å. The result shows that the two bipolarons can combine to become a biexciton state not only on chains as mentioned above but also at the interface of the heterojunction. Note also the high quantum formation yield of biexcitons (73%). The results are expected to be qualitatively valid for other multiple-layer PLEDs.

These behaviors of biexciton formation are reflected in the energy levels and occupation numbers. As an example, the evolution of the energy levels with time corresponding to Figure 1a along with their occupation numbers are plotted in Figure 3. The energy levels of the bipolaron state are closed-shell configurations; the up-spin electron wave function of every energy level is the same as that of the down-spin electron. Figure 3a shows that there are four localized electronic energy levels in the energy gap, which are localized electronic states corresponding to the two lattice defects before the collision. We use ε_{L1} (ε_{R1}) and ε_{L2} (ε_{R2})

to denote the upper level and the lower level, respectively, corresponding to the defect at the left (right) side. Initially, ε_{L1} and ε_{R1} (ε_{L2} and ε_{R2}) are degenerate, because the two bipolarons are far apart. As time increases, the degeneracy is broken both by the electric field due to the Stark effect and by the coupling of the two bipolarons when they come closer; that is, ε_{R1} (ε_{R2}) goes downward, and ε_{L1} (ε_{L2}) goes upward. After the collision, these energy levels oscillate with time, corresponding to the amplitude oscillation of the lattice deformations. Simultaneously, two localized levels (ε_{L1} and ε_{R2}) gradually merge into the continuum, and the remainder (of ε_{R1} and ε_{L2}) go deeper into the gap to form a self-trapped biexciton state corresponding to a single large lattice deformation. For the occupation numbers of upper localized energy levels (ε_{L1} , ε_{R1}) and lower localized energy levels (ε_{L2} , ε_{R2}), see Figure 3b. In the initial state, ε_{R1} and ε_{R2} are both occupied by two electrons with opposite spin and ε_{L1} and ε_{L2} are empty. This indicates that a hole bipolaron is located on the left side of the chain and an electron bipolaron is located on the right side. When the constant lattice distortion is formed after collision, the occupation numbers for ε_{L1} and ε_{L2} remain ~ 0 and ε_{R2} remains ~ 2.0 , while the electron population in ε_{R1} changes to ~ 1.45 . From the above analysis, the main products after the scattering of the oppositely charged bipolarons are the biexciton state plus a few free charges excited into the conduction band levels during the combination process. Similar to the scattering process of the two bipolarons on a single chain, the behaviors of biexciton formation on coupled interchains and at a multilayer heterojunction structure are also reflected in the energy levels and occupation numbers (these behaviors are not displayed in this paper).

The yield of the biexciton state can also be calculated by using a projection method that is adopted in our previous research.^{8–10} The evolved wave function of the whole system $|\Psi(t)\rangle$ can be constructed by the single electron evolutionary wave function ($\psi_k(n,t)$) as a Slater determinant. After each evolution step, the evolved state $|\Psi(t)\rangle$ is projected onto the space of eigenstates of the system. The relative yield $I_K(t)$ for a given eigenstate $|\Phi_K\rangle$ is then obtained from $I_K(t) = |\langle\Phi_K|\Psi(t)\rangle|^2$. In our cases, the state $|\Phi_K\rangle$ is constructed using the functions ($\phi_k(n,t)$), which are the eigenfunctions of the electronic part of the Hamiltonian,

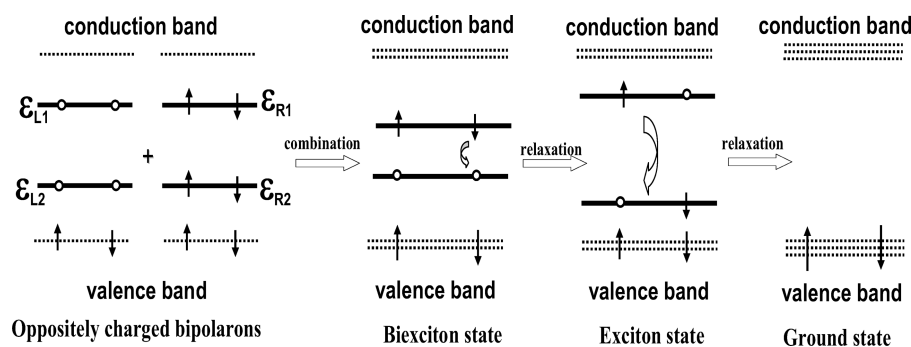


Figure 6. Schematic diagram of the biexciton formation through oppositely charged bipolaron scattering and the radiative decay of the biexciton.

and $|\Phi_K\rangle$ can be any state of interest, for example, the biexciton state. The results show that there is a high quantum yield of biexcitons, which may reach as high as 75%. Simultaneously, another free charge is excited into the higher energy levels in the combination process.

With the above findings, we propose the following possibility: the efficiency of electroluminescence in PLEDs can be highly improved if the hole bipolarons collide with electron bipolarons. The design of an associated multilayer PLEDs device is shown in Figure 5. As a result of the strong electron–lattice interactions, self-trapped elementary excitations can form when the holes and the electrons are injected into the HTL and ETL, respectively. Under the effect of the electric field, these oppositely charged excitations can move through their respective transport materials and accumulate at the heterojunction interface, and the two same charge polarons with antiparallel spins can combine into a singlet bipolaronic state simultaneously.^{25,29} Most importantly, the biexcitons can be formed by the combination of oppositely charged bipolarons, as illustrated in Figure 5.

For a biexciton, there are two localized states in the gap, where the upper one is occupied by two electrons with opposite spin and the lower one is empty. The wave functions of the two localized electronic energy levels of the biexciton have opposite parity. Using the polymer's parameters, which are chosen in this paper, the numerical calculation results show that the radiative process $BE \rightarrow Ex + h\nu$ has large transition dipole moments (8.8 eÅ), so that the biexciton state can decay to exciton state by emitting one photon. After the emission, the biexciton becomes a singlet exciton. In this resultant exciton, there are also two localized states with opposite parity in the energy levels gap, where each of them is occupied by one electron with opposite spin. The numerical calculation result indicates that the radiative process $Ex \rightarrow GS + h\nu$ also has large transition dipole moments (5.5 eÅ), which are the same order of magnitude as those of the biexciton. Finally, the exciton state can decay to the ground state by emitting one photon. In conclusion, besides the previous investigations of the physical principles for improving the quantum efficiency,^{7–11} it should be stressed that the electroluminescence process in PLEDs results partly from the following processes: the formation process $BP^+ + BP^- \rightarrow BE$, the radiative decay process $BE \rightarrow Ex + h\nu$, and finally $Ex \rightarrow GS + h\nu$, as shown in Figure 6.

SUMMARY

In summary, by combining the one-dimensional SSH model and the EHM, the scattering and combination of oppositely charged bipolarons in conjugated polymers have been investigated,

using a nonadiabatic evolution method. Results show that two bipolarons can scatter into singlet biexciton states in both monolayer and/or multiple-layer electroluminescence polymeric materials. The yield of biexcitons in the collision of bipolarons can reach values as high as about 75%. The biexciton state can decay to an exciton state, which can subsequently decay to the ground state, allowing the overall electroluminescent quantum efficiency in PLEDs from all sources to reach values as high as about 75%. These results are important for understanding the experimental fact that the internal quantum efficiency can reach as high as 60%. Consequently, the formation process of biexcitons by the scattering and combination of oppositely charged bipolarons provides an approach for designing a PLED structure with higher electroluminescent efficiency.

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