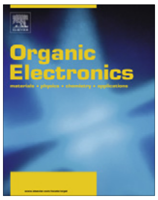
Organic Electronics 13 (2012) 1178–1184

Contents lists available at SciVerse ScienceDirect

Organic Electronics

journal homepage: www.elsevier.com/locate/orgel



The dynamic formation of trions in conjugated polymers

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ARTICLE INFO

Article history:
Received 23 December 2011
Received in revised form 18 March 2012
Accepted 22 March 2012
Available online 6 April 2012

Keywords:
Polymers
Electron–lattice interaction
Trion

ABSTRACT

The dynamic formation process of a trion by recombination of an on-chain bipolaron with an off-chain counterion trapped in a radical molecule, under the influence of an external electric field, has been investigated using a nonadiabatic evolution method. We demonstrate that the dynamic formation of the trion depends sensitively on the strength of the applied electric field, the radical potential, and the coupling between the polymer chain and radical. The trion can be formed efficiently via the bipolaron-trapped counterion reaction under the appropriate conditions. Our simulation provides theoretical evidence for the trion formation channel proposed by Kadashchuk et al. The bipolaron-trapped counterion reaction also makes an additional contribution to electroluminescence in conjugated polymers that lies beyond the set of processes involving polaron recombination.

1. Introduction

In recent years, due to their processing and performance advantages for low-cost and large-area applications, much research has focused on studies of organic electronic devices [1], especially polymer light-emitting diodes (PLEDs) and field-effect transistors, i.e., multilayered devices based on organic polymer films sandwiched between electrodes. Due to strong electron–lattice interactions, electrons or holes injected from the electrodes induce self-localized excitations, such as polarons and bipolarons. A polaron has spin ±1/2 and charge $\pm e$, whereas a bipolaron is spinless with charge $\pm 2e$ [2]. Both polarons and bipolarons are believed to be of fundamental importance in understanding the operation of the optoelectronic devices based on conjugated polymers.

The concept of bipolaron formation was advanced almost 30 years ago [3]. Since then, a number of experimental and theoretical studies have shown the existence of bipolarons especially in doped polymers. For example, through theoretical calculations, Brazovskii et al. concluded that the formation of a bipolaron is energetically favorable as compared to the formation of two polarons for weak electron–electron interactions [4]. The optical data measured by Lane testified directly to the existence of polarons and bipolarons in conjugated polymers [5]. Bipolarons can be created in organic LEDs where charge injection results in a large concentration of polarons [6]. The dynamics simulations show that the charges injected from a metal electrode into a nondegenerate polymer chain can favor the formation of electron (or hole) bipolarons which have better stability than two polarons [7]. The infrared-active vibrational modes around a bipolaron have also been discussed within a two-dimensional Su–Schrieffer–Heeger model [8]. Based on these previous works, it can be stated that the bipolaron is a common type of self-localized excitation that has a large possibility of interacting with other charged defects or impurities in conjugated polymers. In the present work, we demonstrate that an on-chain bipolaron with an off-chain counterion trapped in a radical molecule can be recombined and form a trion under the influence of an external electric field. The trion is essentially a three-particle bound state including two electrons and a hole, or two holes and an electron. It is easy to understand that the trion, like the polaron and the bipolaron, is a

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http://dx.doi.org/10.1016/j.orgel.2012.03.023

self-localized excitation including both charge and lattice distortion. The first observation at room temperature of trions in one-dimensional carbon nanotubes by adding *p*-type dopant has recently been reported [9]. Kadashchuk and coworkers suggested, on the basis of an experimental study of PPV derivatives [10], that a charged trion can also be created by fusion of a free polaron with a neutral polaron pair. We think the evolution of trions might probably be described by our present model irrespectively of rout dominating their formation.

Several theoretical studies have recently pointed out that significant contributions to electroluminescence in conjugated polymers beyond those involving polaron recombination may arise through additional processes, for example, triplet exciton quenching by a polaron [11–13] or bipolaron [14], polaron–polaron interaction-induced bipolaron [15–17], and polaron-bipolaron scattering [18,19]. In these processes, a new self-localized state, the excited polaron, that opens a new channel for improving the electroluminescence efficiency in PLEDs, can be formed. In fact, the excited polaron is equivalent to a charged trion, as can be shown through their electronic states. In the electronic spectrum of a finite polymer chain containing a trion, there are two localized energy levels in the gap: the upper one ε_t^u and the lower one ε_t^d. For the negative trion, ε_t^d is occupied by one electron, and ε_t^u by two; for the positive trion, ε_t^u is occupied by one electron, and ε_t^d is empty. When an electron located in ε_t^u transits to ε_t^d, a photon can be emitted and the trion decays into a normal polaron. Fig. 1 shows the lattice configuration and electronic state of a positive trion. Obviously, as a three-particle-system, the trion possesses a larger binding energy [20] and lattice distortion than does the polaron or bipolaron.

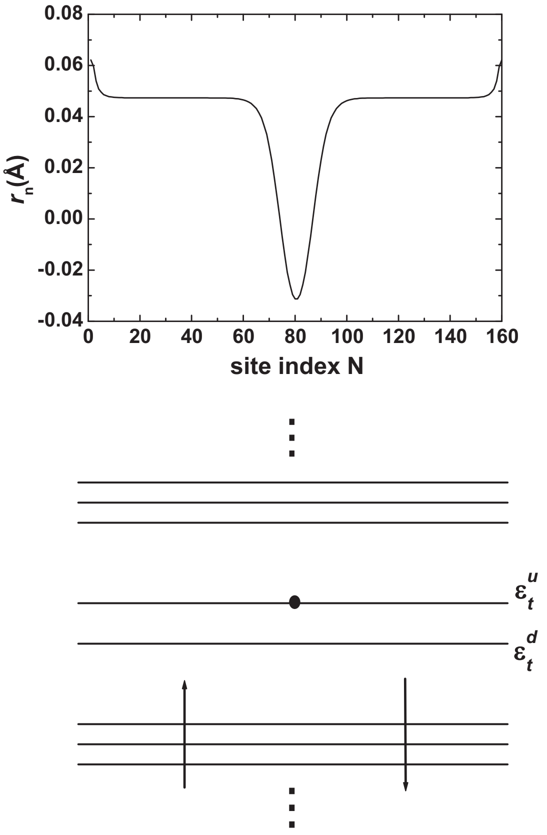

Fig. 1. The lattice configuration and the schematic diagram of energy levels for the positive trion.

Beyond the various processes of trion formation mentioned above, analysis of the electronic spectrum of bipolarons and trions suggests that trions can also be formed by bipolaron-counterion scattering in conjugated polymers. To clarify this point, we investigate the scattering and recombination of an on-chain bipolaron with a trapped counterion coming from a side radical, under the influence of external electric field. The calculations are carried out using an evolution method based on the Su–Schrieffer–Heeger (SSH) model. Such a 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. We focus on investigating the products and their yields in the bipolaron-trapped counterion reaction, and we especially consider, whether this reaction is an efficient mechanism for giving birth to trions. In our calculations, an unpaired electron in the side radical molecule was taken as an off-chain trapped counterion. The dynamics calculations were performed using a nonadiabatic evolution method where electron transitions between instantaneous eigenstates were allowed in contrast to the so-called adiabatic dynamics with fixed level occupation.

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 that of the SSH model with a Brazoskii-Kirova-type symmetry-breaking term and including the applied electric field effect:

$$H = H_{\mathrm{SSH}} + H_{\mathrm{ext}} + H_{\mathrm{SR}}. \tag{1}$$

The first term of Eq. (1) expresses the Su–Schrieffer–Heeger (SSH) Hamiltonian [21]:

$$H_{\mathrm{SSH}} = -\sum_{n,s} t_n (c_{n,s}^{\dagger} c_{n+1,s} + h.c.) + \frac{K}{2}\sum_n (u_{n+1} - u_n)^2 + \frac{M}{2}\sum_n \dot{u}_n^2, \tag{2}$$

here, $t_n = t_0 - \alpha(u_{n+1} - u_n) + (-1)^n t_e$ is the hopping integral between intrachain sites n and $n+1$with t_0 being the transfer integral of π electrons in a regular lattice, α is the electron–lattice coupling constant, and u_n the lattice displacement of the nth site from its equidistant position. The term t_e is introduced to lift the ground-state degeneracy in nondegenerate polymers [22]. K is the elastic constant due to the σ bonds, and M is the mass of a CH group. H_{ext} is the additional potential energy induced by the applied electric field E, and has the form:

$$H_{\mathrm{ext}} = E\sum_{n,s} |e| [na + u_n] \left[c_{n,s}^{\dagger} c_{n,s} - \frac{1}{2} \right], \tag{3}$$

where e is the electron charge, and a is the lattice constant.

The contribution to the Hamiltonian from the side radical is described by:

$$H_{\mathrm{SR}} = -t_1(c^{\dagger}_{P,s}c_{n_i,s} + h.c.) + V_{\mathrm{SR}}c^{\dagger}_{n_i,s}c_{n_i,s}, \tag{4}$$

Here the side radical is taken to be bonded at the pth site of the chain. In addition, t_1 is the hopping integral between the on-chain pth site and the side radical molecule (labeled as n_ith site), and V_{SR} the strength of the side radical potential. Although the parameters used here are taken as those chosen for polyacetylene [3], i.e., $t_0 = 2.5$ eV, α = 4.1 eV/Å, $t_e = 0.05$ eV, K = 21 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.

The temporal evolution of the lattice configuration is determined by the equation of motion:

$$M\ddot{u}_n = -K(2u_n - u_{n+1} - u_{n-1}) + 2\alpha\sum_S[\rho^s_{n,n+1}(t) - \rho^s_{n,n-1}(t)] - |e|E(t)\sum_s[\rho^s_{n,n}(t)], \tag{5}$$

where the density matrix ρ is defined as:

$$p^s_{n,n\prime}(t) = \sum_k \Phi^s_{n,k}(t) f_{k,s} \Phi^{s^*}_{n\prime,k}(t), \tag{6}$$

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

$$i\hbar\dot{\Phi}^s_{n,k}(t) = -t_n\Phi^s_{n+1,k}(t) - t_{n-1}\Phi^s_{n-1,t}(t) + V_{\mathrm{SR}}\Phi^s_{n,k}(t)\delta_{n,n_i} \tag{7}$$

The coupled differential Eqs. (5) and (7) can be solved with a Runge–Kutta method of order 8 with step-size control [23], which has proven to be an effective approach in investigating polaron [24–26] and soliton [27] dynamics and photoexcitation dynamics [28] in conjugated polymers.

3. Results and discussions

In our simulations, a polymer chain containing 160 CH-units with a side radical molecule containing 1 site was considered. Initially, the bipolaron was located at the 40th site while the radical was located at the 100th site of the main chain. They were well enough separated to ensure they were initially non-interacting. At first, the strength of the radical potential was taken as $V_{\mathrm{SR}} = 0.33$ eV, and the coupling between the chain and the radical was $t_1 = 0.1$ eV. Starting from the initial conditions, we investigated the collision processes of a positive bipolaron driven by the external field with a counterion trapped in the side radical. For convenience of discussion, we introduce the bond structure parameter r_n defined as:

$$r_n = (-1)^n \frac{u_{n-1} + u_{n+1} - 2u_n}{4} \tag{8}$$

The external electric field with a direction from left to right was applied. In order to reduce lattice vibrations during the acceleration process of the bipolaron, the electric field was turned on in a smooth way, as described in Ref. [24].

Fig. 2 shows the lattice configuration evolution for the bipolaron–radical collision at different electric field strengths. The light gray regions represent perfect dimerization ($r_n \sim 0.04$ Å), and the darker gray regions indicate the center of the bipolaron (before collision) and/or new states formed via the bipolaron–radical collision. One can see that the bipolaron is first accelerated and then approaches its saturation velocity. When the bipolaron meets the side radical, a collision takes place. After that, they recombine quickly into a new stable local state with larger lattice distortion than that of the bipolaron. In the above processes, the behaviors of both the bipolaron and the new state depend on the field strength. We identify basically three regions of the electric field strength.

(1) In a weak electric field (E < 0.26 × 10^5 V/cm), such as 0.25 × 10^5 V/cm, the new state is confined and oscillates around the side radical. See Fig. 2(a). We have examined this case for a few picoseconds, and find that the new state has little chance of escaping from the radical and moving further along the chain. In this case, the wave functions of the bipolaron and radical have a large overlap, which makes charge transfer between them easy. In the initial state, the main polymer contains a charge of $+2e$ trapped in the bipolaron while the side radical is neutral. As the bipolaron begins to enter into contact and interact with the radical, the system becomes unstable and negative charges start to be injected into the polymer from the radical. The total charges of polymer and radical then oscillate as the new state is pinned by the radical. It is easy to see that the weak field can not offer enough energy for the new state to depart from the radical.

(2) At an intermediate electric field (0.27 × 10^5 V/cm $\leqslant E \leqslant$ 1.1 × 10^5 V/cm), such as 0.5 × 10^5 V/cm, after oscillating around the radical for a short time, the new state gains sufficient energy from the electric field to enable it to escape from the radical and moves along the chain. See Fig. 2(b). The result of this process is clearly seen in the net charge distributions before and after the collision, as shown in Fig. 3. As the new state departs from the radical, its charge decreases to a constant value of about $+1.1e$ that is close to the charge of a perfect polaron. By comparing the evolution of the lattice configuration with that of the charge distribution it can be seen that they coincide with each other in both space and time. Consequently we can conclude that the bipolaron and the unpaired electron form a positive-polaron-like carrier. From the lattice configuration shown in Fig. 2, it may be seen there are some lattice oscillations left after the collision. Such oscillations are new phonon modes created in the collision process [29].

Due to the one-dimensional nature of conjugated polymers, the lattice configuration depends sensitively on the electronic state. Once the latter is changed, the bond structure of the polymer undergoes distortion. To recognize the new state we draw the evolution of energy levels inside and around the gap, as shown in Fig. 4(a). In the initial condition, the levels ε^u_{Bp} and ε^d_{Bp} with values of +0.415 eV and -0.415 eV come from the positive bipolaron, and are empty. The level $\varepsilon_{\mathrm{SR}}$ comes from the side radical and is occupied by an unpaired electron. When the bipolaron approaches and then collides with the radical, the two gap levels of the bipolaron move toward the midgap and form a pair of coupling levels with a narrower gap, which

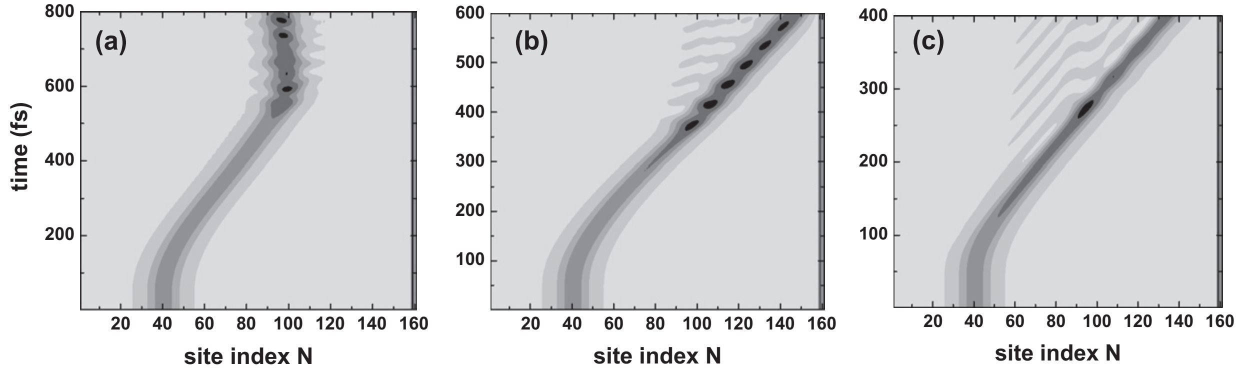

Fig. 2. Temporal evolution of the lattice configuration r_n for the bipolaron-radical collision occuring at different electric field strengths: $E = 0.25 \times 10^5$ V/cm (a); $E = 0.5 \times 10^5$ V/cm (b); $E = 1.5 \times 10^5$ V/cm (c).

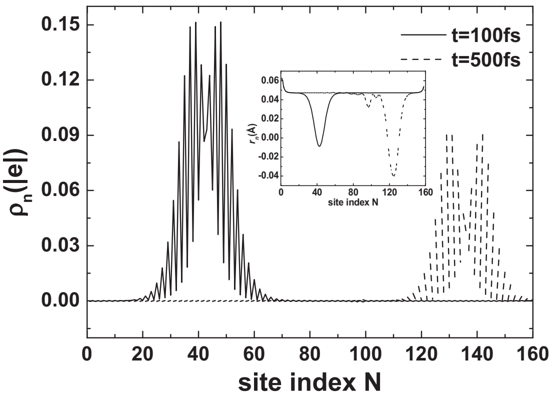

Fig. 3. The charge distribution, ρ_n, and, the bond structure parameter, r_n (inset), at different times before and after the collision, $E = 0.5 \times 10^5$ V/cm.

suggests that the bipolaron–radical interaction results in a new bound state with larger binding energy and lattice distortion than those of bipolaron. We denote the gap levels of the new state by ε_N^d and ε_N^u. It should be noted that the oscillation of the intragap levels is associated with the lattice oscillation caused by the interaction between the bipolaron and the radical.

By analysis of the temporal evolution of the occupation numbers shown in Fig. 4(b), we found that the bipolaron–radical collision induces the unpaired electron to be transfer among the intragap levels ε_N^d, ε_N^u and ε_{SR}, and the conduction-band with different probabilities. We found that there are mainly two electronic states, shown in Fig. 5, that are mixed together in the new state after the collision. State (a) denotes the initial electronic state containing an unpaired electron in the radical and a positive bipolaron; state (b) denotes a charged trion. We do not show the other possible states as we have found that the yields of other states are very small compared with these two states.

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:

$$I_K(t) = |\langle\Psi_K|\Phi(t)\rangle|^2 \quad (9)$$

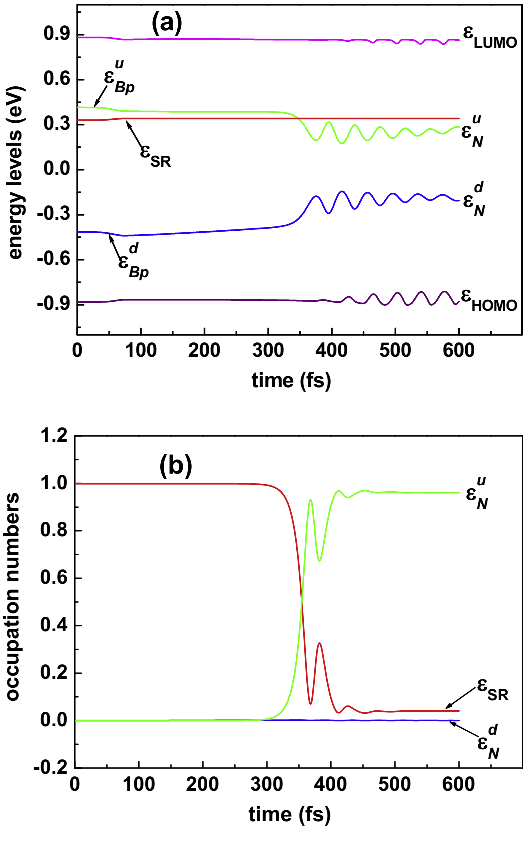

Fig. 4. Evolution with time of the energy levels inside and around the gap (a) and the occupation numbers (b), $E = 0.5 \times 10^5$ V/cm.

Fig. 6 shows the time dependence of yields for states (a) and (b). From the figure, one can see that the yield of state (a) approximates 100% before 300 fs, which corresponds to the situation before the bipolaron-side radical collision. After 300 fs, as the bipolaron begins to interact with the radical, the yield of state (a) drops and then oscillates over a wide range. Meanwhile, the yield of state (b) increases sharply and also oscillates significantly. During this period, the new state is pinned by the radical molecule and the

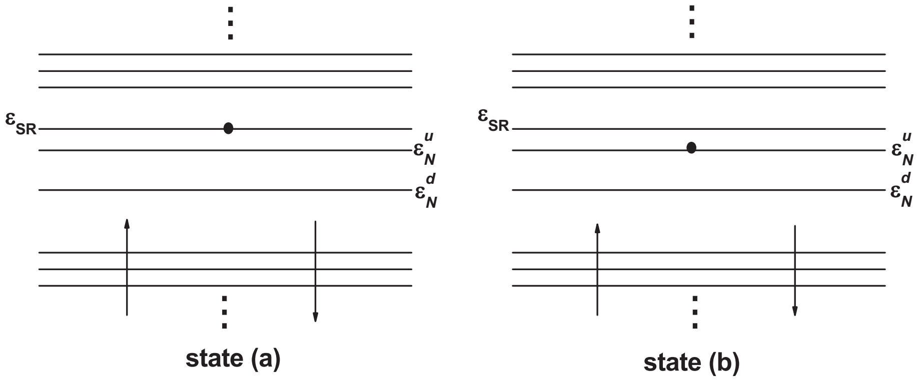

Fig. 5. The electronic state (a) and (b) after the bipolaron-radical collision.

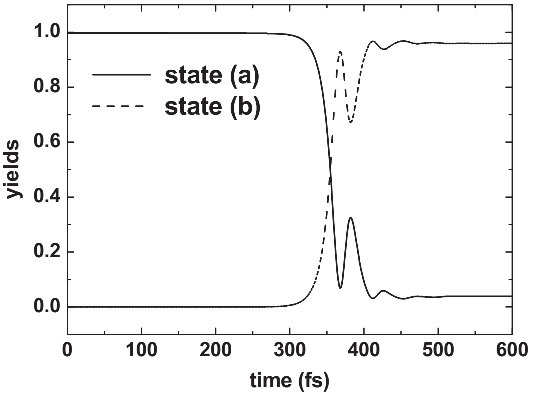

Fig. 6. The temporal evolution of yields for state (a) and (b) (the trion), $E = 0.5 \times 10^5$ V/cm.

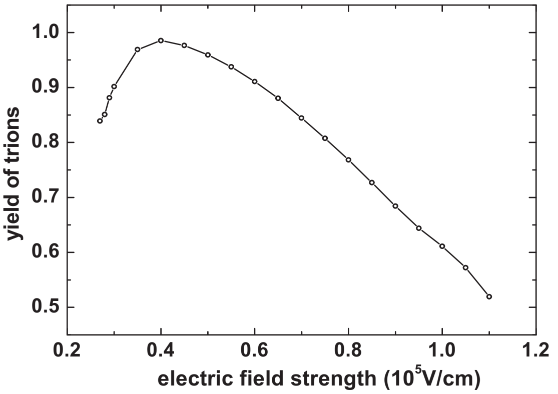

Fig. 7. Yield of charged trions as a function of electric field strength.

charge oscillates violently between the chain and the side radical, which results in the yields of state (a) and (b) also oscillating with the same frequency. After the new state leaves the vicinity of the radical, the yields of states (a) and (b), the trion, approach fixed values of 4% and 96% respectively, from which we can conclude that the trion becomes the main component of the new state.

The above dynamical process shows that the trion is likely to be formed via the recombination of a bipolaron and either a trapped polaron, a charged defect, or an impurity of the opposite sign. This implies that that the model proposed by Kadashchuk et al. [10] is a feasible mechanism for trion formation. Furthermore, like other excitations such as the polaron and bipolaron, the trion can move along the chain as an entity. Due to its larger lattice distortion, the trion saturation velocity is slower than that of either the polaron or the bipolaron under the same external field. The large yield of trions indicates that it plays an important role in the electrical and optical processes of polymers. It is worth noting that trions may decay into a normal polaron with the emission of one photon. Therefore, it can be expected that the reaction of the bipolaron with the trapped counterion can enhance the efficiency of electroluminescence in conjugated polymers.

The above results suggest the following reaction:

$$\mathrm{BP}^{2\pm} + e \rightarrow \mathrm{T}^{\pm}, \qquad (10)$$

Here $\mathrm{BP}^{2\pm}$ denotes the on-chain bipolaron, e the trapped counterion coming from a side radical or a charged defect or impurity, and $\mathrm{T}^{\pm}$ a charged trion. As in the case of a singlet and/or triplet exciton, there are many intrinsic and extrinsic factors that determine the formation and the stability of the trion. The yields of trions at different electric field strengths are depicted in Fig. 7. One can see that the yield of trions first increases as the external electric field strength increases from 0.27 × 105 to 0.4 × 105 V/cm, reaches a maximum value at about $E = 0.4 \times 105$ V/cm, and then decreases as the external electric field becomes larger. This indicates that the formation of the trion depends sensitively on the applied electric field and that a larger electric field is disadvantageous for the formation of trion because of the larger pre-collision velocity of the bipolaron.

We next consider the effect of the strength of the side radical potential on the yield of trions by systematically varying the value of V_{SR} in the presence of an intermediate electric field. Fig. 8 shows the dependence of the trion yield on the radical potential with a fixed field strength. We can see that the yield of trions increases with increasing V_{SR} for $V_{SR} < 0.3$ eV and reaches a broad maximum near $V_{SR} = 0.3$ eV, and then decreases with increasing V_{SR}. For a small value of V_{SR} the radical energy level ε_{SR} is far below the bipolaron level ε_{Bp}^{u} and the electron located in ε_{SR} is unlikely to

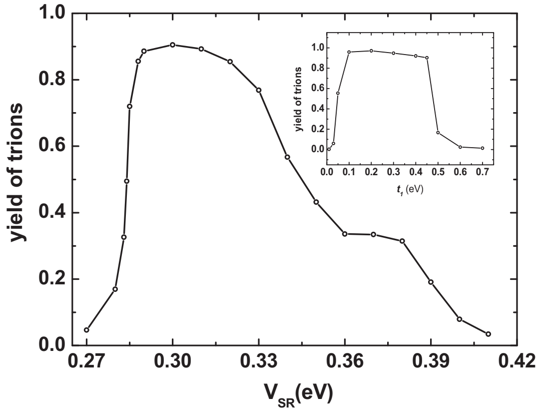

Fig. 8. Yield of trions as a function of the strength of the side radical potential with an electric field of $E = 0.8 \times 10^5$ V/cm .The inset shows the yield of trions as a function of the coupling between the chain and radical.

transit to ε^u_{Bp} due to the large energy barrier, so the trion can not be formed efficiently.

As the value of V_{SR} increases, the electron in ε_{SR} has a greater probability of transiting to ε^u_{Bp} due to the energy barrier decreasing. This process facilitates the formation of a trion, so the yield of trions increases with increasing V_{SR} within a range of $0.27\ \text{eV} < V_{SR} < 0.3$ eV. Increasing the radical potential continues to reduce the difference between the energy levels ε_{SR} and ε^u_{Bp} with the result that there is an even greater coupling between the electronic states of the chain and the radical, and there is a greater rate in the charge transfer. In this case, the bipolaron is likely to be trapped by the radical, so the yield of trions decreases as V_{SR} increases.

The inset in Fig. 8 shows the dependence of the trion yield on the coupling t_1 between the polymer chain and radical. Larger coupling implies a stronger contact between the radical and the polymer. We can see that the bipolaron has a large probability to recombine with the trapped counterion and form a charged trion when t_1 ranges from 0.05 to 0.45 eV. For a small value of t_1 (<0.05 eV), an electron located in the radical has little chance to transit to the chain due to the weak coupling, the bipolarons pass directly through the side radical and few trions are formed. For a larger value of t_1 (>0.45 eV), the charge transfer between the chain and radical becomes intense and the bipolaron is trapped by the radical, few trions can be formed. This indicates that the formation of the trion depends sensitively on the parameters described above.

(3) At a stronger electric field ($E > 1.1 \times 10^5$ V/cm), such as 1.5×10^5 V/cm, after the bipolaron–radical collision, the new state oscillates around the radical for a short time and then departs, continuing to move with more or less the same velocity as the bipolaron. See Fig. 2(c). In this case, the yield of bipolarons is larger than that of charged trions, which indicates that the main component of the new state is the bipolaron. This process can be regarded as the bipolaron passing directly through the radical.

In addition, many theoretical results strongly suggest that disorder is important to the transport process of polarons in conjugated polymers [30]. The symmetry breaking supplied by disorder is essential to obtain creation times [31] and diagonal disorder fosters electronic localization and small-polaron formation [32]. Therefore, the disorder may also have a significant influence on the trion formation and motion. The dynamics in a disorder organic system is a complex task. To describe the formation and dynamics processes of a trion towards the disorder conjugated polymers, our model needs to be extended and will be studied in the further works.

4. Summary

In conclusion, we have simulated the collision processes of a positive bipolaron driven by the external field with a counterion trapped in the side radical using a nonadiabatic evolution method. The bipolaron can pass through the side radical, recombine with the counterion to form a charged trion, or be pinned by the radical, depending on the field strength, the radical potential, and the coupling between the polymer chain and radical. The trion can be formed efficiently via the bipolaron-trapped counterion reaction under the appropriate conditions. Our simulation provides theoretical evidence for the trion formation channel proposed by Kadashchuk et al. It is worthy of note that a trion can decay into a polaron through emission of a photon, so the bipolaron-trapped counterion reaction provides a contribution to the electroluminescence in conjugated polymers.

Acknowledgments

The authors would like to acknowledge the financial support from the National Natural Science Foundation of China (No. 11074064), Hebei Provincial Outstanding Youth Science Fund (No. A2009001512), Key Project of Ministry of Education of China (No. 210021), and Natural Science Fund of Hebei Province, China (No. A2010000357).

References

[1] I.H. Campbell, D.L. Smith, Solid State Phys. 55 (2001) 1.
[2] P.A. Lane, X. Wei, Z.V. Vardeny, in: N.S. Sariciftci (Ed.), Spindependent Recombination Processes in π-Conjugated Polymers, World Scientific, Singapore, 1997, p. 292.
[3] A.J. Heeger, S. Kivelson, J.R. Schreiffer, W.P. Su, Rev. Mod. Phys. 60 (1988) 781.
[4] S. Brazovskii, N. Kirova, Z.G. Yu, A.R. Bishop, A. Saxena, Opt. Mater. 9 (1998) 502.
[5] P.A. Lane, X. Wei, Z.V. Vardeny, Phys. Rev. Lett. 77 (1996) 1544.
[6] C.H. Lee, G. Yu, A.J. Heeger, Phys. Rev. B 47 (1993) 15543.
[7] Y.H. Yan, Z. An, C.Q. Wu, K. Nasu, Eur. Phys. J. B 48 (2005) 501.
[8] Z. Xie, Y.M. Kang, Z. An, Y.C. Li, Phys. Rev. B 61 (2000) 1096.
[9] R. Matsunaga, K. Matsuda, Y. Kanemitsu, Phys. Rev. Lett. 106 (2011) 37404.
[10] A. Kadashchuk, V.I. Arkhipov, C.H. Kim, J. Shinar, et al., Phys. Rev. B 76 (2007) 235205.
[11] Y. Meng, X.J. Liu, B. Di, Z. An, J. Chem. Phys. 131 (2009) 244502.
[12] M. Segal, M.A. Baldo, M.K. Lee, J. Shinar, Z.G. Soos, Phys. Rev. B 71 (2005) 245201.
[13] S. Li, J.F. Luo, T.F. George, Synth. Met. 160 (2010) 2023.
[14] Z. Sun, Y. Li, S.J. Xie, Z. An, D.S. Liu, Phys. Rev.B 79 (2009) 201310(R).
[15] L.S. Swanson, J. Shinar, A.R. Brown, D.D.C. Bradley, R.H. Friend, et al., Phys. Rev B 46 (1992) 15072.
[16] G. Li, C.H. Kim, P.A. Lane, J. Shinar, Phys. Rev. B 69 (2004) 165311.
[17] B. Di, Y. Meng, Y.D. Wang, X.J. Liu, Z. An, J. Phys. Chem. B 115 (2011) 964.
[18] Z. Sun, Y. Li, K. Gao, D.S. Liu, Z. An, S.J. Xie, Org. Electron. 11 (2010) 279.

[19] L. Ge, S. Li, T.F. George, X. Sun, Phys. Lett. A 372 (2008) 3375.
[20] H.Y. Choi, M.J. Rice, Phys. Rev. B 44 (1991) 10521.
[21] W.P. Su, J.R. Schrieffer, A.J. Heeger, Phys. Rev. Lett. 42 (1979) 1698 [Phys. Rev. B 22 (1980) 2099.].
[22] S.A. Brazovskii, N. Kirova, Sov. Phys. JETP 33 (1981) 4.
[23] R.W. Brankin, I. Gladwell, L.F. Shampine, RKSUITE: a suite of Runge-Kutta codes for the initial value problem for ODEs, Softreport 92-S1, Department of Mathematics, Southern Methodist University, Dallas, Texas, USA, 1992. see <http://www.netlib.org>.
[24] C.Q. Wu, Y. Qiu, Z. An, K. Nasu, Phys. Rev. B 68 (2003) 125416.
[25] A. Johansson, S. Stafström, Phys. Rev. Lett. 86 (2001) 3602.
[26] S.V. Rakhmanova, E.M. Conwell, Appl. Phys. Lett. 75 (1999) 1518.
[27] Y. Ono, A. Terai, J. Phys. Soc. Jpn. 59 (1990) 2893.
[28] Z. An, C.Q. Wu, X. Sun, Phys. Rev. Lett. 93 (2004) 216407.
[29] Z. An, B. Di, H. Zhao, C.Q. Wu, Eur. Phys. J. B 63 (2008) 71.
[30] Z. Qu, Y. Li, W. Liu, D.W. Kang, S.J. Xie, Phys. Lett. A 373 (2009) 2189.
[31] P.H. de Oliveria Neto, W.F. da Cunha, L.F. Roncaratti, R. Gargano, G.M. e Silva, Chem. Phys. Lett. 493 (2010) 283.
[32] D. Emin, M.N. Bussac, Phys. Rev. B 49 (1994) 14290.