Dynamics of charge injection into an open conjugated polymer: A nonadiabatic approach

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The dynamic process of charge injection is investigated for an open conjugated polymer chain in contact with a metal electrode in the framework of a nonadiabatic approach. It is found that the injected charges form wave packets due to the strong electron-lattice interactions in the conjugated polymer. A wave packet may contain any quantity of charges up to two electronic units, which depends upon the injection condition. As the system is spin degenerate within the present model, a wave packet has no spin. Discrete energy levels will appear in the gap accompanying the wave packet, which results in potential asymmetry of the charge injection and ejection between the metal electrode and the polymer. The asymmetry can be used to explain the electrical hysteresis in organic devices. It is found that there exists an upper critical field or forming field, beyond which the injected charges could not form a wave packet. Under a strong driving electric field, it is also found that a wave packet will dissociate into an extended state. The dependence of the dissociating field on the charge quantity a wave packet contains is studied.

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I. INTRODUCTION

Conjugated organic materials have been attracting much theoretical and experimental interest both because of the novel physics that occurs in these materials and because of the technological potential of electronic devices fabricated from them.[1–3] In particular, they are already the basis of effective light-emitting diodes (LEDs) and a wider range of devices and applications such as organic spin valves and magnetic resistance.[4,5] In these electronic devices, conjugated polymers are used as the light-emitting and charge-transporting layers. Electrons and/or holes are injected from the metal electrode into the polymer layer and transported under the driving of an external electric field. The essence of the charged carriers in organic polymers has been widely investigated. It has been predicted that doped electrons or holes will form self-trapping states called solitons (only in *trans*-polyacetylene),[6] polarons,[7] or bipolarons,[8] which serve as the transport carriers in conjugated polymers. A polaron is the self-trapping state of one electron or hole and it carries one electronic charge with 1/2 spin, while a bipolaron is the self-trapping state of two electrons or holes and it carries two electronic charges with no spin.

Up to now, there have been extensive studies on polaron dynamics in conjugated polymers under driving electric fields.[9,10] It is found that a polaron will dissociate into an extended state when the field is over 1.0×10^6 V/cm.[11] From a nonadiabatic approach, Wu *et al.* studied the formation process of a polaron by considering injecting a doped electron from a metal electrode into a polymer chain.[12] Stoneham *et al.* summarized the present investigations on electron flow in polymers and indicated the intrinsic difference between a polymer and a conventional semiconductor with the same dimensions.[13] Davids *et al.* gave a picture of bipolaron lattice formation at metal/polymer interfaces with a nondegenerate continuum model.[14] All these investigations seem to show that the electrons are injected one by one from the electrode to the polymer. However, in an organic device, one electronic state belongs to the whole system composed of the open metal electrode and the open polymer layer. It is inexplicable for one electronic state to completely transfer into the polymer layer instantaneously. In this paper, we will follow the evolution of the electronic states in a metal/polymer system driven by an external electric field. In the following section, the model is described and the dynamical evolution method based on a nonadiabatic approach is presented. The results are analyzed in Sec. III. Finally in Sec. IV, a summary is given.

II. MODEL AND METHOD

We consider a one-dimensional metal/polymer structure. The Hamiltonian consists of three parts,

$$H = H_e + H_{latt} + H_{ext}. \tag{1}$$

The electronic part is described with the Su-Schrieffer-Heeger model[6] including a Brazovskii-Kirova-type symmetry breaking term,[15]

$$H_e = -\sum_{n,\sigma} e_n a^\dagger_{n,\sigma} a_{n,\sigma} + \sum_{n,\sigma} t_{n,n+1}(a^\dagger_{n+1,\sigma} a_{n,\sigma} + a^\dagger_{n,\sigma} a_{n+1,\sigma}) \tag{2}$$

where e_n denotes the on-site electron energy of an atom (site) and $t_{n,n+1}$ the hopping integral between sites n and $n+1$. We set $t_{n,n+1}=t_0$ for a bulk metal electrode and $t_{n,n+1}=t_0-\alpha(u_{n+1}-u_n)-(-1)^n t_e$ for a bulk polymer with α the electron-phonon coupling constant and u_n the displacement of the nth site (CH group) from its equidistant position. t_e is introduced to lift the ground-state degeneracy for a nondegenerate polymer. $a^+_{n,\sigma}(a_{n,\sigma})$ denotes the electron creation (annihilation) operator at site n with spin σ ($\sigma=\uparrow,\downarrow$). Here the internal electron-electron interactions are neglected. It has been predicted that the electron-lattice interactions will dominate the properties of polymers if the electron-electron interactions are not too strong.[16,17]

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The Hamiltonian due to the lattice distortion in the polymer is described classically by

$$H_{latt} = \frac{1}{2}\sum_n K(u_{n+1} - u_n)^2 + \frac{M}{2}\sum_n \dot{u}_n^2 \tag{3}$$

where K denotes the elastic constant and M the mass of a CH group.

Interfacial coupling between the metal electrode and the polymer is described by the hopping integral $t_{M\text{-}P} = \beta t_0$ with β the weighting parameter. It has been pointed out that $\beta > 1$ means an interface of a potential well, whereas $\beta < 1$ indicates an interface of a potential barrier.[18]

The contribution from an external electric field is

$$H_{ext} = \sum_{n,\sigma} V_n(t)(a_{n,\sigma}^{\dagger} a_{n,\sigma} - 1) \tag{4}$$

where $V_n(t)$ is the lift potential energy of the electrode for the charge injection $V_n(t) = V(t)$, or the driving field for the moving of the injected charges in the polymer chain, $V_n(t) = -|e|E(t)[(n-n_0)a + u_n]$, where e is the electronic charge, n_0 the interfacial site index of the polymer, and a the lattice constant.

The evolution of the electronic state $|\Phi_{\mu,\sigma}(t)\rangle = \Sigma_n \psi_{\mu,\sigma}(n,t)|n\rangle$ is obtained by solving the time-dependent Schrödinger equation,

$$i\hbar\dot{\psi}_{\mu,\sigma}(n,t) = -t_{n,n+1}\psi_{\mu,\sigma}(n+1,t) - t_{n-1,n}\psi_{\mu,\sigma}(n-1,t) + V_n(t)\psi_{\mu,\sigma}(n,t). \tag{5}$$

The lattice configuration $\{u_n\}$ of the system is inversely determined classically by the electronic states in a nonadiabatic approach,

$$M\ddot{u}_n(t) = K[u_{n+1}(t) + u_{n-1}(t) - 2u_n(t)] + 2\alpha[\rho_{n,n+1}^c(t) - \rho_{n-1,n}^c(t)] - |e|E(t)[\rho_{n,n}^c(t) - 1]. \tag{6}$$

For the metal electrode, we set $u_n = 0$. $\rho_{n,n'}^c$ is defined by the elements of the density matrix $\rho_{n,n'}^{\sigma}$

$$\rho_{n,n'}^{\sigma}(t) = \sum_{\mu} \psi_{\mu,\sigma}^*(n,t) f_{\mu,\sigma} \psi_{\mu,\sigma}(n',t), \tag{7}$$

$$\rho_{n,n'}^c(t) = \rho_{n,n'}^{\sigma}(t) + \rho_{n,n'}^{-\sigma}(t), \tag{8}$$

where $f_{\mu,\sigma}$ is the time-independent distribution function determined by initial occupation (being 0, 1). The coupled differential equations (5) and (6) can be solved numerically with a Runge-Kutta method of order 8 with step-size control,[19] which has been proven to be an effective approach.[9,10] It should be mentioned that $\psi_{\mu,\sigma}(n,t)$ is not the instantaneous eigenstate $\phi_{\mu,\sigma}(n,t)$, which satisfies $H\phi_{\mu,\sigma}(n,t) = \varepsilon_{\mu,\sigma}\phi_{\mu,\sigma}(n,t)$. At the beginning, we have $\psi_{\mu,\sigma}(n,t=0) = \phi_{\mu,\sigma}(n,t=0)$. The occupation of $\psi_{\mu,\sigma}(n,t)$ is supposed to be unchanged during the dynamic process.

Dynamical evolution starts from a system with a static structure, which is given by the static lattice configuration obtained through the minimum of the total energy of the system,

$$u_n = \frac{1}{2}\left(u_{n-1} + u_{n+1} + \frac{2\alpha}{K}\sum_{\mu,\sigma}{}'[\psi_{\mu,\sigma}(n+1,t=0)\psi_{\mu,\sigma}(n,t=0) - \psi_{\mu,\sigma}(n,t=0)\psi_{\mu,\sigma}(n-1,t=0)]\right). \tag{9}$$

We present calculations on a one-dimensional metal/polymer system with the polymer layer containing 200 sites and the metal electrode 100 sites, which is long enough for the present investigation. The parameters for the polymer are those referring to *cis*-polyacetylene with no loss of universality,[20] $t_0 = 2.5$ eV, $t_e = 0.05$ eV, $\alpha = 41$ eV/nm, $K = 2100$ eV/nm^2, and $M = 134\,914$ eV fs^2/nm^2. The on-site energies of both layers are supposed to be zero, which means that the Fermi level of the bulk metal is almost at the middle of the band gap of the bulk polymer. Therefore the highest-occupation electronic state is confined in the metal electrode before the external field is applied.

To show the particularity of charge injection into an organic polymer, we present a comparison of an organic system to an inorganic one with the same gaps. A rigid inorganic semiconductor is modeled by setting $\alpha = 0$ and $t_e = 0.43$ eV to get the same gap of 1.76 eV as that of pristine polyacetylene. This kind of rigid-band semiconductor will have a rigid lattice structure and its band structure will remain unchanged during the injection process.

In the calculation, we suppose the external bias to be turned on smoothly, that is, we let $V(t) = V_0 \exp[-(t-t_c)^2/t_w^2]$ for $0 < t < t_c$ and $V(t) = V_0$ for $t \geqslant t_c$, with t_c being a smooth turn-on period and t_w the width. The applied electric field $E(t)$ is also turned on smoothly with the same mode, i.e., $E(t) = E_0 \exp[-(t-t_c)^2/t_w^2]$ for $0 < t < t_c$ and $E(t) = E_0$ for $t \geqslant t_c$. In calculations, we take $t_c = 30$ fs and $t_w = 25$ fs.

III. RESULTS AND DISCUSSION

An isolated pristine polymer chain has a dimerized lattice structure with an energy gap of $E_g = 1.76$ eV and the lowest unoccupied molecular orbital (LUMO) level at 0.88 eV in the present parameters. The initial structure of the metal/polymer system is obtained by solving the static Schrödinger equation and the equilibrium condition with an iterative method. The Fermi level of the bulk metal is supposed to be at the middle of the band gap of the bulk polymer by setting $e_n = 0$ as stated above.

Now a voltage bias is added to lift the Fermi level of the metal electrode. At the same time, an electric field is applied to drive the injected charges into moving along the chain. For a metal/rigid semiconductor system, the effective barrier height experienced by the injected electrons is the energy difference between the LUMO level of the semiconductor and the Fermi level of the metal electrode, or 0.88 eV in the present parameters. It is found that only when the bias nears 0.88 eV are the electronic charges apparently injected into the semiconductor and the injected charges then extend over the whole semiconductor layer.

For a metal/polymer system, it was predicted that, due to the existence of the virtual polaron level,[13] charges could be injected into the polymer layer even when the Fermi level of

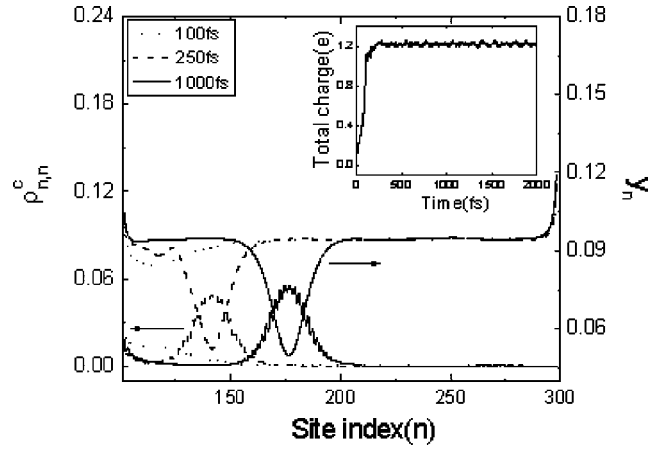

FIG. 1. Injected charge distribution $\rho^c_{n,n}$ (down) and staggered lattice configuration y_n (up) of the polymer chain at a few typical times with $\beta=0.4$. The bias $V_0=0.94$ eV and the field $E_0=5\times10^3$ V/cm. The inset shows the evolution of the total injected charges in the polymer chain.

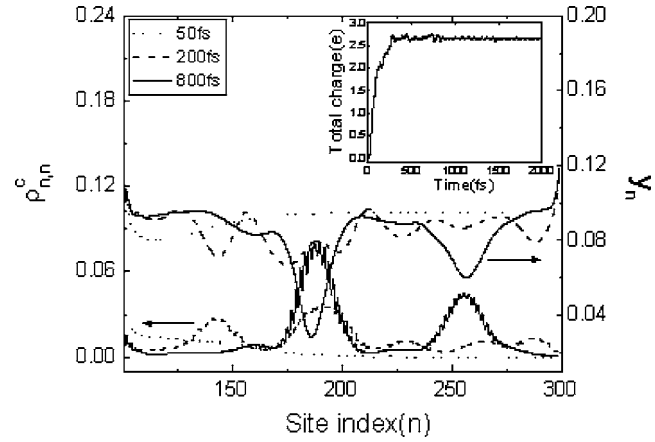

FIG. 2. Injected charge distribution $\rho^c_{n,n}$ (down) and the staggered lattice configuration y_n (up) of the polymer chain at a few typical times with $\beta=0.4$. The bias $V_0=1.05$ eV and the field $E_0=5\times10^3$ V/cm. The inset shows the evolution of the total injected charges in the polymer chain.

the metal is just above the virtual polaron level, or 0.71 eV in the present parameters. However, in an actual system, this virtual polaron level does not exist before charge injection. Now let us turn on a voltage bias and the driving electric field. It is found that charges are injected into the polymer apparently only when the bias $V_0\approx0.88$ eV, which means that charge injection happens only when the Fermi level of the electrode nears the LUMO level of the polymer, which is consistent with the prediction in Ref. 18.

The injected charge distribution $\rho^c_{n,n}$ and staggered lattice configuration $y_n=(-1)^n(u_{n+1}-u_n)$ (in angstroms) of the polymer chain at a few typical times are shown in Fig. 1 with interfacial coupling parameter $\beta=0.4$ at voltage bias $V_0=0.94$ eV and electric field $E_0=5\times10^3$ V/cm. To clarify the property of the injected charges, let us recall a polaron in an isolated polymer chain. When one extra electron is added to the chain, it will occupy the LUMO level. Due to the strong electron-lattice interactions, this level will fall into the gap and its eigenstate becomes localized. Here in the dynamic process of an open polymer chain in contact with a metal electrode, an electronic state belongs to the whole metal/polymer system. The electronic state should have probabilities both in the electrode and in the polymer layer. From the figure, it is found that a localized wave packet forms in the polymer layer, which means that the injected charges will get together due to the strong electron-lattice interactions. The wave packet behaves like a quasiparticle and serves as the transporting carrier in the polymer layer. The evolution of the total injected charges is shown in the inset of Fig. 1. Apparently, the whole injection process will have take a take duration of about 250 fs and then the two layers reach a dynamical balance. At the present bias, it is obtained that about $1.22e$ are injected into the polymer layer, of which about $0.06e$ are confined at the interface. By increasing the bias, more charges will be injected and the wave packet may contain two electronic charges with opposite spin orientations. In this case, it is found that a complete spatial electronic state transfers into the polymer layer and the wave packet is a double-charged bipolaron. On increasing the bias further, another electronic state will begin to transfer toward the polymer and another wave packet will form. Therefore, each wave packet contains no more than two electronic charges. The results at $V_0=1.05$ eV are plotted in Fig. 2. It is found that about $2.7e$ are injected into the polymer layer, of which about $0.1e$ are confined at the interface. There form two wave packets in the polymer layer, one with two electronic units and the other with about $0.6e$. From the evolution at $t=200$ fs, it is also found that the formation of a stable wave packet is not instantaneous but needs a process of charge accumulation. It has been indicated that a polaron moves faster than a bipolaron due to the bigger mass of the latter.[21,22] Here we find that a wave packet with fewer charges moves faster than that with more charges, which implies that charge accumulations will slow down the carriers transportation or decrease the conductance in polymers. It should be mentioned that the result of noninteger charge injection is a consequence of the wave characteristic of electrons and the model in which the metal and the polymer are considered as one composite system, as opposed to considering them as two different systems. For a real metal/polymer device with coupling at the interface, one may get some information due to the wave packets in the polymer layer, but one cannot recognize an isolated noninteger charged wave packet.

Within the present approach, the system is spin degenerate, which means that each spatial eigenstate can contain two electrons with spin up and down separately and each formed wave packet contains a charge quantity of $0-2e$. As charge injection has the same probability for spin up on down due to the spin degeneracy of the system, the wave packet is always spinless. It should be mentioned that, within the present model, the formation of a double-charged bipolaron is favored over two separate singly charged polarons. Unless we fix the spin orientation, we cannot get a spin polaron.

From Figs. 1 and 2, it is also found that a localized lattice defect is induced by the wave packet, and the amplitude of the lattice defect is dependent upon the charge quantity of the

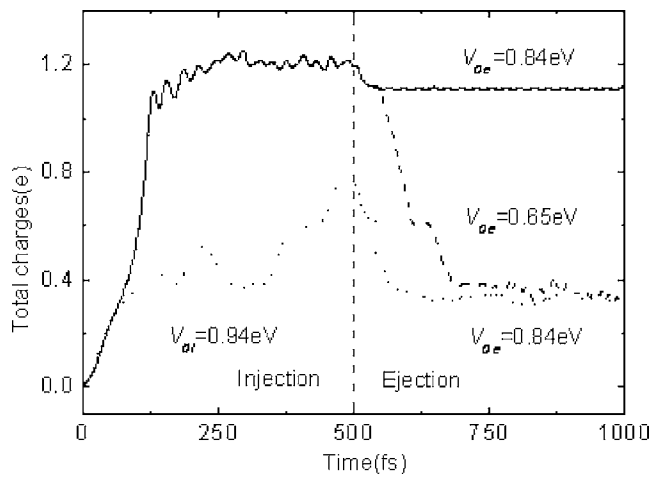

FIG. 3. Evolution of the total injected charges in the polymer chain. At t=500 fs, the bias is adjusted and the field is reversed. The injection bias V_{0i}=0.94 eV, the ejection bias V_{0e}=0.84 (solid line) and 0.65 eV (dashed line) for a metal/soft polymer system and V_{0e}=0.84 eV (dotted line) for a metal/rigid semiconductor system. The strength of the field $E_0=5\times10^3$ V/cm.

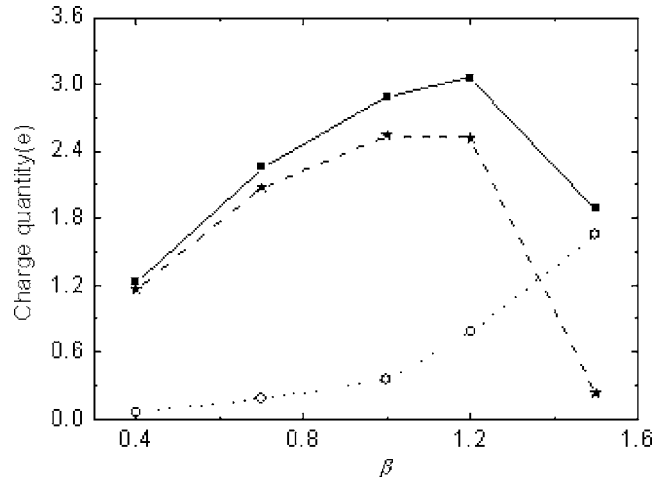

FIG. 4. Dependence of the total injected charge in the polymer chain (solid line) including that being confined at the interface (dotted line) and that departing from the interface into the polymer (dashed line) on the interfacial coupling β. The voltage bias V_0 =0.94 eV and the field $E_0=5\times10^3$ V/cm.

wave packet. If it contains one electronic charge (half with spin up and half with spin down within the present approach), the wave packet behaves like a moving polaron, whereas if it contains two electronic charges, the wave packet behaves as a moving bipolaron.

It is interesting to follow the evolution of the highest occupation level, defined by $\varepsilon_{HO}=\langle\Phi_{HO,\sigma}(t)|H|\Phi_{HO,\sigma}(t)\rangle$, which is the Fermi level of the metal electrode before charge injection. When the Fermi level nears the original LUMO level of the polymer, the charge injection begins. It is found that the level ε_{HO} will fall into the original gap of the polymer and the electronic state corresponding to this level becomes localized in the polymer layer. In fact, the wave packet and the localized state appear simultaneously, which results from the strong electron-lattice interactions in the polymer. The shift of the highest-occupation energy level will result in an interesting phenomenon if we consider the process of charge ejection from the polymer to an equivalent electrode. To mimic the charge ejection in a normal device with two electrodes, a reverse field is applied in the present system after the charges are injected into the polymer layer. As shown in Fig. 3, at t=500 fs, the direction of the electric field is reversed when the bias is adjusted from V_{0i}=0.94 eV (injection bias) to a slightly lower value, i.e., V_{0e}=0.84 eV (ejection bias), which makes the original Fermi level lower than the original LUMO level. If the band is rigid, which is the case for the metal electrode/rigid semiconductor system, the injected charges will return to the metal electrode, as shown in Fig. 3 by the dotted line. But for the metal electrode/soft polymer system, as shown in Fig. 3 by the solid line, the injected charges cannot return to the electrode. To do so, we have to adjust the bias to a much lower value, i.e., V_{0e}=0.65 eV, at which the original Fermi level lies below the occupied ε_{HO}, or about 0.71 eV in the present parameters. The ejection process is shown in Fig. 3 by the dashed line. The asymmetry of the injection and ejection in the metal/polymer structure results from the emergence of localized wave packets with discrete levels, which has been confirmed experimentally by the hysteretic current characteristic.[23] In addition, due to the rigid-band characteristic of the inorganic semiconductor, the magnitude of the total injected charges is also smaller than that for the conjugated polymer in the process of charge injection.

It has been indicated that the interface with coupling strength $\beta<1$ acts as a potential barrier and the injected charges tend to depart from the interface, while the interface with $\beta>1$ acts as a potential well and the injected charges tend to be confined at the interface. Therefore, the process of charge injection (or ejection) is also affected by the interfacial coupling, as shown in Fig. 4 for the fixed bias and electric field chosen as in Fig. 1. It is found that the injected charges departing from the interface into the polymer will reach a maximum value at β=1. The interfacial charge accumulation will increase apparently when the coupling $\beta>1$, which shows the characteristic of the interface as a potential well in this case. With strengthening of the coupling ($\beta>1.2$), more and more charges will be confined at the interface. In this case, the effect of the interface on charge injection will become very important. Due to the softness of organic polymers, it is easy to form a self-adjusting interface between the polymer and the contact electrode.[5] Therefore, the interface can be optimized to realize an effective charge injection in organic devices.

All the discussions above are presented under a weak driving electric field. In fact, the formation of a wave packet is dependent upon the strength of the driving field. It is found that there is an upper critical value of the electric field (forming field) for the forming of a stable wave packet, beyond which the injected charges cannot get together. As shown in Fig. 5 by the solid line, the formation field increases nearly linearly with the quantity of the injected charges. The existence of a formation field can be understood from the competition between the driving field and the confinement of the

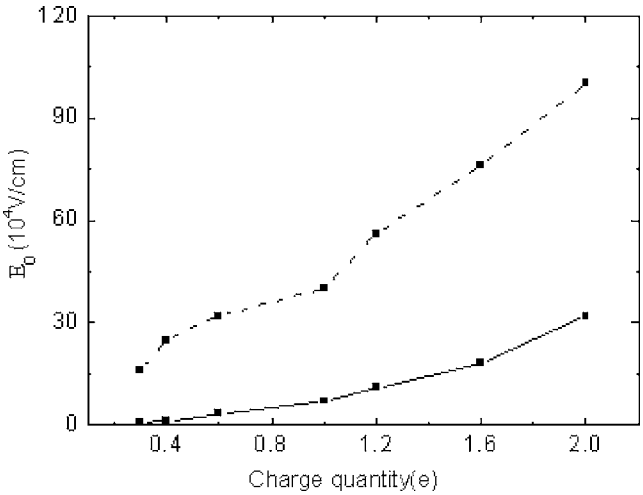

FIG. 5. Dependence of the formation (solid line) and dissociation field (dashed line) on the charge quantity of a wave packet.

lattice on the injected charges. The electron-lattice interactions are inclined to confine the injected charges and are in favor of wave-packet formation, while an external electric field is inclined to drive the injected charges and get rid of the lattice confinement. The evolution of the injected charges at a stronger electric field is shown in the inset of Fig. 6, in which the value of the injected charges is almost the same as in the case of Fig. 2 except for a weaker driving field for the latter. However, it is found that, unlike the case in Fig. 2, although about 2.72e are injected into the polymer, only one wave packet with charge 2e forms. The extra charges (about 0.72e) could not get together and become extended at the present field ($E_0=9\times10^4$ V/cm). If we increase the field to a high value ($\geqslant 3.2\times10^5$ V/cm), it is found that the wave packet with 2e cannot form either and all the injected charges become extended.

It should be pointed out that the electron-electron interactions may also affect the stability of a wave packet. We give a simple calculation in the Hubbard model with the mean

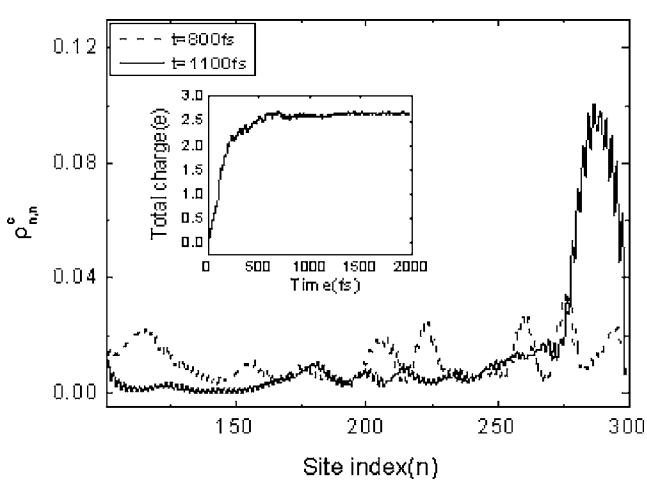

FIG. 6. Injected charge distribution $\rho^c_{n,n}$ at a few typical times with $\beta=0.4$. The voltage bias $V_0=0.94$ eV and the field $E_0=9\times10^4$ V/cm. The inset shows the evolution of the total injected charges in the polymer chain.

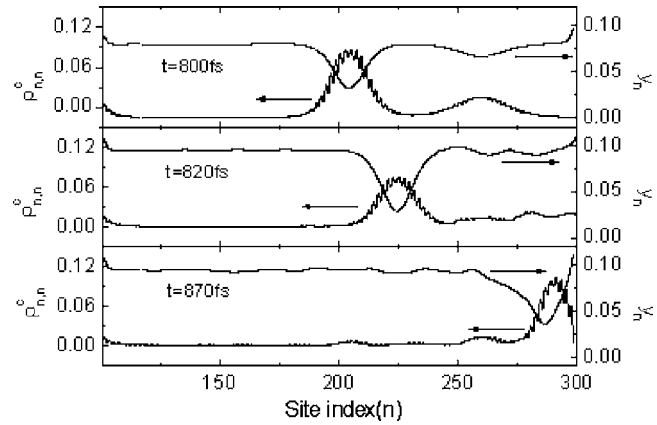

FIG. 7. Injected charge distribution $\rho^c_{n,n}$ (down) and the staggered lattice configuration y_n (up) of the polymer chain at a few typical times with $\beta=0.4$. The voltage bias $V_0=1.01$ eV and the field $E_0=5\times10^3$ V/cm. At $t=800$ fs, the bias and the driving field are turned to $V_0=0.98$ eV and $E_0=5\times10^5$ V/cm separately.

field treatment[24,25] by setting the on-site repulsion $U=t_0$ and the nearest-neighbor repulsion $V=U/3$. It is obtained that the formation field for a wave packet containing two electronic charges changes from 3.2×10^5 to 2.6×10^5 V/cm due to the electron-electron interactions.

Experimentally, the values of the electric fields applied in LED or organic LED devices are about 10^5-10^6 V/cm.[23,26] In this region, as predicted above, wave packets, such as polarons or bipolarons, can keep their integrity. However, experimental investigation also reveals a different behavior at a strong field beyond 10^7 V/cm from that at a low one. It was found that the electric current would have an apparent increase under such a strong electric field.[27] We attribute that to the intrinsic changes of the carriers due to the effect of the external electric field. In other words, the large current increase may come from the dissociation of wave packets, as the mobility of an extended electron is much greater than that of a wave packet. The dissociation of a polaron has been widely studied recently. Our investigation shows that a wave packet containing charges 0–2e may also dissociate at a strong field (dissociation field). It is interesting to note that the formation field is not equal to the dissociation one in values for a wave packet and this difference is more apparent for a larger wave packet. As shown in Fig. 5 with the dashed line, the dissociation field is apparently larger than the formation field. In addition, similar to the case of formation of a wave packet, the upper critical field for dissociation of a wave packet also increases with the charge quantity it contains. An example is given in Fig. 7 for the dissociation process. The injected charges form two wave packets with charges 2e and 0.32e separately at a driving field $E_0=5\times10^3$ V/cm. Then we increase the field to $E_0=5\times10^5$ V/cm at $t=800$ fs. It is found that the smaller wave packet dissociates into an extended state 20 fs later, while the larger wave packet still keeps its integrity.

IV. CONCLUSION

The dynamic process of charge injection is investigated for an open conjugated polymer chain in contact with a metal

electrode in the framework of a nonadiabatic approach. By adjusting the voltage bias of the electrode and the driving field applied on the polymer chain, electronic charges can be injected from the electrode into the polymer layer. The injected charges will form wave packets due to the strong electron-lattice interactions in the conjugated polymer. Each wave packet contains charges of $0-2e$ depending upon the injection conditions. A wave packet with two electronic charges means that a complete spatial electronic state transfers into the polymer. As the system is spin degenerate in the present model, the wave packet has no spin. With the formation of a wave packet, discrete energy levels will appear in the band gap of the conjugated polymer, which results in potential asymmetry of the charge injection and ejection between the metal electrode and the polymer. Further, we studied the effect of the driving electric field on the formation and dissociation of a wave packet. It is obtained that there is an upper critical field of a wave packet for each case and the dissociation field is greater than the formation one. The injected charge cannot form a localized wave packet if the driving electric field is greater than that of formation. Similarly, a wave packet will become an extended state if the field is greater than that of dissociation.

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