Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Polaron spin filtering in an organic ferromagnetic polymer: A dynamics simulation

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Section 1. The explanation of the reason why polaron binding energies are different for two different spins.

When considering the antiferromagnetic correlation of the polaron on the backbone with the side radicals, the energy levels of the up and down polarons are not spin degenerate. In our simulations, the spin-down electron occupies the lower LUMO level while the spin-up electron occupies the higher LUMO+1 level. When the polaron is far away from the side radical, the spin splitting of the two levels are eliminated, as shown in Figure S1 (the red lines). When the polaon dissociates into free electrons, the two levels are delocalized with a spin splitting of about 0.01 eV (the black lines in Figure S1). Thus, the binding energy of spin-up polaron is a little higher than that of spin-down polaron.

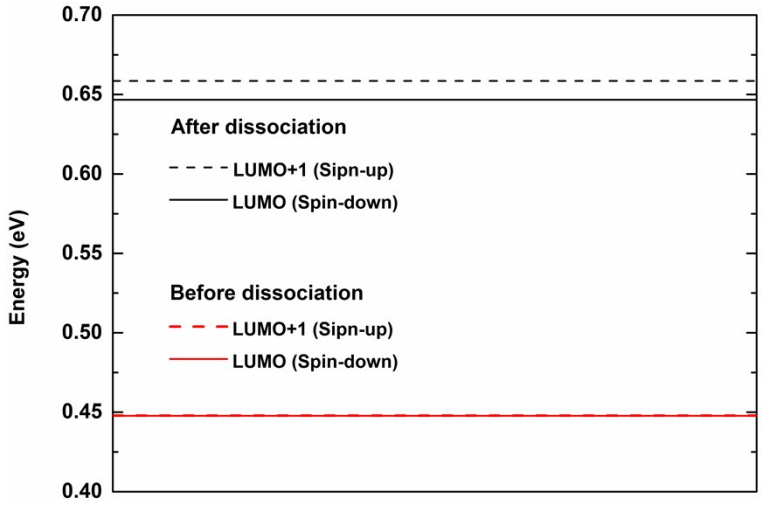

Figure S1. The energy of LUMO and LUMO+1 levels before and after the dissociation of the polaron. The value of the spin coupling parameter is $J_f = 0.3t_0$, and the side radical with up spin is connected to the 120*th* site.

Section 2. The results of the condition with negative electric fields.

The condition with negative electric fields has been calculated and the results are shown in Figure S2. The phenomenon of spin filtering is not affected by the direction of the electric field according to our calculations.

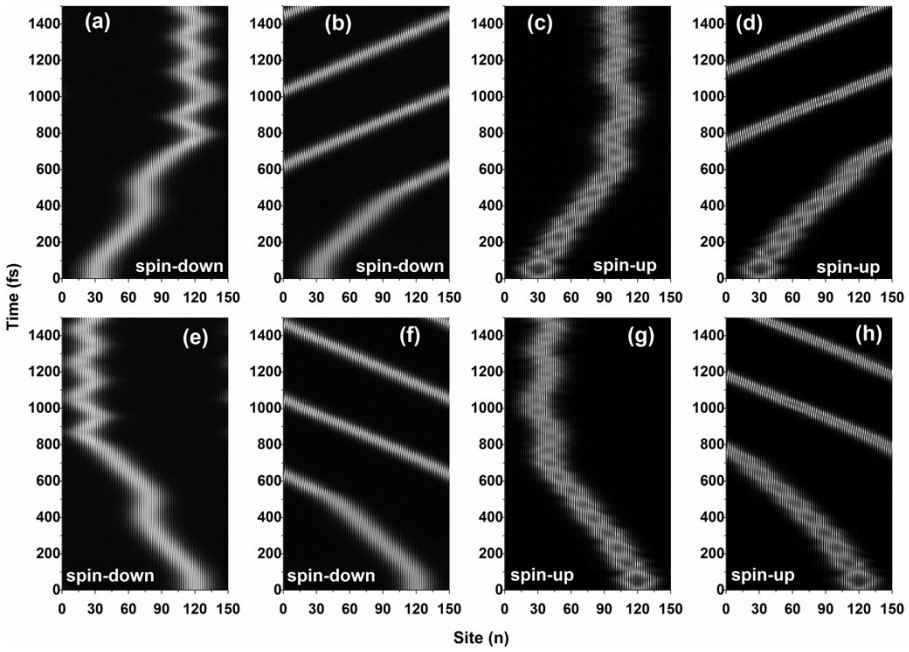

Figure S2. Time evolution of polaron-charge distributions in the presence of different strength of electric field. The driven electric field is E_0=1.4×10^{-3} V/nm for (a), E_0=1.5×10^{-3} V/nm for (b), E_0=3.5×10^{-3} V/nm for (c), E_0=3.8×10^{-3} V/nm for (d), E_0=-1.4×10^{-3} V/nm for (e), E_0=-1.5×10^{-3} V/nm for (f), E_0=-3.5×10^{-3} V/nm for (g) and E_0=-3.8×10^{-3} V/nm for (h). The value of the spin coupling parameter is $J_f = 0.3t_0$. For Figure 3 (a), (b), (c) and (d), the initial polaron center is on the 30*th* site and the side radical is connected to the 120*th* site; for Figure 3 (e), (f), (g) and (h), the initial polaron center is on the 120*th* site and the side radical is connected to the 20*th* site.

Section 3. The results of the condition with different side radical positions.

We also calculated the condition in which the side radical position is changed, and the results of the spin-down polaron are shown in Figure S3 as an example. According to our simulations, the spin filtering behavior is not affected by the side radical positions.

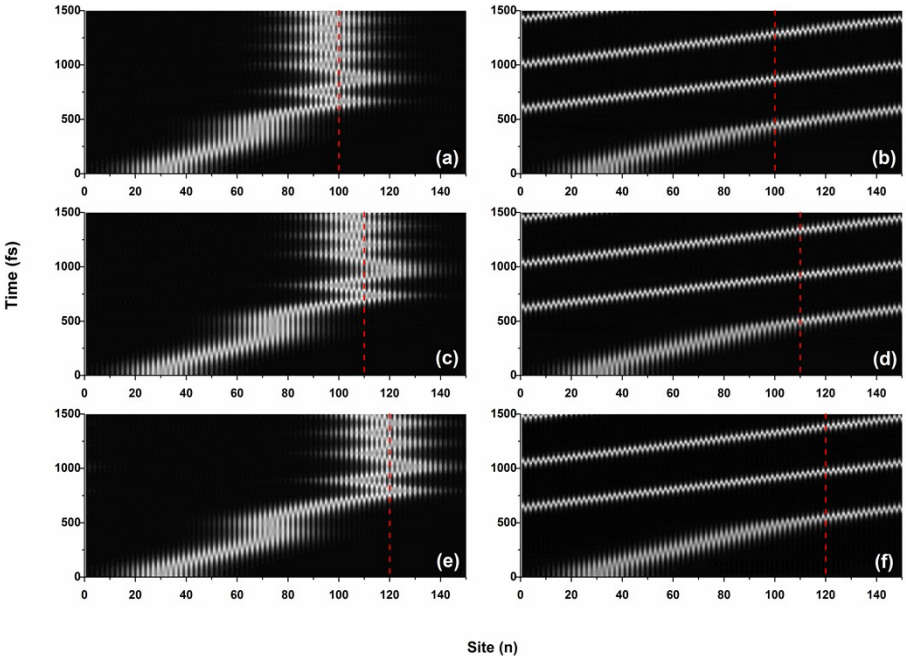

Figure S3. Time evolution of spin-down polaron-charge distributions in the presence of different strength of electric field. The driven electric fields are E_0=1.4×10^{-3} V/nm [(a), (c) and (e)] and E_0=1.5×10^{-3} V/nm [(b), (d), and (f)]. The initial polaron center is on the 30*th* site and the side radical is connected to the 100*th* site[Figure 4 (a) and (b)], 110*th* site [Figure 4 (c) and (d)], and 120*th* site [Figure 4 (e) and (f)], respectively.