Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

A Pair of Conjoined Donor–Acceptor Butterflies as Promising Solution-Processable Aggregation-Enhanced Emission FR/NIR EL Emitters

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Contents

SI. Experimental Section

Computational Details. The ground-state geometries were optimized under the B3LYP/6-31G(d, p) level, which is well known to provide molecular geometries in good agreement with the experiment. Based on the optimized configuration of ground-state (S_0), the high excitation energy levels of singlet and triplet states were evaluated using TD-M06-2X/6-31G(d, p). In order to examine the character of excited-states, natural transition orbitals (NTOs) were evaluated for the ten lowest excited-states, involving both singlet and triplet states. This approach provides the most compact representation of the electronic transitions in terms of an expansion into single particle orbitals by diagonalizing the transition density matrix associated with each excitation.

Lippert-Mataga model. The influence of solvent environment on the optical property of our compounds can be understood using the Lippert-Mataga equation, a model that describes the interactions between the solvent and the dipole moment of solute:

$$hc(\upsilon_a - \upsilon_f) = hc(\upsilon_a^0 - \upsilon_f^0) - \frac{2(\mu_e - \mu_g)^2}{a^3} f(\varepsilon, n)$$

where f is the orientational polarizability of solvents, μ_e is the dipole moment of excited state, μ_g is the dipole moment of ground state; a is the solvent cavity (Onsager) radius, ε and n are the solvent dielectric and the solvent refractive index, respectively.

The method of measuring/calculating external quantum efficiency (EQE)

The measured parameters included luminance, current and EL spectrum. EQE was calculated according to the formula below:

$$EQE = \frac{\pi \cdot L \cdot e}{683 \cdot I \cdot h \cdot c} \cdot \frac{\int_{380}^{780} I(\lambda) \cdot \lambda d\lambda}{\int_{380}^{780} I(\lambda) \cdot K(\lambda) d\lambda}$$

where L (cd m^{-2}) is the total luminance of device, I (A) is the current flowing into the EL device, λ (nm) is EL wavelength, I(λ) is the relative EL intensity at each wavelength and obtained by measuring the EL spectrum, K(λ) is the Commision International de L'Eclairage chromaticity (CIE) standard photopic efficiency function, e is the charge of an electron, h is the Planck's constant, c is the velocity of light.

SII. Figures (Figure S1-Figure S9)

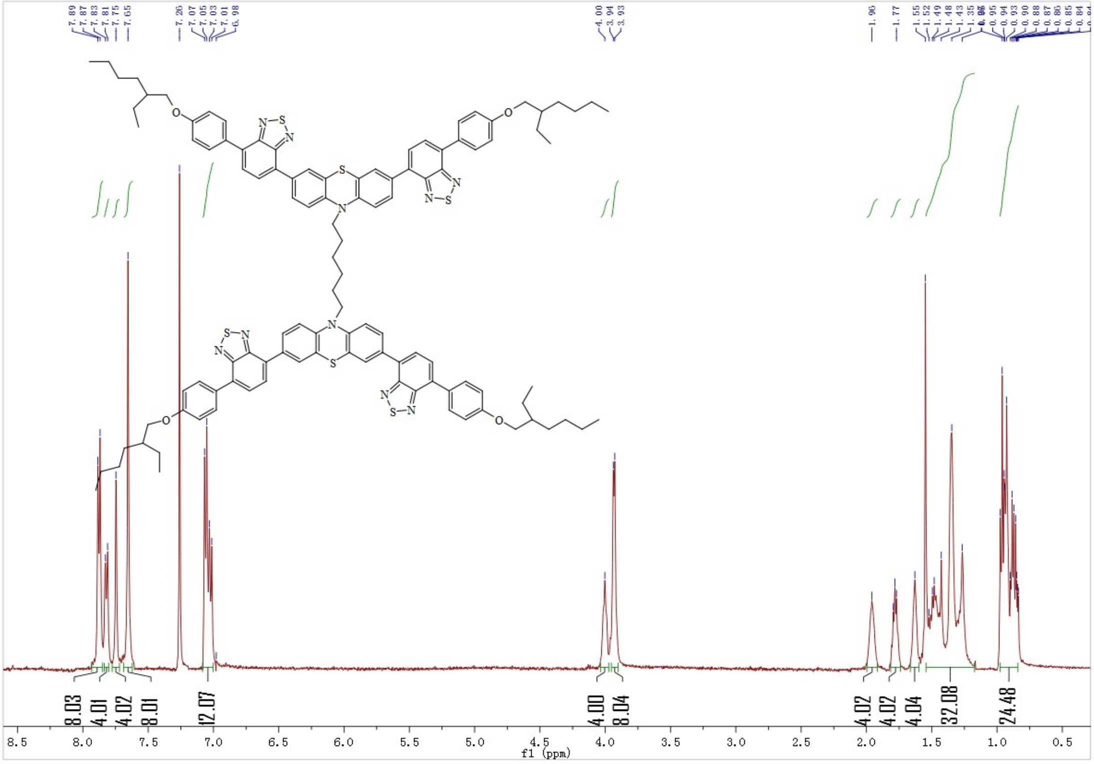

Figure S1. ^{1}H NMR spectrum in deuterated $CDCl_3$ for SP6.

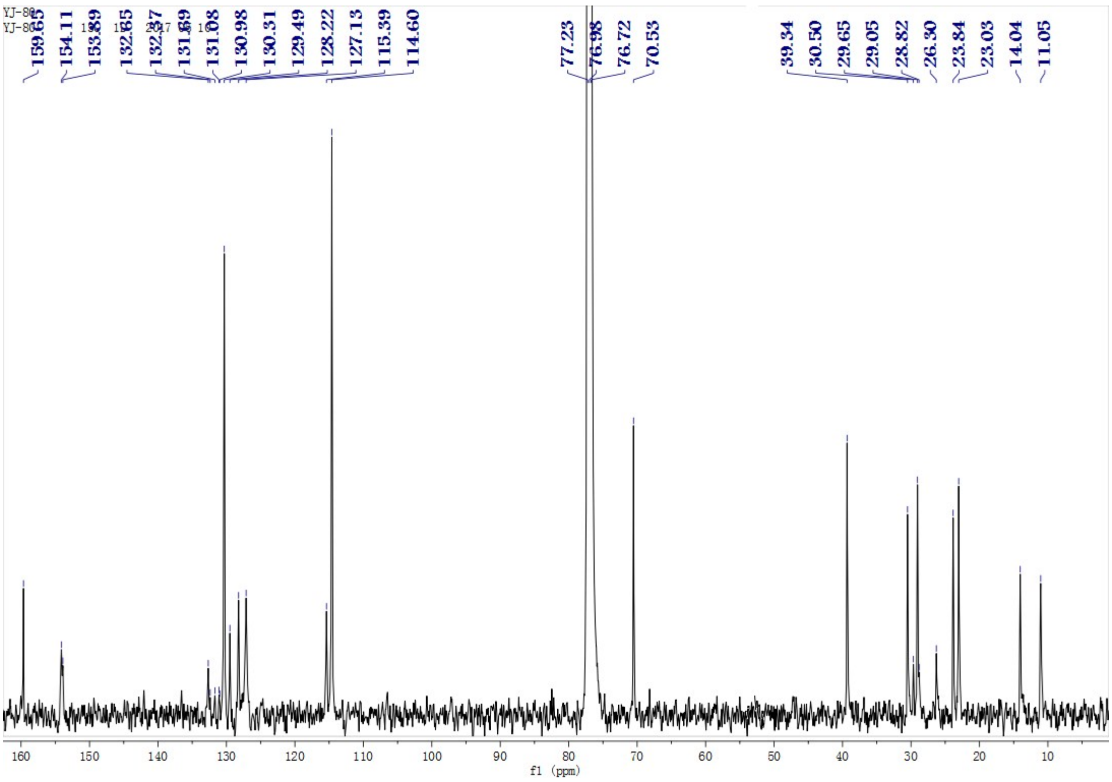

Figure S2. ^{13}C NMR spectrum in deuterated $CDCl_3$ for SP6.

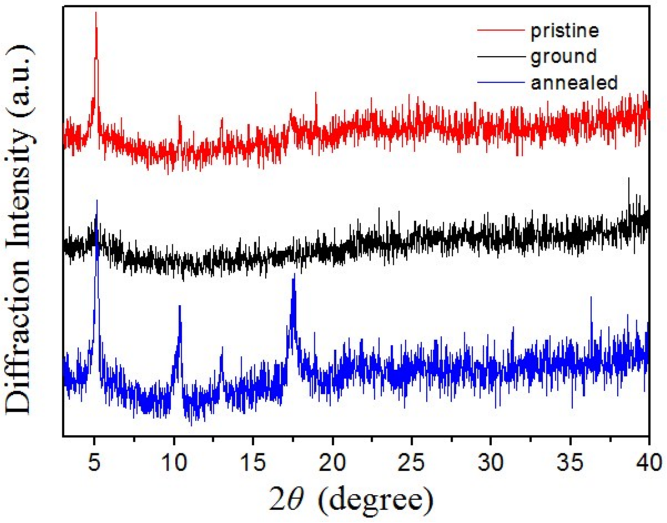

Figure S3. XRD curves of **SP6** solid samples under different conditions.

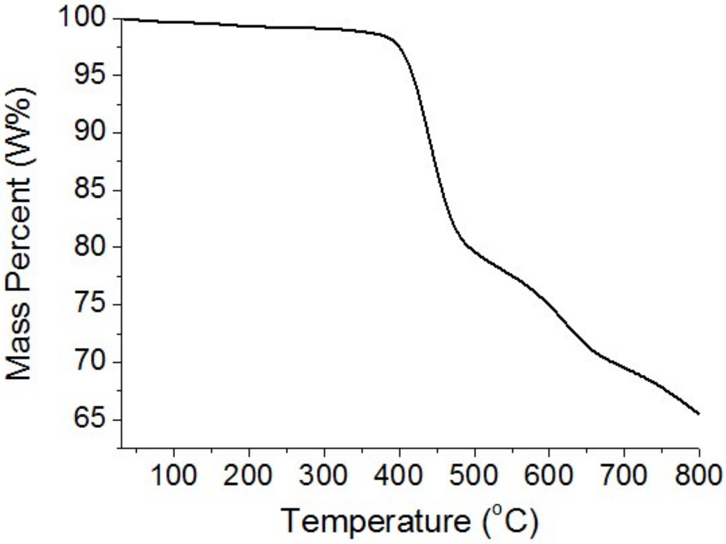

Figure S4. The TGA of SP6.

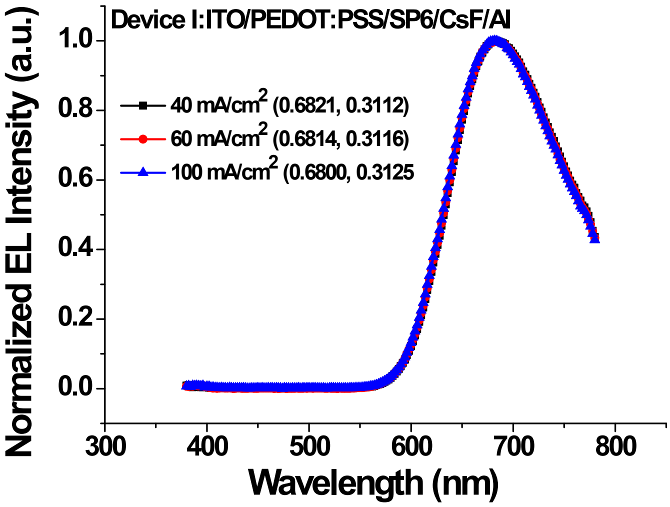

Figure S5. The EL spectra of **SP6** device I under the different current density.

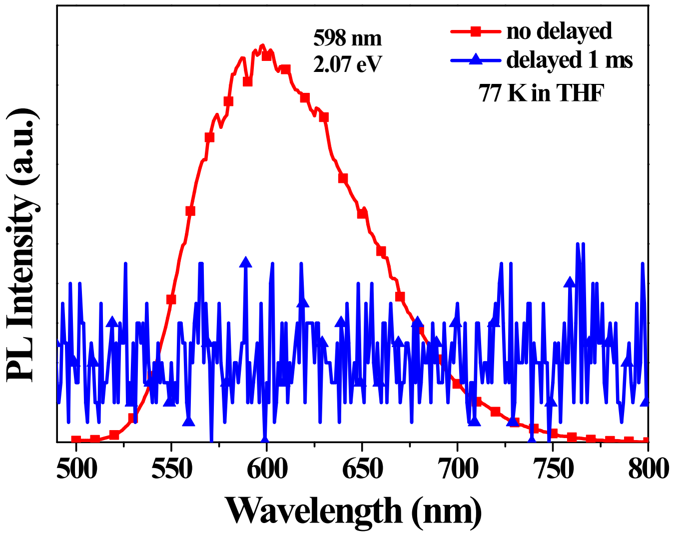

Figure S6. The fluorescence and phosphorescence spectra in THF at 77 K**.**

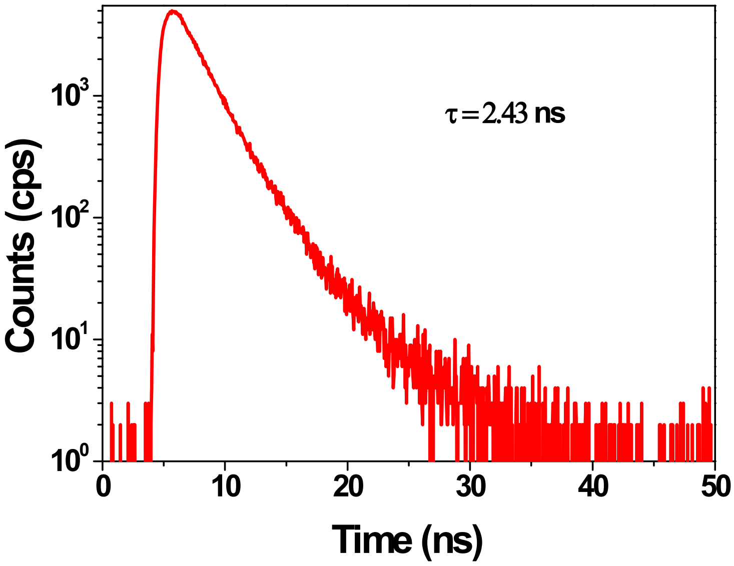

Figure S7. The transient photo-luminescence decay curve of **SP6** solution in THF.

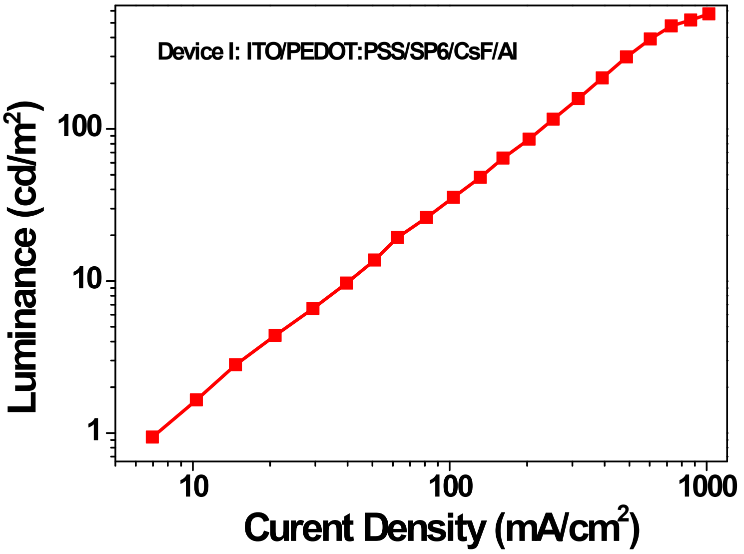

Figure S8. The luminance-current density characteristics of the ITO/PEDOT:PSS/ **SP6**/ CsF (1 nm)/ Al (100 nm).

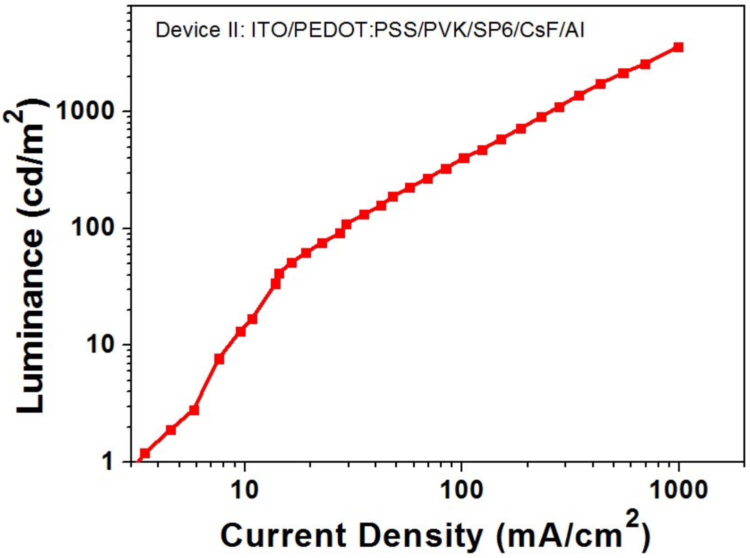

Figure S9. The luminance-current density characteristics of the ITO/PEDOT:PSS/ PVK/**SP6**/ CsF (1 nm)/ Al (100 nm).

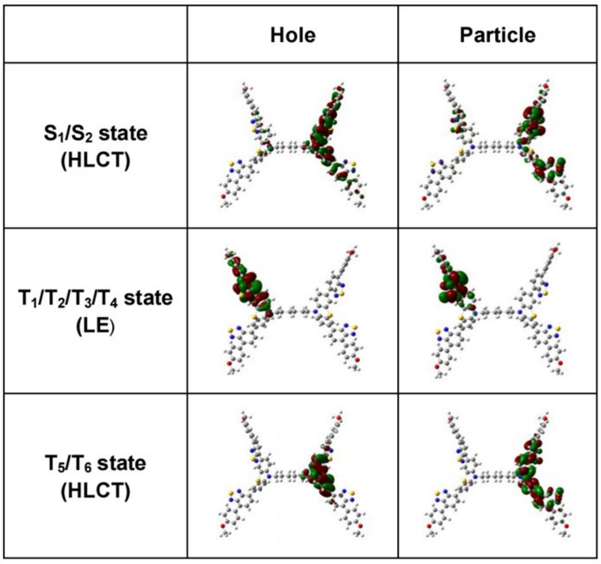

Figure S10. Natural transition orbitals for S_1/S_2, T_1/ T_2/ T_3/ T_4 and T_1/T_6.