Supporting Information for

Molecular stacking effect on photoluminescence quantum yield and charge mobility of organic semiconductors

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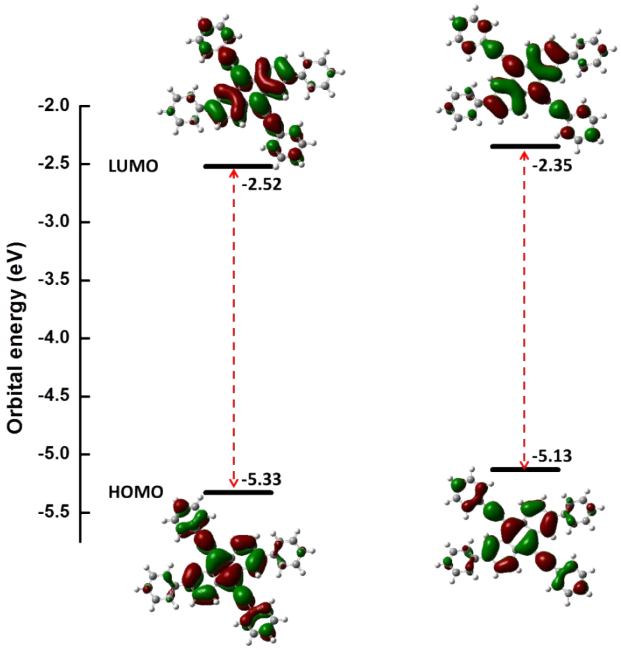

Figure S1. Spatial distributions of HOMO and LUMO as well as their orbital energies for DP-BPEA in THF (left) and solid phase (right) respectively.

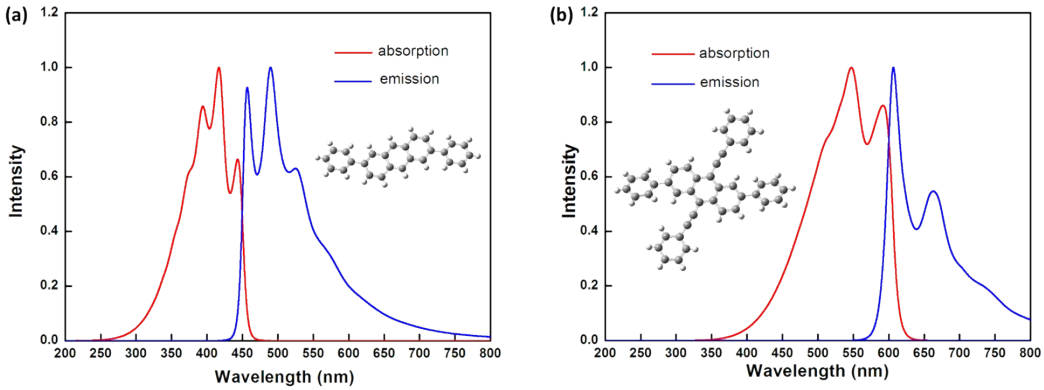

Figure S2. Vibronic resolved UV-vis (red line) and fluorescent (blue line) spectra of DPA (a) and DP-BPEA (b) in THF.

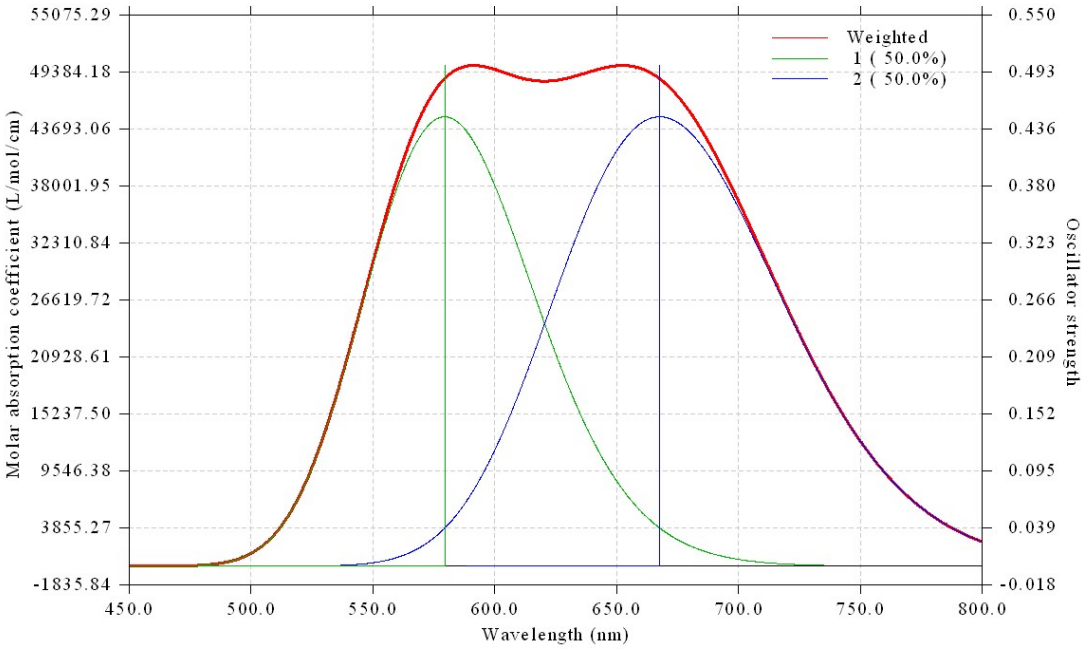

Figure S3. Weight fluorescence spectra (red line) of monomer (green line) and excimer (blue line) with the assumed ratio is 1:1.

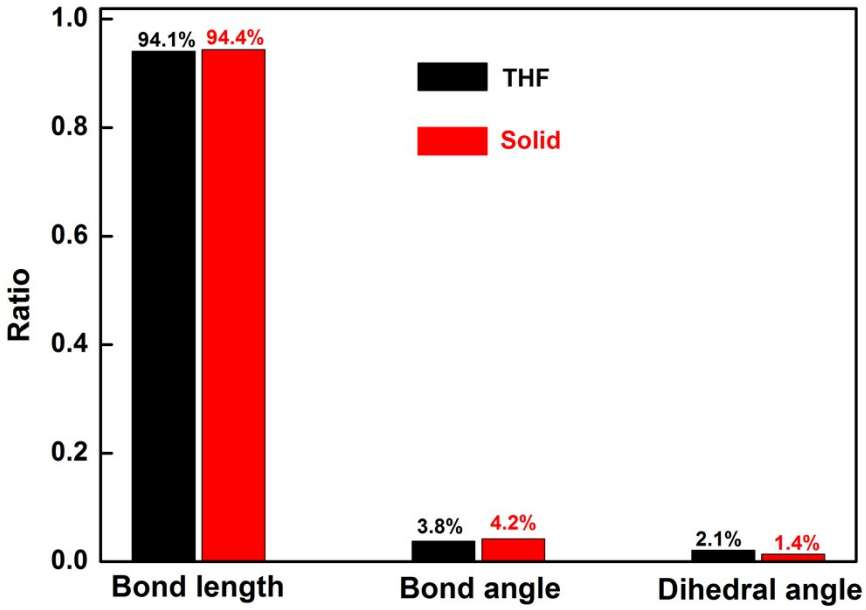

Figure S4. Contributions to the reorganization energies from bond length, bond angle and dihedral angle of DP-BPEA in THF (black) and solid phase (red).

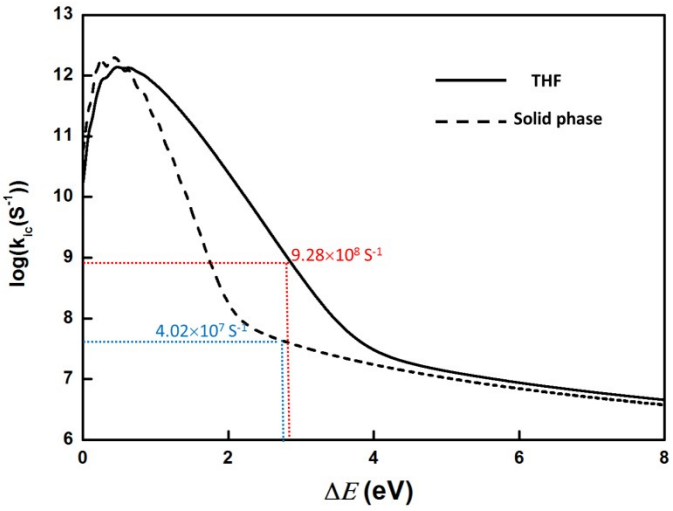

Figure S5. Internal conversion rate k_{IC} from S1 to S0 versus the energy gap ΔE in both THF (solid line) and solid phase (dotted line) for DPA. The vertical line indicates the position of the adiabatic energy gap.

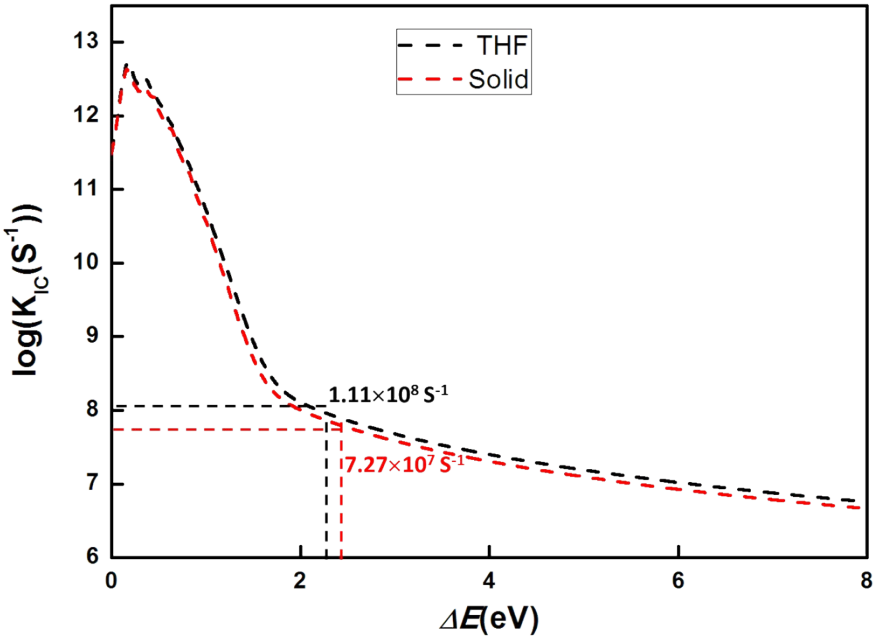

Figure S6. Internal conversion rate k_{IC} from S1 to S0 versus the energy gap ΔE in both THF (black) and solid phase (red) for DP-BPEA. The vertical line indicates the position of the adiabatic energy gap.

Table S1. Calculated vertical excitation energy (VEE), oscillator strength (*f*), electric transition diploe moment (EDM) and the assignment for S1 of DPA are listed.

	VEE	*f*	EDM	assignment
THF	3.11eV (399nm)	0.175	3.85 D	HOMO→LUMO (98.8%)
Solid	3.01eV (412nm)	0.185	4.02 D	HOMO→LUMO (98.3%)

Table S2. Calculated vertical excitation energy (VEE), oscillator strength (*f*), electric transition diploe moment (EDM) and the assignment for S1 of DP-BPEA are listed.

	VEE	*f*	EDM	assignment
THF	2.36eV (526nm)	0.772	3.66 D	HOMO→LUMO (99.8%)
Solid	2.41eV (516nm)	0.551	3.06 D	HOMO→LUMO (99.6%)

Table S3. Reorganization energies (meV) from bond length, bond angle, and dihedral angle of DP-BPEA in THF and solid phase are listed respectively.

	THF	Solid	$\Delta_{\text{THF-Solid}}$
Bond length	144.6	122.5	22.1
Bond angle	5.8	5.4	0.4
Dihedral angle	3.2	1.8	1.4
Total	153.6	129.7	23.9