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

Supporting Information for

High efficient T-shape deep-red thermally activated delayed fluorescence emitter: substitution position effect

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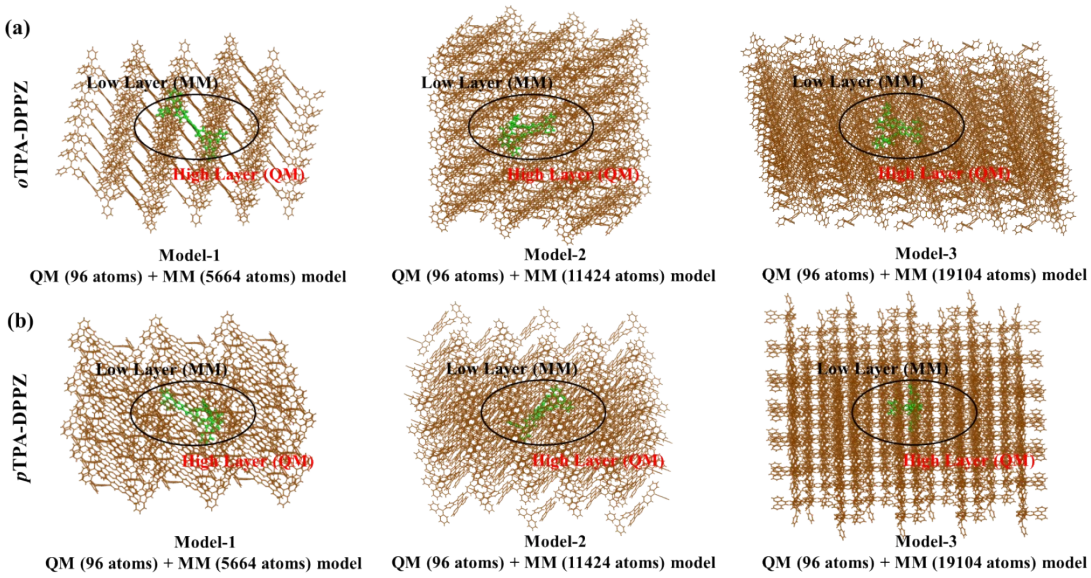

Figure S1. ONIOM model to simulate the aggregation in crystal state for *o*TPA-DPPZ (a) and *p*TPA-DPPZ(b). 60 molecular model named as Model-1, 120 molecular model named as Model-2, 200 molecular model named as Model-3.

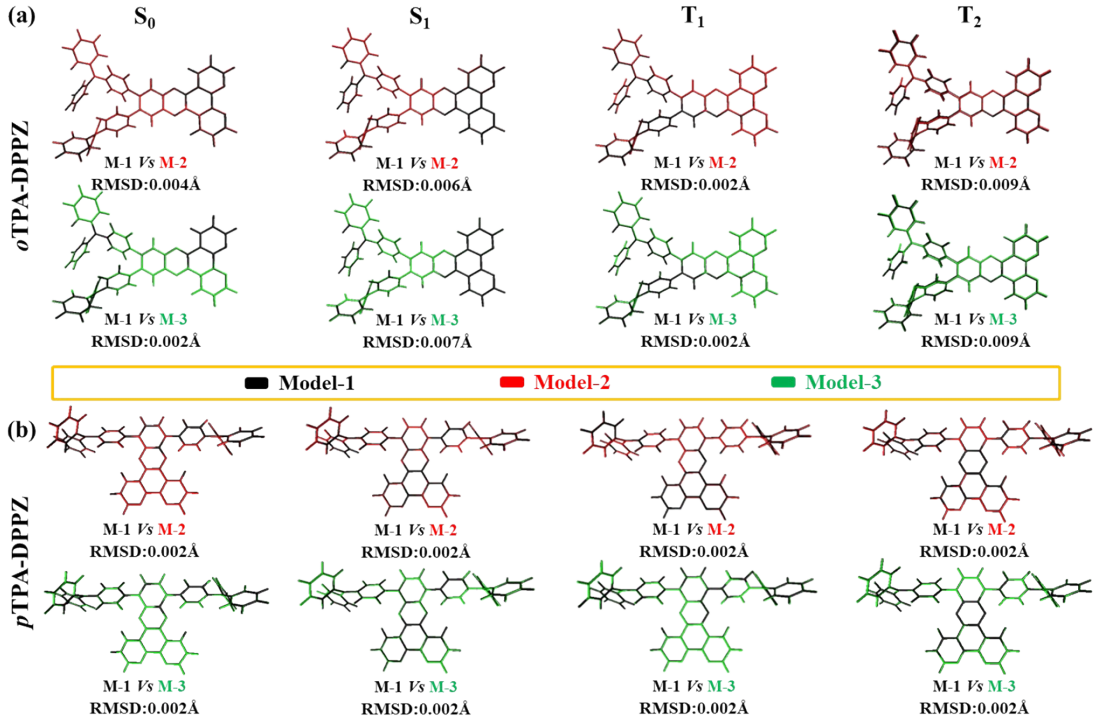

Figure S2. Geometry comparisons between of OTPA-DPPZ and pTPA-DPPZ in Model-1 (black), Model-2 (red) and Model-3 (green).

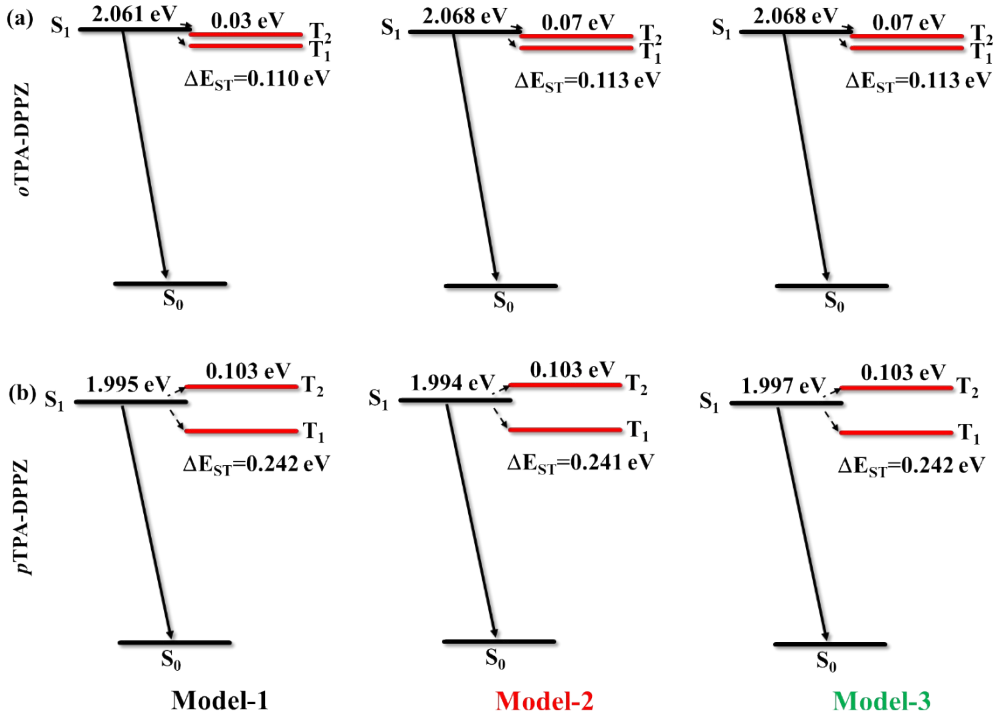

Figure S3. Adiabatic excitation energies for *o*TPA-DPPZ and *p*TPA-DPPZ in Model-1, Model-2 and Model-3.

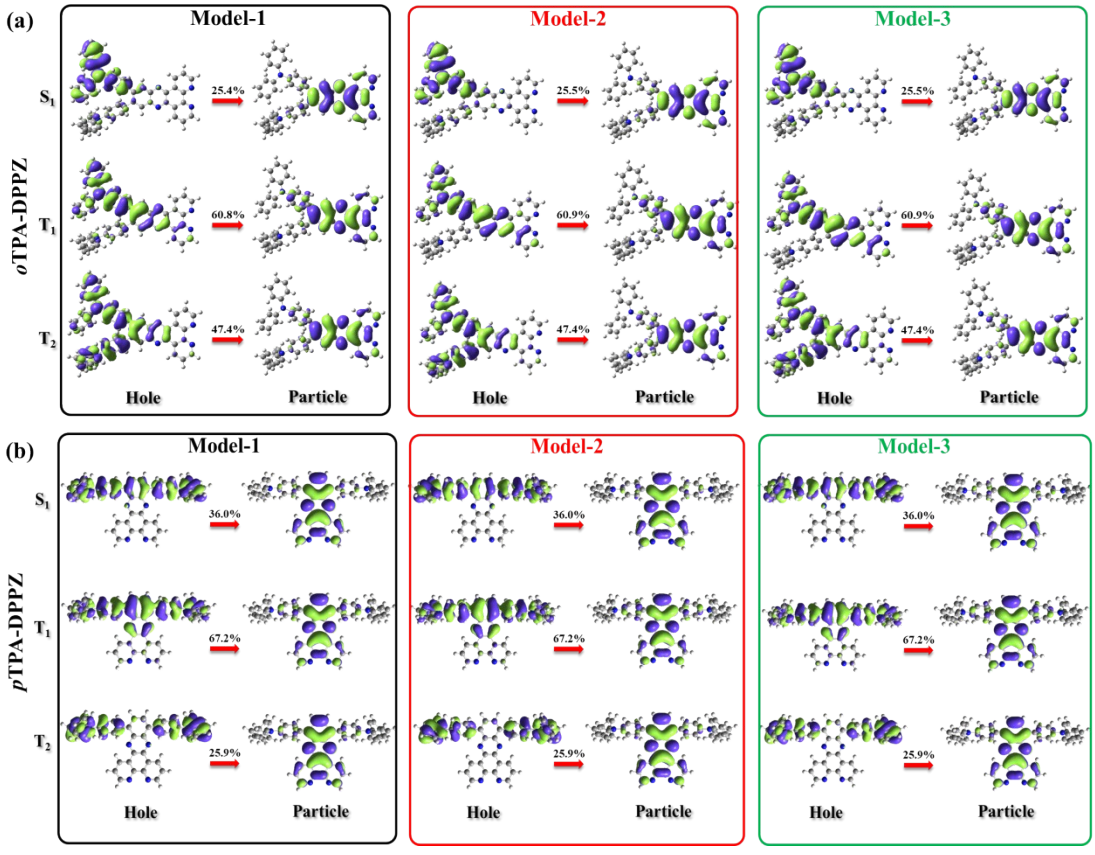

Figure S4. Transition characteristics of *o*TPA-DPPZ and *p*TPA-DPPZ in Model-1, Model-2 and Model-3.

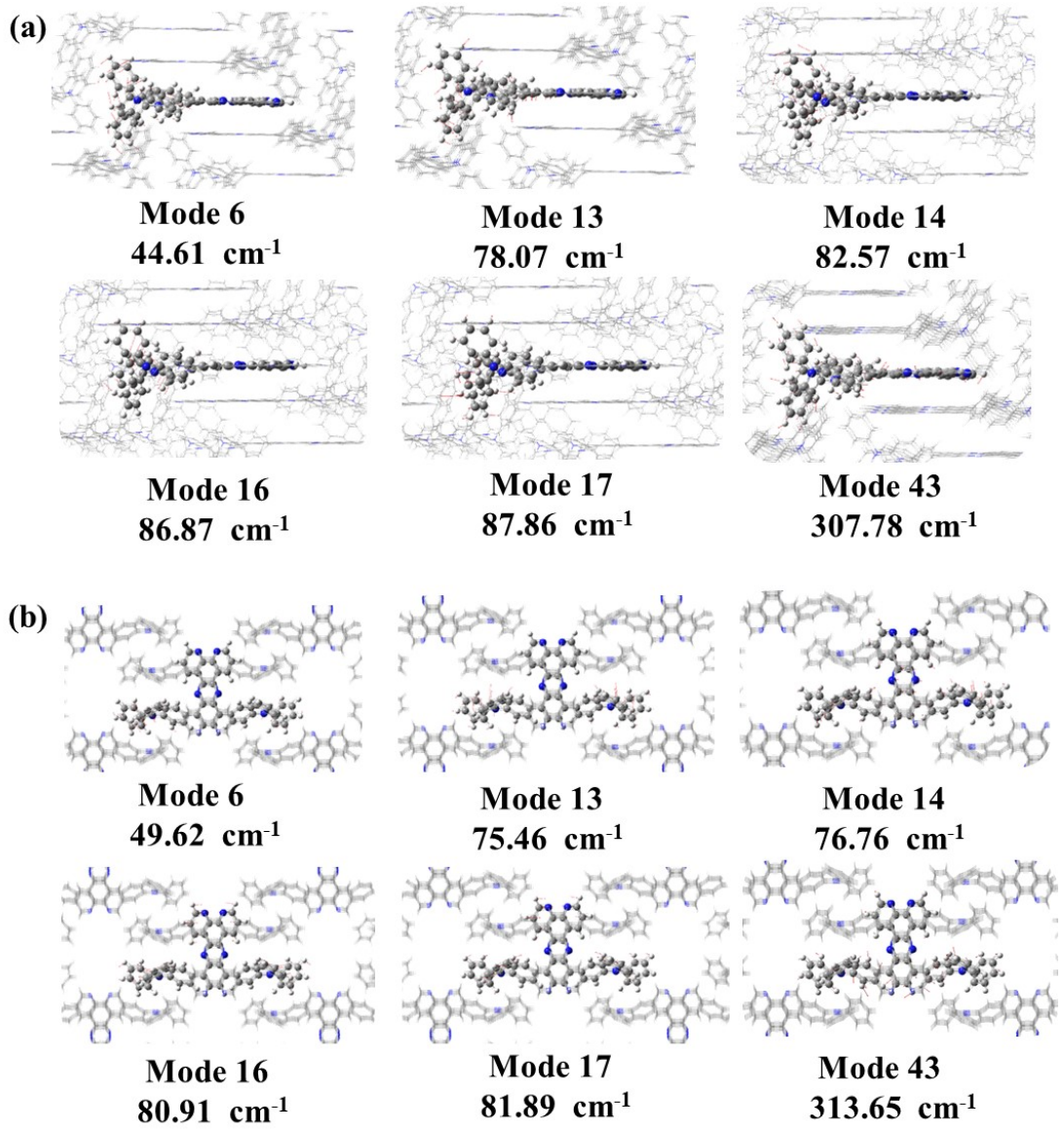

Figure S5. Diagrammatic illustration of selected normal modes with large reorganization energies (λ) for S_0 of *o*TPA-DPPZ (a) and *p*TPA-DPPZ (b) in crystal.

Table S1. The emission wavelength and oscillator strength of of *o*TPA-DPPZ and *p*TPA-DPPZ in Model-1, Model-2 and Model-3.

	***o*TPA-DPPZ**			***p*TPA-DPPZ**		
	Model-1	**Model-2**	**Model-3**	**Model-1**	**Model-2**	**Model-3**
λ_{em} **(nm)**	639	637	637	669	670	669
f	0.105	0.106	0.106	0.144	0.144	0.144

Table S2. Calculated SOC constants and transition dipole moments, radiative (K_{rt}) and non-radiative rates (K_{nrt}) from T_1 to S_0.

		SOC (cm^{-1})	μ (Debye)	K_{rt} (s^{-1})	K_{nrt} (s^{-1})
***o*TPA-DPPZ**	T_1-S_0	0.437	1.92×10^{-4}	3.01×10^{-2}	5.62×10^{0}
***p*TPA-DPPZ**	T_1-S_0	0.472	2.32×10^{-4}	2.74×10^{-2}	4.56×10^{2}

Table S3. Frequencies of each mode ω_j, normal-mode displacement (ΔQ), Huang-Rhys factors (S_j) and reorganization energy (λ) for S_0 of *o*TPA-DPPZ and *p*TPA-DPPZ in crystal.

***o*TPA-DPPZ**					***p*TPA-DPPZ**				
mode	$\omega_j(cm^{-1})$	ΔQ	S_j	λ_j(meV)	mode	$\omega_j(cm^{-1})$	ΔQ	S_j	λ_j(meV)
6	44.51	-94.03	0.90	39.91	6	49.62	-16.75	0.03	1.57
13	78.07	-59.31	0.63	48.84	13	75.46	-0.66	0.00	0.00
14	82.57	-60.01	0.68	55.92	14	76.76	0.41	0.00	0.00
16	86.87	-45.09	0.40	34.95	16	80.91	-23.57	0.10	8.29
17	87.86	52.23	0.55	47.98	17	81.89	7.54	0.01	0.87
43	307.78	-16.90	0.20	61.61	43	313.65	-5.74	0.02	7.39