Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

"**Efficient fluorescent OLEDS based on assistant acceptor modulated HLCT emissive state for enhancing singlet Exciton Utilization"**

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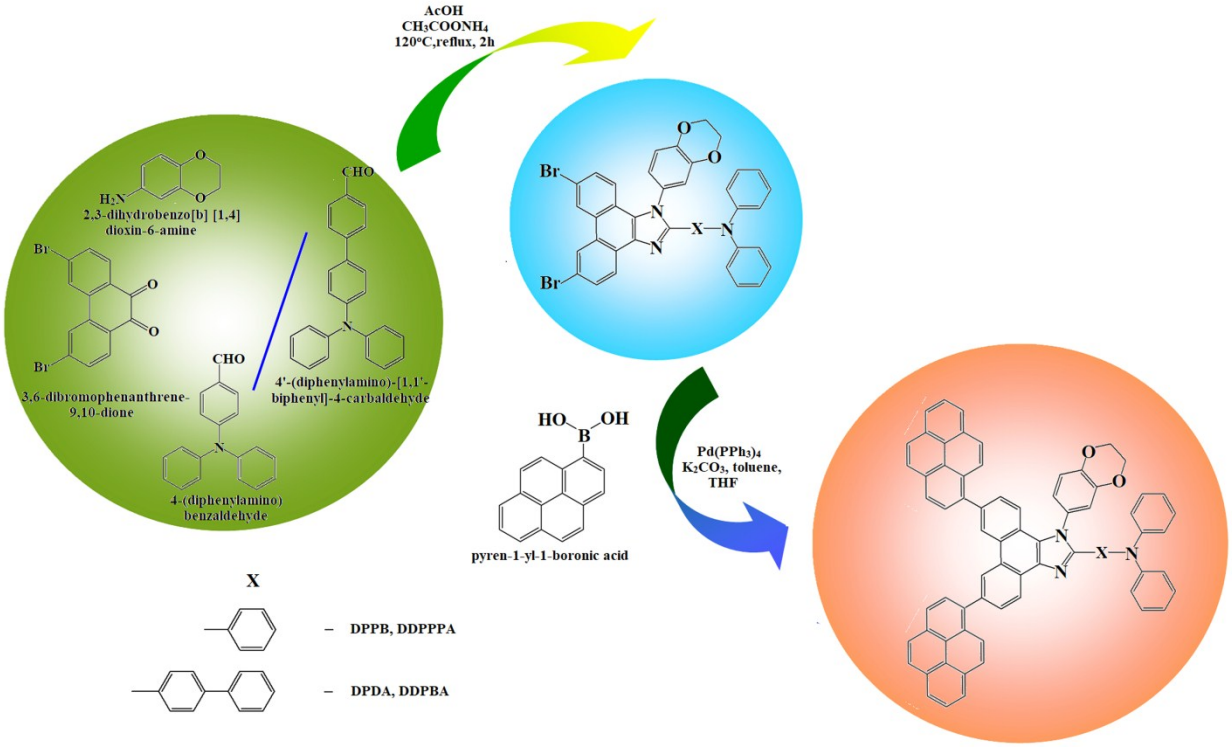
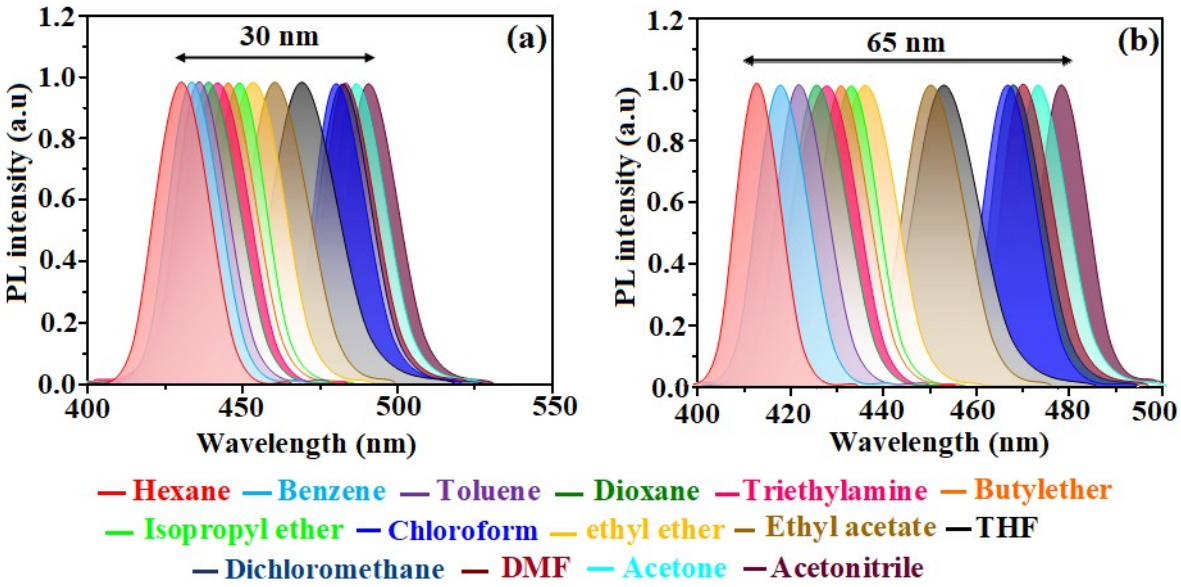
Scheme S1. Synthetic route of DDPPPA and DDPBA.



SI–I: Figures

Figure S1. Normalized emission spectra of a) DDPPPA and b) DDPBA.



SI–II: Charge-Transfer intexes

The hole-particle pair interactions have been related to the distance covered during the excitations one possible descriptor Δr intex could be used to calculate the average distance which is weighted in function of the excitation coefficients.

$$\Delta r = \frac{\Sigma_{ia} k_{ia}^2 \left| \langle \varphi_a | r | \varphi_a \rangle - \langle \varphi_i | r | \varphi_i \rangle \right|}{\Sigma_{ia} K_{ia}^2} \quad \text{…….. (S1)}$$

Where $\left| \langle \varphi_i | r | \varphi_i \rangle \right|$ is the norm of the orbital centroid [1–4]. Δr–index will be expressed in Å.

The density variation associated to the electronic transition is given by

$$\Delta\rho(r) = \rho_{EX}(r) - \rho_{GS}(r) \quad \text{..... (S2)}$$

Where $\rho_{GS}(r)$ and $\rho_{EX}(r)$ are the electronic densities of to the ground and excited states, respectively. Two functions, $\rho_+(r)$ and $\rho_-(r)$, corresponds to the points in space where an increment or a depletion of the density upon absorption is produced and they can be defined as follows:

$$\rho_+(r) = \begin{Bmatrix} \Delta\rho(r) & if\ \Delta\rho(r) > 0 \\ 0 & if\ \Delta\rho(r) < 0 \end{Bmatrix} \quad \text{..... (S3)}$$

$$\rho_-(r) = \begin{Bmatrix} \Delta\rho(r) & if\ \Delta\rho(r) < 0 \\ 0 & if\ \Delta\rho(r) > 0 \end{Bmatrix} \quad \text{..... (S4)}$$

The barycenters of the spatial regions R_+ and R_- are related with $\rho_+(r)$ and $\rho_-(r)$ and are shown as

$$R_+ = \frac{\int r\rho_+(r)dr}{\int \rho_+(r)dr} = (x_+, y_+, z_+) \quad \text{..... (S5)}$$

$$R_- = \frac{\int r\rho_-(r)dr}{\int \rho_-(r)dr} = (x_-, y_-, z_-) \quad \text{..... (S6)}$$

The spatial distance (D_{CT}) between the two barycenters R_+ and R_- of density distributions can thus be used to measure the CT excitation length

$$D_{CT} = \left|R_+ - R_-\right| \quad \text{(S7)}$$

The transferred charge (q_{CT}) can be obtained by integrating over all space $\rho_+(\rho_-)$,. Variation in dipole moment between the ground and the excited states (μ_{CT}) can be computed by the following relation:

$$\|\mu_{CT}\| = D_{CT}\int \rho_+(r)dr = D_{CT}\int \rho_-(r)dr \quad \text{(S8)}$$

$$= D_{CT}q_{CT} \quad \text{(S9)}$$

The difference between the dipole moments $\|\mu_{CT}\|$ have been computed for the ground and the excited states $\Delta\mu_{ES-GS}$. The two centroids of charges (C^+/C^-) associated to the positive and negative density regions are calculated as follows. First the root-mean-square deviations along the three axis (σ_{aj}, j = x, y, z; a = + or –) are computed as

$$\sigma_{a,j} = \sqrt{\frac{\sum_i \rho_a(r_i)(j_i - j_a)^2}{\sum_i \rho_a(r_i)}} \quad \text{(S10)}$$

The two centroids (C_+ and C_-) are defined as

$$C_+(r) = A_+ e\left(-\frac{(x-x_+)^2}{2\sigma_{+x}^2} - \frac{(y-y_+)^2}{2\sigma_{+y}^2} - \frac{(z-z_+)^2}{2\sigma_{+z}^2}\right) \quad \text{(S11)}$$

$$C_-(r) = A_- e\left(-\frac{(x-x_-)^2}{2\sigma_{-x}^2} - \frac{(y-y_-)^2}{2\sigma_{-y}^2} - \frac{(z-z_-)^2}{2\sigma_{-z}^2}\right) \quad \text{(S12)}$$

The normalization factors (A+ and A_) are used to impose the integrated charge on the centroid to be equal to the corresponding density change integrated in the whole space:

$$A_{+} = \frac{\int \rho_{+}(r)dr}{\int e\left(-\frac{(x-x_{-})^2}{2\sigma_{+x}^2} - \frac{(y-y_{-})^2}{2\sigma_{+y}^2} - \frac{(z-z_{-})^2}{2\sigma_{+z}^2}\right)dr} \quad \text{..... (S13)}$$

$$A_{-} = \frac{\int \rho_{-}(r)dr}{\int e\left(-\frac{(x-x_{-})^2}{2\sigma_{-x}^2} - \frac{(y-y_{-})^2}{2\sigma_{-y}^2} - \frac{(z-z_{-})^2}{2\sigma_{-z}^2}\right)dr} \quad \text{..... (S14)}$$

H index is defined as half of the sum of the centroids axis along the D–A direction, if the D–A direction is along the X axis, H is defined by the relation:

$$H = \frac{\sigma_{+x} + \sigma_{-x}}{2} \quad \text{..... (S15)}$$

The centroid along X axis is expected. The t intex represents the difference between D_{CT} and H:

$$t = D_{CT} - H \quad \text{..... (S16)}$$

Figure S2. Natural transition orbital pairs with transition character analysis for singlet states (S_1-S_{10}) of (HONTOs and LUNTOs) DDPPPA [*f*-oscillator strength and % weights of

hole-particle].

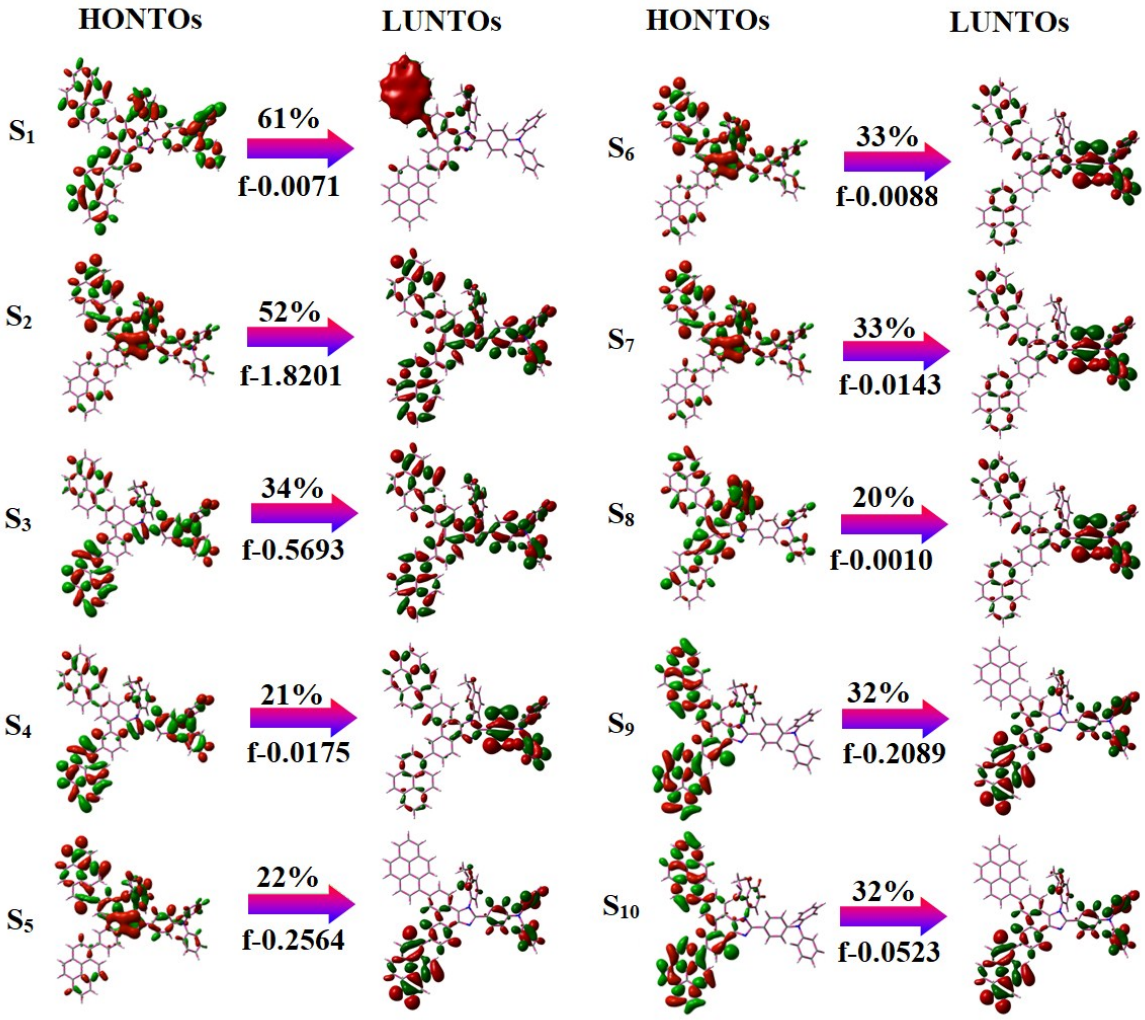


Figure S3. Natural transition orbital pairs with (HONTOs and LUNTOs) transition character analysis for singlet states (S_1-S_{10}) of DDPBA [*f*-oscillator strength and % weights of hole-particle].

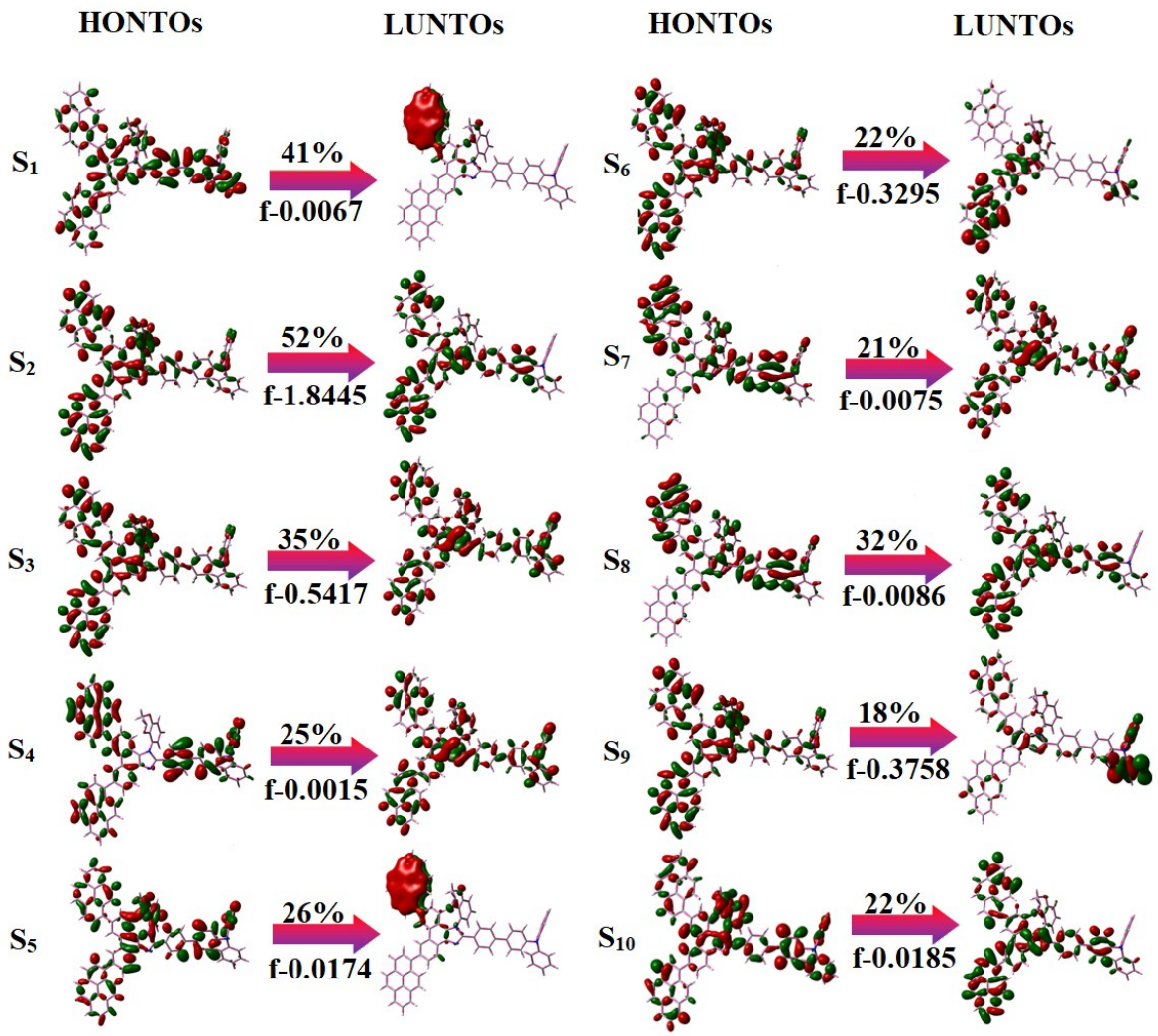


Figure S4. Scheme of exciton decay process after hole and electron recombination in OLEDs of D-π-A molecules.

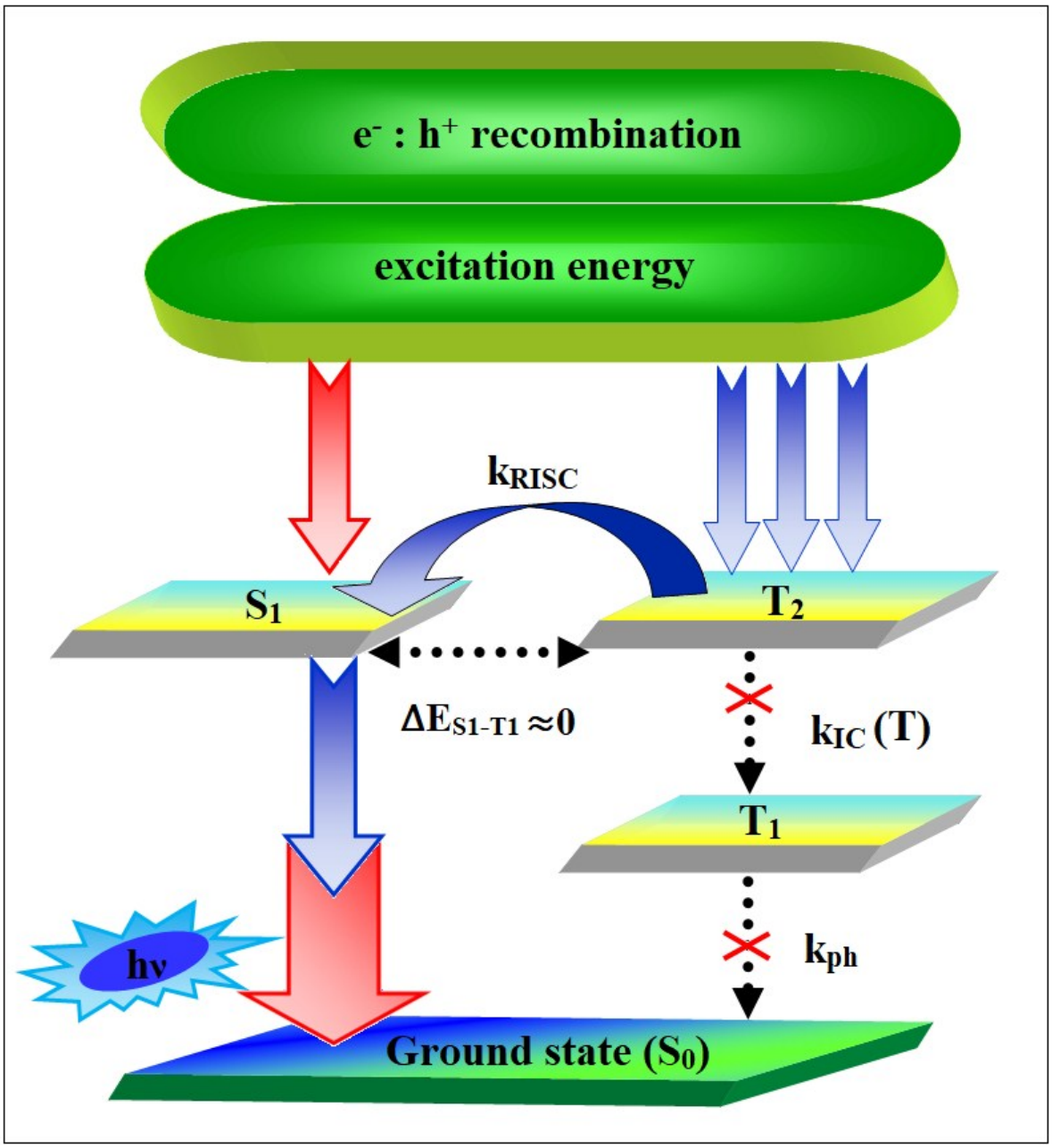


Figure S5. (a) Reverse intersystem crossing; (b) Hybridization process of LE and CT states of DDPPPA and DDPBA.

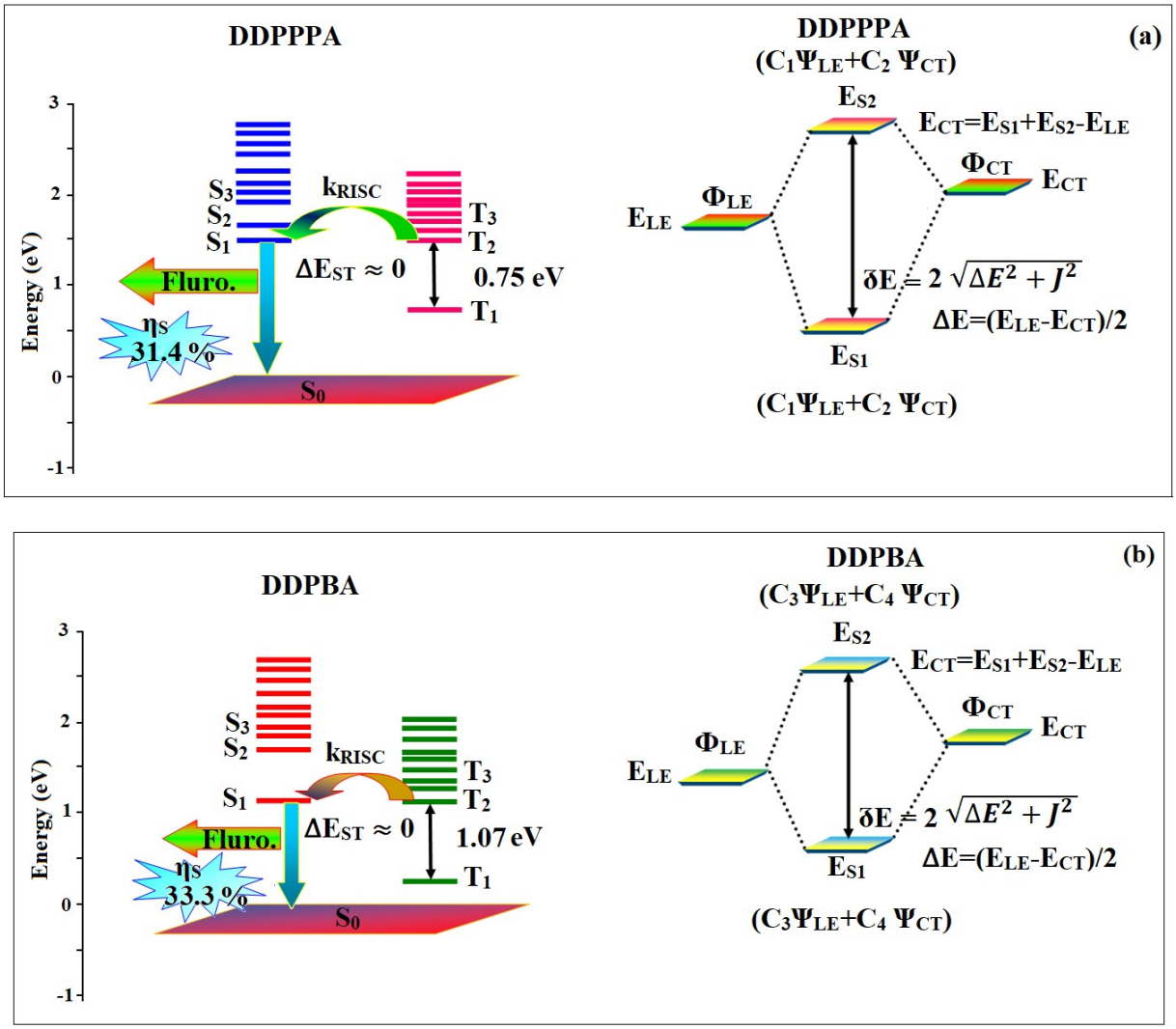


Figure S6. Hole and particle distribution [green - increasing electron density and blue - decreasing electron density and Contour plots of transition density matrices (TDM) of DDPPPA for [S_1-S_4 states: density=transition=n /IOp(6/8=3)].

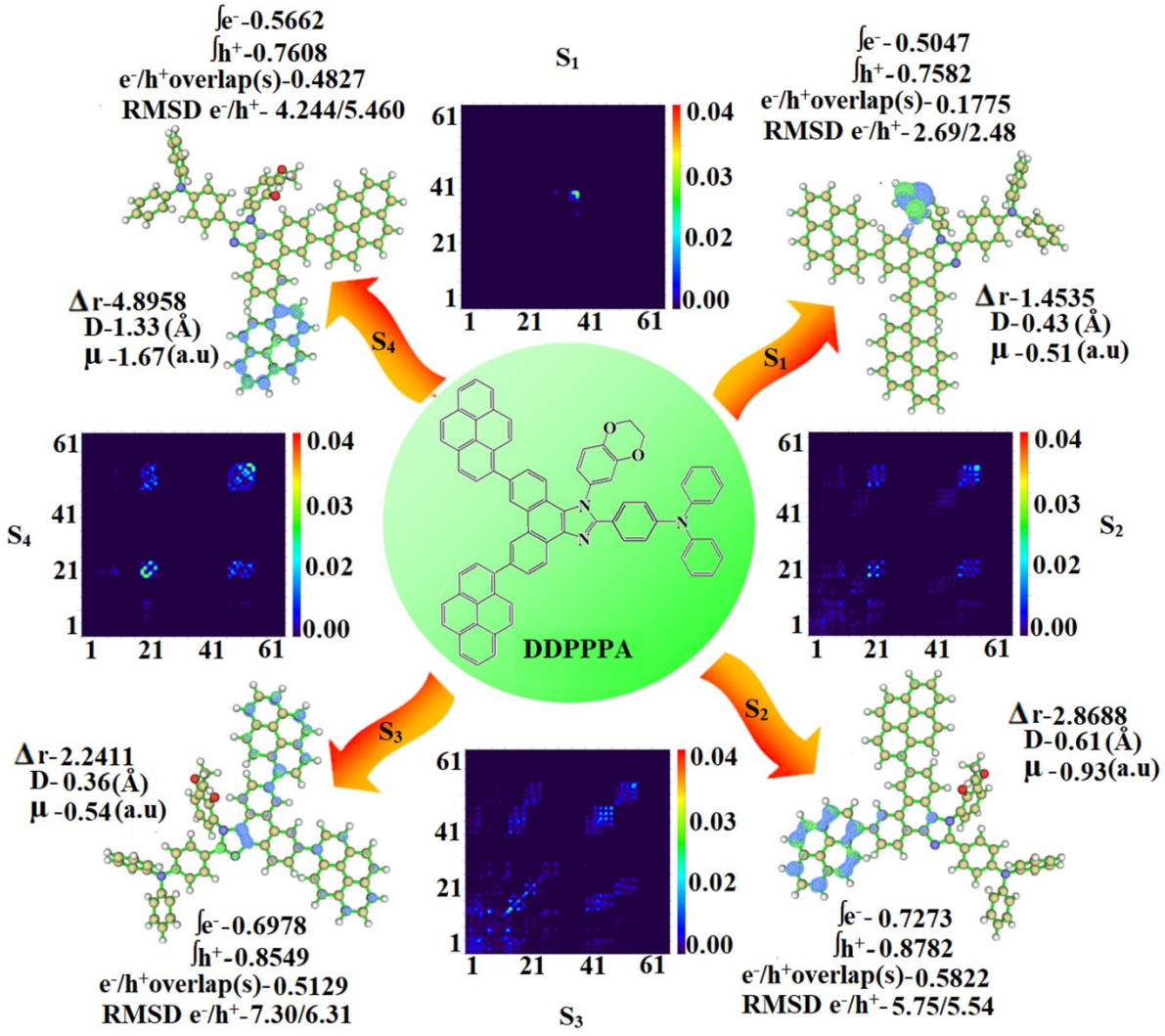


Figure S7. Hole and particle distribution green - increasing electron density and blue - decreasing electron density and Contour plots of transition density matrices (TDM) of DDPBA for [S_1-S_4 states: density=transition=n /IOp(6/8=3)].

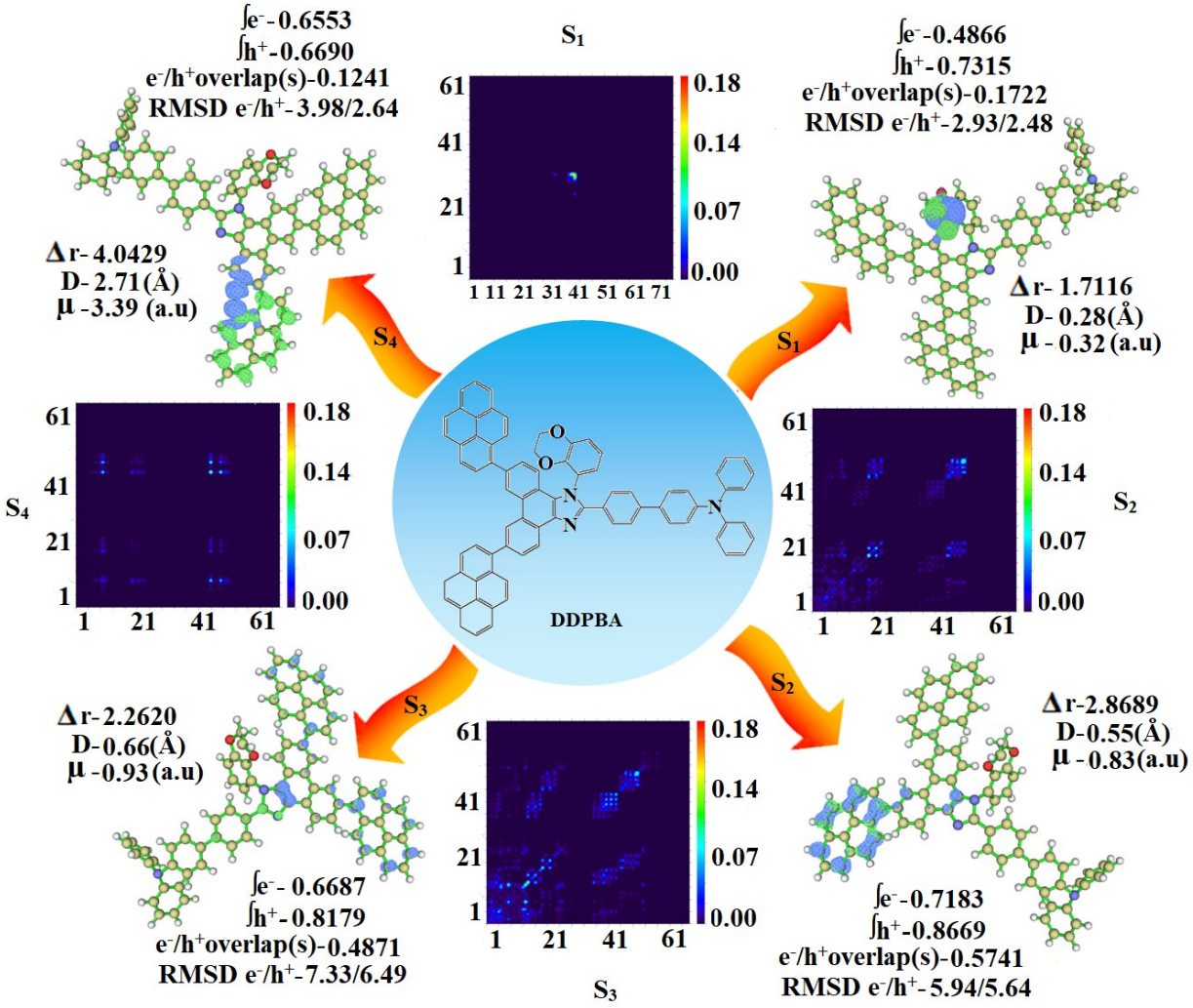


Figure S8. Graphical representation of D_{CT} and centroid of charges [C+(r) / C-(r); isosurface for DDPPPA and for DDPBA (0.1 a.u)]

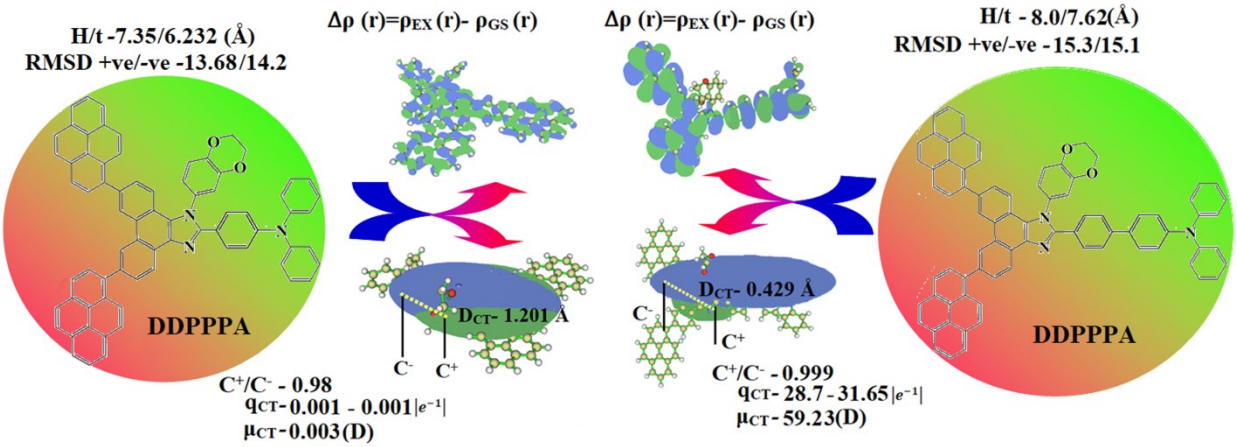
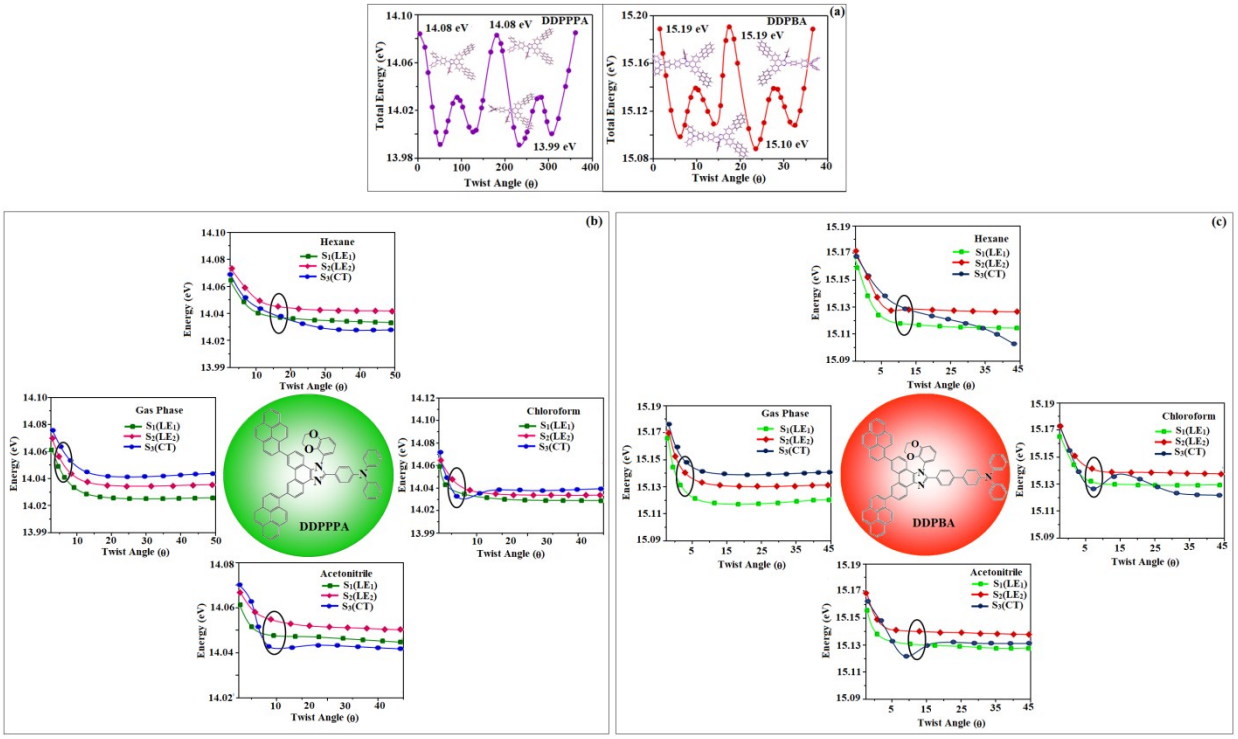


Figure S9. Potential energy surface scan (PES) diagram of (a) DDPPPA and DDPBA; (b) Potential energy scan (PES) of S_1-S_3 excited states of (b) DDPPPA and (c) DDPBA with increasing solvent polarity.



SI–III: Tables

Table S1: Photophysical properties of DDPPPA in different solvents.

Solvents	ε	n	f(ε,n)	λ_{ab} (nm)	ν_{ab} (cm^{-1})	λ_{flu} (nm)	ν_{flu} (cm^{-1})	ν_{ss} (cm^{-1})
Hexane	1.88	1.37	0.0004	345	28985.51	430	23255.81	5729.69
Benzene	2.28	1.43	0.0266	348	28735.63	432	23148.15	5587.48
Toluene	2.38	1.49	0.014	346	28901.73	435	22988.51	5913.23
Dioxane	2.22	1.42	0.0214	344	29069.77	438	22831.05	6238.72
Triethylamine	2.42	1.40	0.048	345	28985.51	440	22727.27	6258.23
Butylether	3.08	1.39	0.096	347	28818.44	444	22522.52	6295.92
Isopropylether	3.88	1.37	0.145	344	29069.77	449	22271.71	6798.05
Chloroform	4.81	1.45	0.148	342	29069.77	480	22123.89	6945.87
Ethyl ether	4.34	1.35	0.167	345	28985.51	450	22222.22	6763.28
Ethyl acetate	6.09	1.41	0.1866	341	29325.51	460	21739.13	7586.38
Tetrahydrofuran	7.52	1.40	0.2096	341	29325.51	469	21321.96	8003.55
dichloromethane	9.08	1.42	0.2183	344	29239.77	481	20833.33	8406.43
Dimethylformamide	36.7	1.43	0.276	344	29069.77	482	20746.89	8322.88
Acetone	21.01	1.35	0.2847	341	29325.51	486	20576.13	8749.38
Acetonitrile	37.5	1.34	0.3053	340	29411.76	490	20408.16	9003.60

Table S2: Photophysical properties of DDPBA in different solvents.

Solvents	**ε**	**n**	**f(ε,n)**	**λ_{ab} (nm)**	**ν_{ab} (cm^{-1})**	**λ_{flu} (nm)**	**ν_{flu} (cm^{-1})**	**ν_{ss} (cm^{-1})**
Hexane	1.88	1.37	0.0004	330	30303.03	415	24096.39	6206.64
Benzene	2.28	1.426	0.0266	334	29940.12	420	23809.52	6130.59
Toluene	2.38	1.494	0.014	335	29850.75	424	23584.91	6265.84
Dioxane	2.22	1.422	0.0214	334	29940.12	428	23364.49	6575.63
Triethylamine	2.42	1.401	0.048	332	30120.48	430	23255.81	6864.67
Butylether	3.08	1.399	0.096	332	30120.48	433	23094.69	7025.79
Isopropylether	3.88	1.368	0.145	330	30303.03	435	22988.51	7314.52
Chloroform	4.81	1.446	0.1482	334	29940.12	469	22935.78	7004.34
Ethyl ether	4.34	1.352	0.167	329	30395.14	455	21978.02	8417.11
Ethyl acetate	6.09	1.413	0.1866	330	30303.03	438	22831.05	7471.98
Tetrahydrofuran	7.52	1.40	0.2096	333	30030.03	452	22123.89	7906.14
Dichloromethane	9.08	1.42	0.2183	334	29940.12	470	21321.96	8618.16
Dimethylformamide	36.7	1.427	0.276	338	29585.8	472	21186.44	8399.36
Acetone	21.01	1.35	0.2847	335	29850.75	475	21052.63	8798.11
Acetonitrile	37.5	1.34	0.3053	332	30120.48	480	20833.33	9287.15

Table S3. Computed [zindo (Singlet or Triplet, n states=10)] singlet (E_S) and triplet (E_T) energies (eV), oscillator strength (*f*), dipole moment (μ, D) and singlet-triplet splitting (ΔE_{ST}, eV) of DDPPPA from NTOs.

Energy level	**E_S**	**Oscillator strength (f)**	**μ**	**NTO Transitions**	**E_T**	**ΔE_{ST}**	**NTO Transitions**
1	1.48	0.0071	0.51	$177 \xrightarrow{61\%} 196$	0.71	0.77	$182 \xrightarrow{24\%} 184$
2	1.69	1.8201	0.93	$182 \xrightarrow{52\%} 183$	1.47	0.22	$181 \xrightarrow{22\%} 183$
3	1.88	0.5693	0.54	$181 \xrightarrow{34\%} 183$	1.59	0.29	$182 \xrightarrow{21\%} 183$
4	2.05	0.0175	1.67	$181 \xrightarrow{21\%} 184$	1.69	0.36	$182 \xrightarrow{21\%} 183$
5	2.26	0.2564	2.56	$182 \xrightarrow{22\%} 185$	1.77	0.49	$182 \xrightarrow{21\%} 183$
6	2.35	0.0088	0.66	$182 \xrightarrow{33\%} 184$	1.86	0.49	$182 \xrightarrow{24\%} 184$
7	2.48	0.0143	0.21	$182 \xrightarrow{33\%} 184$	1.92	0.56	$177 \xrightarrow{61\%} 196$
8	2.55	0.0010	3.64	$174 \xrightarrow{20\%} 184$	2.01	0.54	$177 \xrightarrow{61\%} 196$
9	2.68	0.2089	1.19	$179 \xrightarrow{32\%} 185$	2.11	0.57	$177 \xrightarrow{61\%} 196$
10	2.75	0.0523	0.62	$179 \xrightarrow{32\%} 185$	2.21	0.54	$182 \xrightarrow{23\%} 197$

Table S4. Computed [zindo (Singlet or Triplet, n states=10)] singlet (E_S) and triplet (E_T) energies (eV), oscillator strength (*f*), dipole moment (μ, D) and singlet-triplet splitting (ΔE_{ST}, eV) of DDPBA from NTOs.

Energy level	**E_S**	**Oscillator strength (f)**	**μ**	**NTO Transitions**	**E_T**	**ΔE_{ST}**	**NTO Transitions**
1	1.60	0.0067	0.32	41% 190 → 211	0.52	1.08	24% 196 → 198
2	1.93	1.8445	0.83	52% 196 → 197	1.60	0.33	22% 195 → 197
3	2.06	0.5417	0.93	35% 196 → 198	1.62	0.44	20% 196 → 197
4	2.14	0.0015	3.39	25% 192 → 198	1.64	0.5	22% 195 → 197
5	2.25	0.0174	0.40	26% 189 → 211	1.75	0.5	22% 195 → 197
6	2.32	0.3295	3.14	22% 196 → 199	1.86	0.46	24% 196 → 198
7	2.45	0.0075	0.56	21% 195 → 198	1.90	0.55	22% 195 → 197
8	2.56	0.0086	0.56	32% 195 → 197	2.03	0.53	24% 196 → 198
9	2.67	0.3758	0.95	18% 196 → 136	2.14	0.53	20% 196 → 197
10	2.75	0.0185	0.81	22% 184 → 197	2.21	0.54	20% 196 → 197

Table S5: Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipole moment (μ) for singlet states of DDPPPA.

State	Hole integral	Electron integral	Integral of transition density	Integral overlap of h^+- e^- (S)	Centroid of hole (Å)			Centroid of electron (Å)			D (Å)	μ (a.u)
					x	y	z	x	y	z		
S1	0.7582	0.5047	-0.0095	0.1775	-2.0284	-3.8305	2.1826	-1.7175	-4.1161	2.2644	0.43	0.51
S2	0.8782	0.7273	0.0018	0.5822	4.6385	3.5532	0.0529	5.2460	3.6272	-0.0100	0.61	0.93
S3	0.8549	0.6978	0.0003	0.5129	3.4878	-0.4737	0.0012	3.3615	-0.8073	-0.0967	0.36	0.54
S4	0.7608	0.5662	0.0016	0.4827	4.5179	4.4771	0.0570	5.3327	5.5388	0.0093	1.33	1.67
S5	0.7420	0.5856	0.0035	0.3399	1.9813	-1.5988	0.0592	-0.0506	-1.8080	-0.0315	2.04	2.56
S6	0.7041	0.5178	0.0010	0.4434	4.1592	-4.4182	-0.2014	3.6564	-4.1301	-0.2078	0.57	0.66
S7	0.5742	0.4369	0.0035	0.2966	2.4688	-0.5593	0.1268	2.3253	-0.7205	0.0813	0.22	0.21
S8	0.7232	0.6790	-0.0027	0.1395	2.6389	4.5505	0.3070	4.9704	6.0034	0.1086	2.75	3.64
S9	0.7017	0.5324	-0.0054	0.3412	-2.0744	0.7939	-0.2136	-1.1353	0.4840	0.0674	1.02	1.19
S10	0.5686	0.4170	-0.0038	0.2914	-1.6902	0.8456	-0.0593	-2.2545	0.4756	-0.0592	0.67	0.62

Table S6: Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipole moment (μ) for triplet states of DDPPPA.

State	Hole integral	Electron integral	Integral of transition density	Integral overlap of h^+- e^- (S)	Centroid of hole (Å)			Centroid of electron (Å)			D (Å)	μ (a.u)
					x	y	z	x	y	z		
T1	0.7593	0.6111	0.0012	0.5229	5.3239	5.7740	0.0469	5.5117	5.7606	0.0368	0.19	0.24
T2	0.6974	0.5586	0.0033	0.4637	4.6972	-5.7342	-0.2867	4.4411	-5.3899	-0.2474	0.43	0.51
T3	0.4361	0.3365	0.0020	0.2191	-1.3452	0.6366	0.0619	-2.1211	0.6907	0.0845	0.78	0.57
T4	0.2418	0.1731	-0.0043	0.1276	-3.6779	0.4487	-0.3056	-3.0428	0.0793	-0.1777	0.74	0.29
T5	0.2237	0.1559	-0.0052	0.1151	-3.4828	-0.2566	-0.3592	-3.8496	0.1283	-0.2165	0.55	0.20
T6	0.6066	0.4239	0.0055	0.3667	4.4420	-5.2823	-0.2400	4.3843	-4.9832	-0.2104	0.31	0.30
T7	0.4380	0.2813	0.0007	0.2510	-6.3588	1.3311	-0.1735	-7.1210	1.0120	-0.1458	0.83	0.56
T8	0.4706	0.2985	-0.0027	0.2655	-7.0105	0.7439	-0.0160	-8.3512	0.6881	0.0629	1.34	0.98
T9	0.7312	0.4885	0.0094	0.1725	-2.0499	-3.8592	2.1945	-1.7186	-4.0136	2.2043	0.36	0.42
T10	0.7798	0.5377	-0.0001	0.4836	5.2364	5.9467	0.0162	5.5042	5.8485	0.0128	0.28	0.35

Table S7: Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipole moment (μ) for singlet states of DDPBA.

State	Hole integral	Electron integral	Integral of transition density	Integral overlap of h^+- e^- (S)	Centroid of hole (Å)			Centroid of electron (Å)			D (Å)	μ (a.u)
					x	y	z	x	y	z		
S1	0.7315	0.4866	-0.0098	0.1722	-0.1004	-4.1282	3.3013	0.17408	-4.1730	3.2522	0.28	0.32
S2	0.8669	0.7183	0.0016	0.5741	5.3817	3.7410	-0.1871	5.8856	3.8104	-0.4112	0.55	0.83
S3	0.8179	0.6687	0.0003	0.4871	4.6297	1.0043	-0.1194	3.9683	0.9793	-0.1411	0.66	0.93
S4	0.6690	0.6553	0.0026	0.1241	3.5005	4.8091	0.7625	5.5483	6.3044	-0.2099	2.71	3.39
S5	0.8271	0.6151	-0.0006	0.5537	5.6641	5.7582	-0.2859	5.8251	6.0081	-0.3272	0.30	0.40
S6	0.7346	0.5884	0.0065	0.3309	3.3694	-1.9550	0.0880	0.8709	-2.1188	0.3662	2.51	3.14
S7	0.6741	0.5022	0.0006	0.4078	3.9918	-1.8714	-0.2232	4.1865	-2.3397	-0.2640	0.50	0.56
S8	0.6741	0.5022	0.0006	0.4078	3.9918	-1.8714	-0.2232	4.1865	-2.3397	-0.2640	0.50	0.56
S9	0.6252	0.4856	-0.0042	0.3631	1.0778	0.8006	0.2322	1.9097	0.4323	0.3107	0.91	0.95
S10	0.5944	0.5098	-0.0010	0.2346	4.0912	-4.2746	-0.0291	4.5071	-4.4989	-0.6514	0.78	0.81

Table S8: Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipole moment (μ) for singlet states of DDPBA.

State	Hole integral	Electron integral	Integral of transition density	Integral overlap of h^+- e^- (S)	Centroid of hole (Å)			Centroid of electron (Å)			D (Å)	μ (a.u)
					x	y	z	x	y	z		
T1	0.7421	0.6001	-0.0002	0.5101	5.8538	6.2305	-0.2957	5.8395	6.1302	-0.3369	0.11	0.14
T2	0.7055	0.5630	-0.0003	0.4740	5.7616	-5.1761	-1.0074	5.7379	-5.1737	-0.9329	0.08	0.09
T3	0.4008	0.3127	-0.0051	0.2151	1.5584	0.6390	0.8530	1.0215	0.5173	0.8923	0.55	0.37
T4	0.3356	0.2333	-0.0065	0.1829	-1.7035	-0.9262	0.6226	-2.1787	-1.1937	0.5599	0.55	0.29
T5	0.3180	0.2361	0.0044	0.1715	-4.7701	0.5602	0.5347	-3.5841	0.2954	0.7936	1.24	0.65
T6	0.5577	0.3901	-0.0030	0.3226	4.6288	-4.4003	-0.8903	5.0215	-4.7702	-0.8707	0.54	0.48
T7	0.2912	0.1933	-0.0072	0.1507	-8.0548	1.3346	-0.6761	-9.5778	1.6501	-1.1251	1.62	0.74
T8	0.1888	0.1292	-0.0082	0.0797	-3.6189	0.4868	0.3305	-3.4437	0.2588	0.9597	0.69	0.21
T9	0.5766	0.3617	0.0006	0.3249	-8.9966	-1.3163	-1.1419	-10.0492	-1.0531	-1.3935	1.11	0.99
T10	0.7935	0.5462	-0.0009	0.5051	5.8344	6.3749	-0.3711	5.7555	6.2335	-0.3786	0.16	0.20

Table S9: Computed RMSD of electron and hole, H index and t index for singlet states of DDPPPA.

State	RMSD (Electron)				RMSD (Hole)				H index				t index			
	x	y	z	total	x	y	z	total	x	y	z	Total	x	y	z	Total
S1	1.634	1.699	1.314	2.699	1.526	1.709	0.967	2.487	1.580	1.704	1.140	2.588	-1.269	-1.419	-1.058	2.178
S2	2.293	5.232	0.714	5.757	2.756	4.755	0.740	5.545	2.524	4.993	0.727	5.642	-1.917	-4.919	-0.664	5.321
S3	4.052	5.696	0.757	7.031	3.330	5.307	0.782	6.314	3.691	5.501	0.770	6.669	-3.565	-5.168	-0.672	6.314
S4	2.523	3.339	0.706	4.244	3.494	4.129	0.741	5.460	3.009	3.734	0.723	4.850	-2.194	-2.672	-0.676	3.523
S5	4.634	3.770	0.802	6.028	3.762	4.094	0.810	5.619	4.198	3.932	0.806	5.808	-2.166	-3.723	-0.715	4.366
S6	3.600	4.245	0.772	5.619	2.744	4.155	0.769	5.038	3.172	4.200	0.770	5.319	-2.669	-3.912	-0.764	4.797
S7	3.394	4.481	0.791	5.676	3.475	4.587	0.842	5.816	3.435	4.534	0.816	5.746	-3.291	-4.373	-0.771	5.527
S8	1.926	2.668	0.687	3.361	1.801	2.459	0.467	3.084	1.863	2.563	0.577	3.221	0.468	-1.111	-0.378	1.263
S9	4.596	3.320	0.804	5.727	5.144	3.570	0.854	6.319	4.870	3.445	0.829	6.023	-3.931	-3.135	-0.548	5.058
S10	4.717	3.140	0.858	5.731	5.051	3.287	0.858	6.087	4.884	3.214	0.858	5.909	-4.319	-2.844	-0.858	5.242

Table S10: Computed RMSD of electron and hole, H index and t index for triplet states of DDPPPA.

State	RMSD (Electron)				RMSD (Hole)				H index				t index			
	x	y	z	total	x	y	z	total	x	y	z	Total	x	y	z	Total
T1	2.159	2.947	0.696	3.719	2.459	2.799	0.723	3.795	2.309	2.873	0.709	3.753	-2.121	-2.859	-0.699	3.628
T2	2.476	3.020	0.746	3.976	2.223	2.707	0.749	3.582	2.349	2.864	0.747	3.779	-2.093	-2.519	-0.708	3.351
T3	4.058	2.406	0.818	4.788	4.273	2.532	0.846	5.038	4.165	2.469	0.832	4.913	-3.389	-2.415	-0.810	4.240
T4	4.044	2.856	0.938	5.039	4.151	3.038	0.947	5.230	4.097	2.947	0.943	5.134	-3.462	-2.578	-0.815	4.393
T5	4.309	3.164	0.997	5.438	3.777	3.146	0.973	5.011	4.043	3.155	0.985	5.222	-3.676	-2.770	-0.842	4.679
T6	2.627	3.355	0.788	4.334	2.501	3.035	0.780	4.009	2.564	3.195	0.784	4.171	-2.506	-2.896	-0.754	3.903
T7	4.515	2.944	1.101	5.502	5.293	3.148	1.054	6.247	4.904	3.046	1.077	5.873	-4.142	-2.727	-1.050	5.069
T8	3.628	2.610	1.135	4.611	5.159	2.972	1.083	6.052	4.393	2.791	1.109	5.322	-3.053	-2.735	-1.030	4.226
T9	1.783	1.890	1.373	2.938	1.495	1.659	0.956	2.430	1.639	1.774	1.165	2.682	-1.308	-1.620	-1.155	2.381
T10	2.475	2.669	0.707	3.708	3.287	2.375	0.755	4.125	2.881	2.522	0.731	3.898	-2.613	-2.424	-0.727	3.638

Table S11: Computed RMSD of electron and hole, H index and t index for singlet states of DDPBA

State	RMSD (Electron)				RMSD (Hole)				H index				t index			
	x	y	z	total	x	y	Z	total	x	y	z	Total	x	Y	Z	Total
S1	1.660	1.924	1.473	2.938	1.435	1.677	1.132	2.481	1.548	1.801	1.303	2.708	-1.273	-1.756	-1.253	2.505
S2	2.171	5.423	1.111	5.946	2.464	4.943	1.187	5.649	2.318	5.183	1.149	5.792	-1.814	-5.113	-0.925	5.504
S3	4.442	5.673	1.375	7.335	3.297	5.437	1.324	6.495	3.869	5.555	1.349	6.903	-3.208	-5.530	-1.328	6.530
S4	2.660	2.791	1.006	3.984	1.505	2.085	0.601	2.641	2.082	2.438	0.804	3.305	-0.034	-0.943	0.169	0.958
S5	2.469	3.169	0.967	4.132	2.662	3.523	1.036	4.536	2.565	3.346	1.002	4.334	-2.404	-3.096	-0.960	4.036
S6	5.363	3.553	1.562	6.620	4.018	3.904	1.463	5.790	4.690	3.728	1.512	6.179	-2.192	-3.564	-1.234	4.362
S7	3.778	4.559	1.326	6.068	4.155	4.676	1.402	6.411	3.967	4.618	1.364	6.238	-3.772	-4.149	-1.323	5.761
S8	3.778	4.559	1.326	6.068	4.155	4.676	1.402	6.411	3.967	4.618	1.364	6.238	-3.772	-4.149	-1.323	5.761
S9	5.127	4.379	1.387	6.884	5.977	4.273	1.346	7.470	5.552	4.326	1.366	7.170	-4.720	-3.958	-1.288	6.293
S10	4.198	3.582	1.219	5.652	2.315	2.410	1.092	3.516	3.257	2.996	1.156	4.574	-2.841	-2.772	-0.533	4.005

Table S12: Computed RMSD of electron and hole, H index and t index for triplet states of DDPBA.

State	RMSD (Electron)				RMSD (Hole)				H index				t index			
	x	y	z	total	x	y	z	total	x	y	z	Total	x	y	z	Total
T1	2.624	3.094	1.037	4.187	2.364	2.862	1.057	3.859	2.494	2.978	1.047	4.023	-2.480	-2.877	-1.006	3.929
T2	2.842	2.894	1.190	4.227	3.136	3.035	1.143	4.512	2.989	2.964	1.167	4.368	-2.965	-2.962	-1.092	4.331
T3	4.110	2.814	1.180	5.119	3.858	2.629	1.118	4.801	3.984	2.721	1.149	4.960	-3.447	-2.599	-1.110	4.458
T4	4.604	2.831	1.280	5.554	4.463	3.129	1.224	5.586	4.534	2.980	1.252	5.568	-4.058	-2.712	-1.189	5.024
T5	5.189	2.550	1.215	5.908	5.504	2.271	1.256	6.085	5.346	2.411	1.235	5.993	-4.160	-2.146	-0.976	4.782
T6	4.224	3.042	1.239	5.351	4.932	3.623	1.256	6.247	4.578	3.333	1.247	5.798	-4.185	-2.963	-1.228	5.273
T7	4.955	2.624	1.285	5.752	5.826	2.598	1.480	6.549	5.390	2.611	1.383	6.147	-3.867	-2.295	-0.934	4.593
T8	4.940	2.558	1.415	5.741	6.268	3.113	1.451	7.148	5.604	2.836	1.433	6.442	-5.429	-2.608	-0.804	6.076
T9	4.760	2.275	1.311	5.436	5.536	2.228	1.452	6.142	5.148	2.251	1.382	5.786	-4.095	-1.988	-1.130	4.691
T10	3.197	2.734	1.092	4.346	2.988	2.532	1.108	4.071	3.093	2.633	1.100	4.208	-3.014	-2.492	-1.093	4.060

Table S13. Transferred charges (q_{CT}), barycentres of electron density loss (R_+) /gain (R-), distance between two barycenters (D_{CT}), dipole moment of CT (μ_{CT}), RMSD of +ve/-ve parts, CT indices (H & t) and overlap integral of C+/C- of DDPPPA and DDPBA.

Blue emissive &Host materials	**q_{CT}** $\lvert e^{-1} \rvert$	**R_+ (Å)**			**R- (Å)**			**D_{CT} (Å)**	**μ_{CT} (D)**	**RMSD of +ve parts**	**RMSD of -ve parts**	**H / t indices (Å)**	**overlap integral of C+/ C-**
		x	y	z	x	y	z						
DDPPPA	0.001 -0.001	0.495	-0.333	-0.049	-0.634	0.079	-0.059	1.201	0.003	13.681	14.152	7.349/6.232	0.9843
DDPBA	28.743 -31.645	1.862	0.427	0.141	1.518	0.177	0.084	0.429	59.228	15.303	15.101	8.044/7.619	0.9985

Table S14: Computed excitation energy (eV), excitation coefficient and Δr intex (Å) for singlet and triplet states of DDPPPA.

State	Singlet			Triplet		
	Excitation energy	**Excitation coefficient**	**Δr intex**	**Excitation energy**	**Excitation coefficient**	**Δr intex**
1	1.4792	0.4317	1.4535	0.7114	0.3673	2.4455
2	1.6881	0.4326	2.8688	1.4713	0.3357	2.0751
3	1.8839	0.4199	2.2411	1.5913	0.2137	4.5605
4	2.0477	0.3606	4.8958	1.6878	0.1148	2.8195
5	2.2623	0.3637	4.7740	1.7704	0.1061	2.0219
6	2.3528	0.3303	3.5192	1.8637	0.2748	4.0050
7	2.4766	0.2800	4.0004	1.9238	0.1925	3.1772
8	2.5467	0.4109	4.3088	2.0111	0.2067	2.1976
9	2.6840	0.3369	3.6357	2.1071	0.4169	1.3995
10	2.7524	0.2697	3.6255	2.2095	0.3525	4.0757

Table S15: Computed excitation energy (eV), excitation coefficient and Δr intex (Å) for singlet and triplet states of DDPBA.

State	Singlet			Triplet		
	Excitation energy	**Excitation coefficient**	**Δr intex**	**Excitation energy**	**Excitation coefficient**	**Δr intex**
1	1.5982	0.4157	1.7116	0.5251	0.3602	2.5285
2	1.9339	0.4274	2.8689	1.5982	0.3385	2.3470
3	2.0592	0.4015	2.2620	1.6194	0.1964	4.6522
4	2.1407	0.3936	4.0429	1.6458	0.1585	2.9743
5	2.2479	0.3901	4.7118	1.7502	0.1520	3.5574
6	2.3200	0.3593	5.0110	1.8613	0.2548	4.8475
7	2.4476	0.3316	4.6645	1.8998	0.1336	3.3529
8	2.5636	0.3222	5.0707	2.0283	0.0877	3.9288
9	2.6706	0.3038	4.1859	2.1363	0.2490	2.5348
10	2.7499	0.3173	4.1176	2.2086	0.3590	5.7523