Electronic Supplementary Material (ESI) for Materials Advances.

Supporting information

Non-doped OLEDs based on tetraphenylethylene phenanthroimidazoles with negligible efficiency roll-off: Effect of end groups regulated stimuli responsive AIE luminogens

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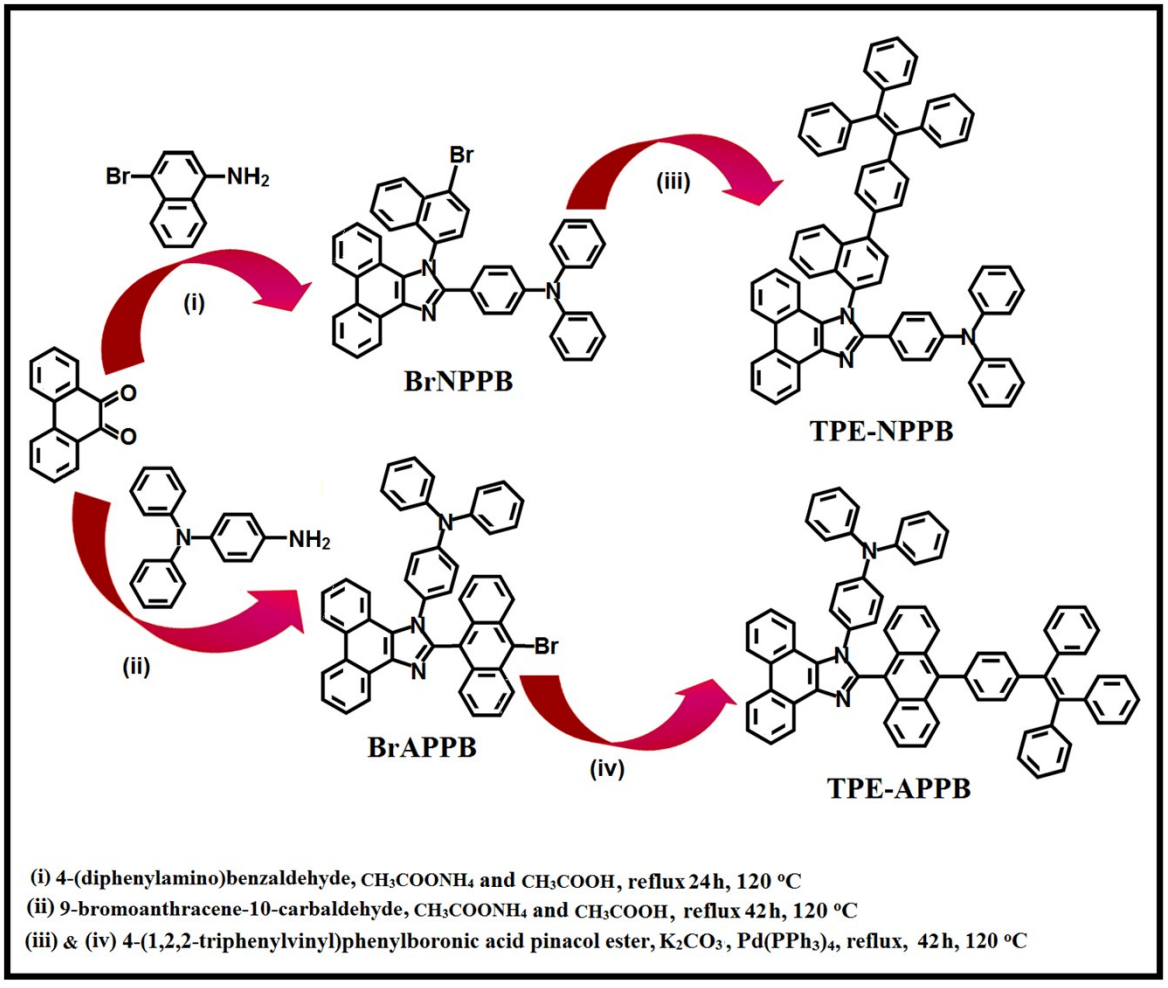
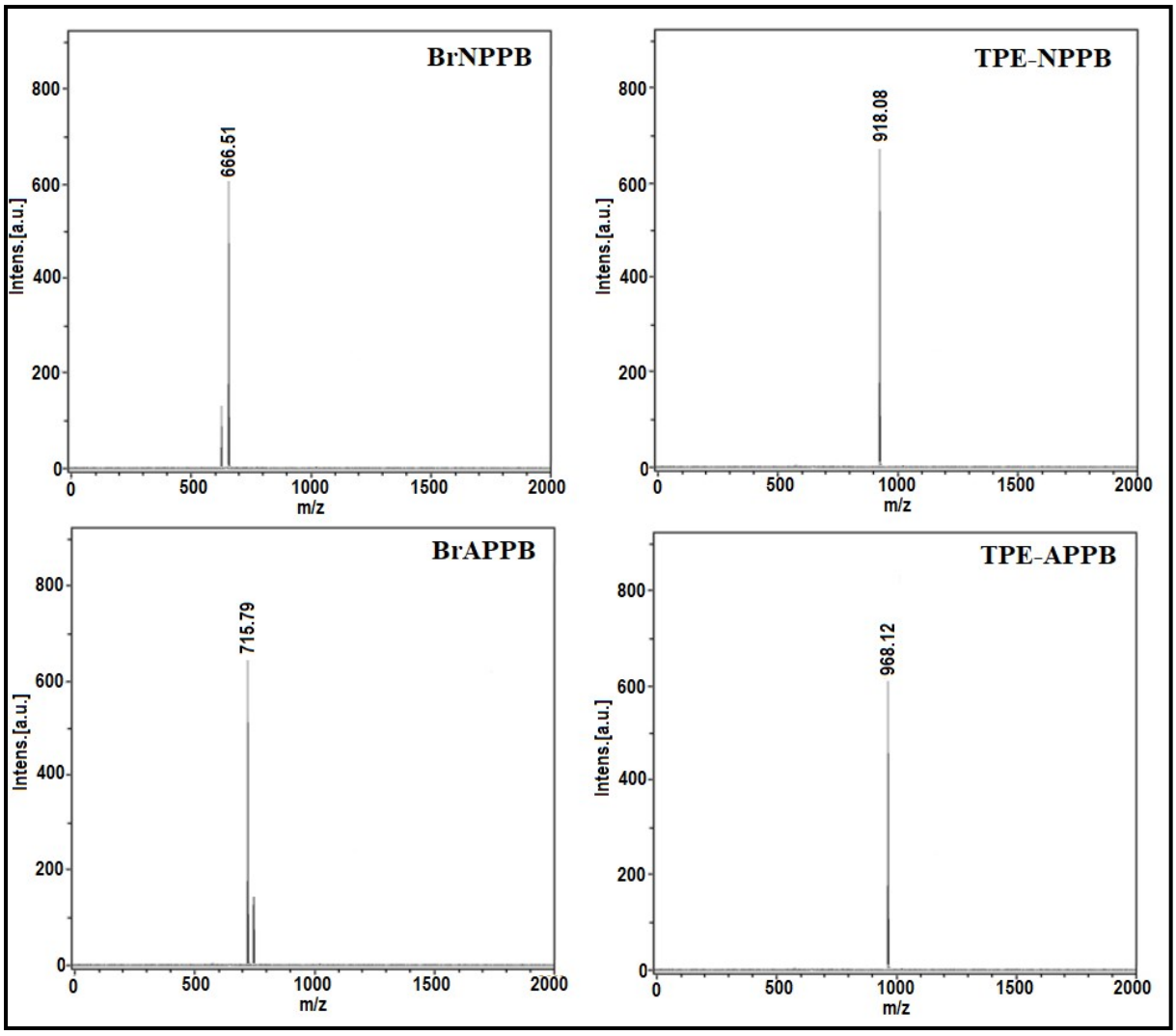
Scheme S1. Synthetic route of emissive materials.



Scheme S2. Mass spectra of BrNPPB, BrAPPB, TPE-NPPB and TPE-APPB.



SI–I: Figures

Figure S1. Frontier molecular orbitals of TPE-NPPB and TPE-APPB.

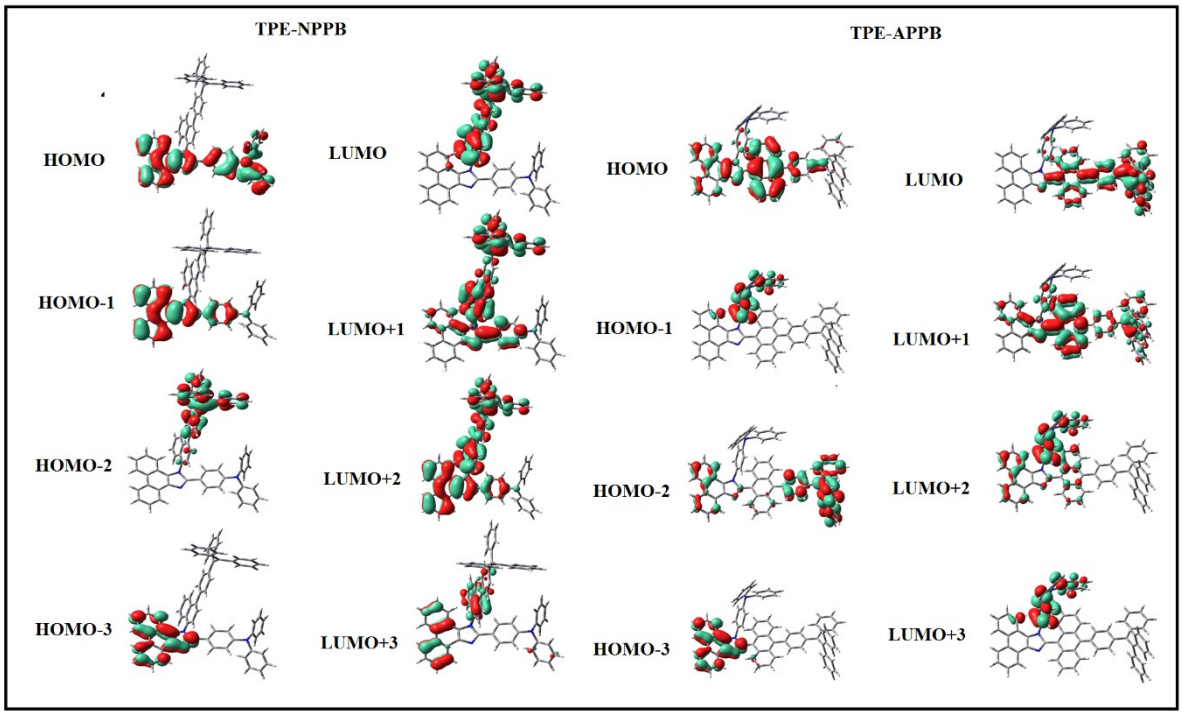


Figure S2. Natural transition orbital pairs (NTOs) with transition character analysis for singlet states of (HONTOs and LUNTOs): (a) TPE-NPPB and (b) TPE-APPB [*f*-oscillator strength and % weights of hole-particle].

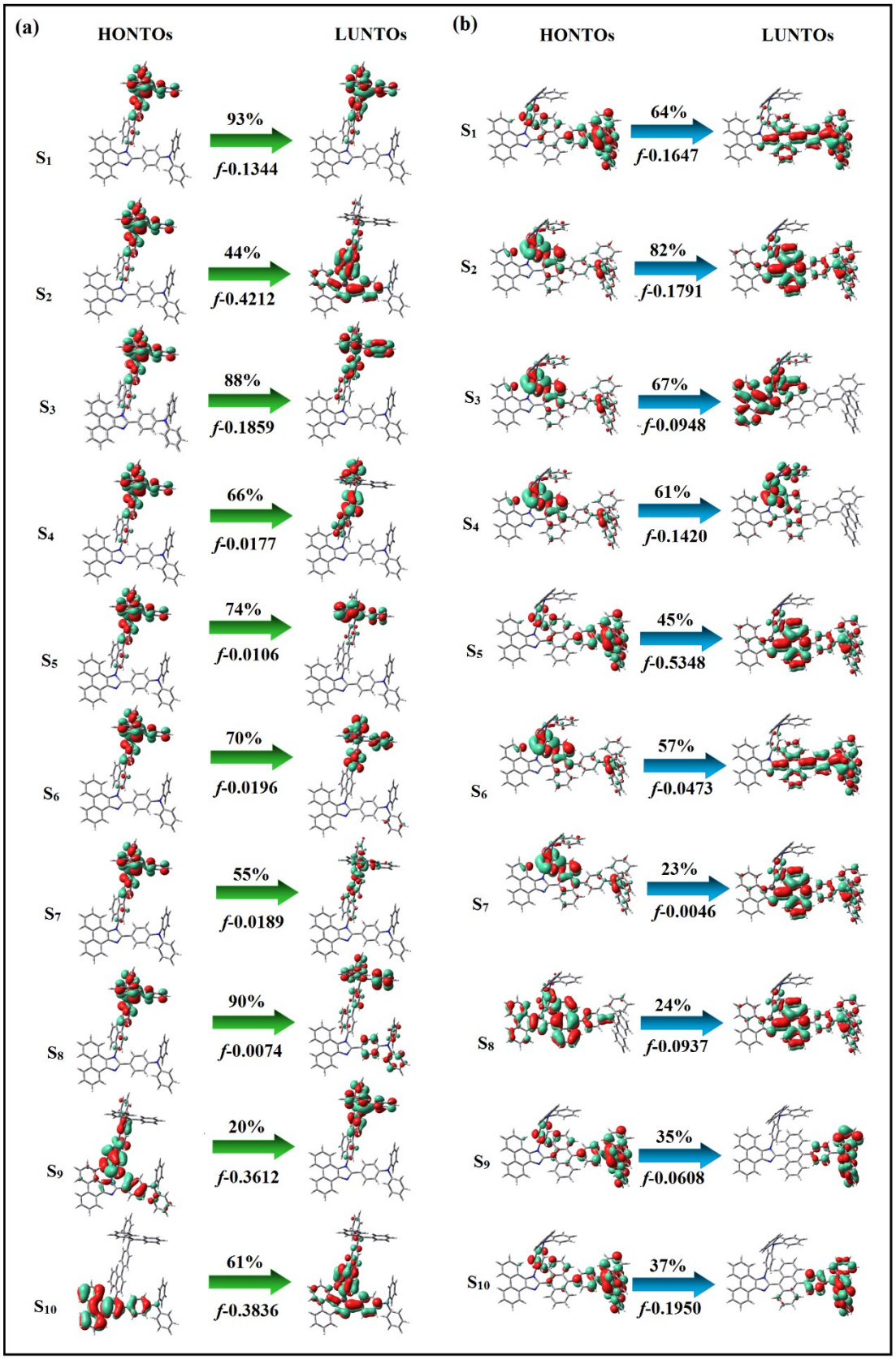


Figure S3. Solvatochromic emission spectra of (a) TPE-NPPB and (b) TPE-APPB.

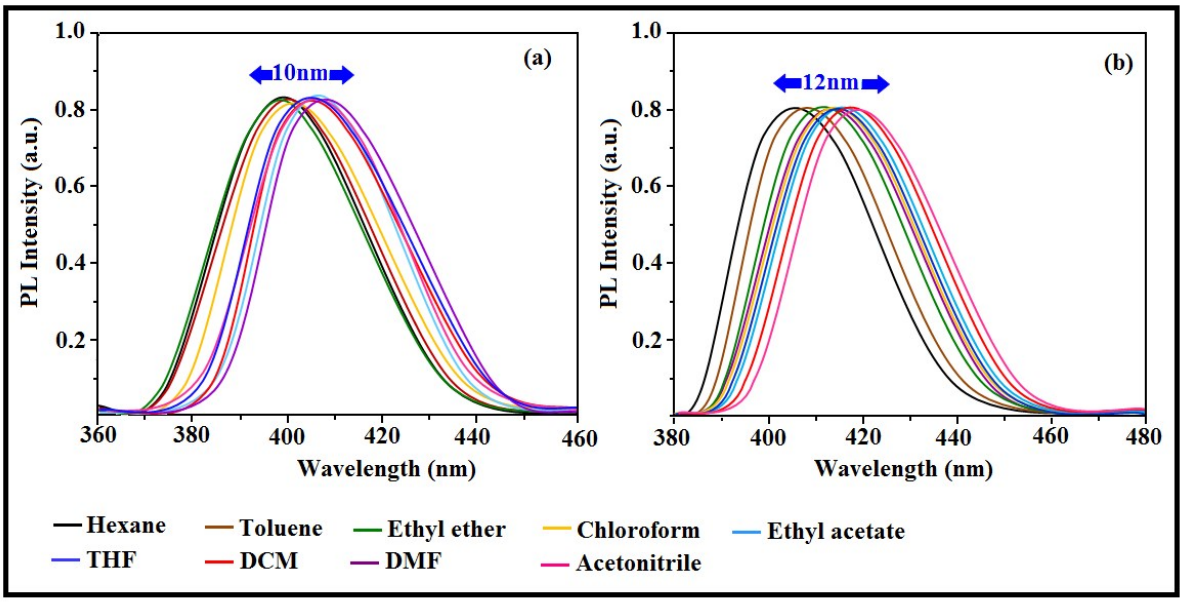


Figure S4. Solvatochromic absorption spectra of (a) TPE-NPPB and (b) TPE-APPB.

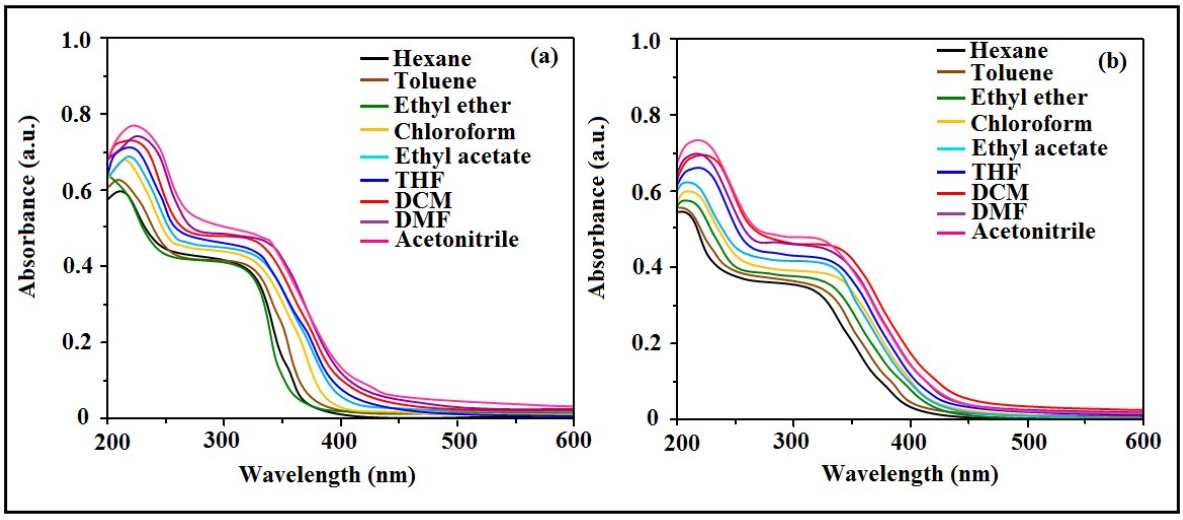


Figure S5. (a) Emission spectra at 90% THF-Water mixture and (b) Intensity vs. Water fraction (%) of TPE-NPPB and TPE-APPB.

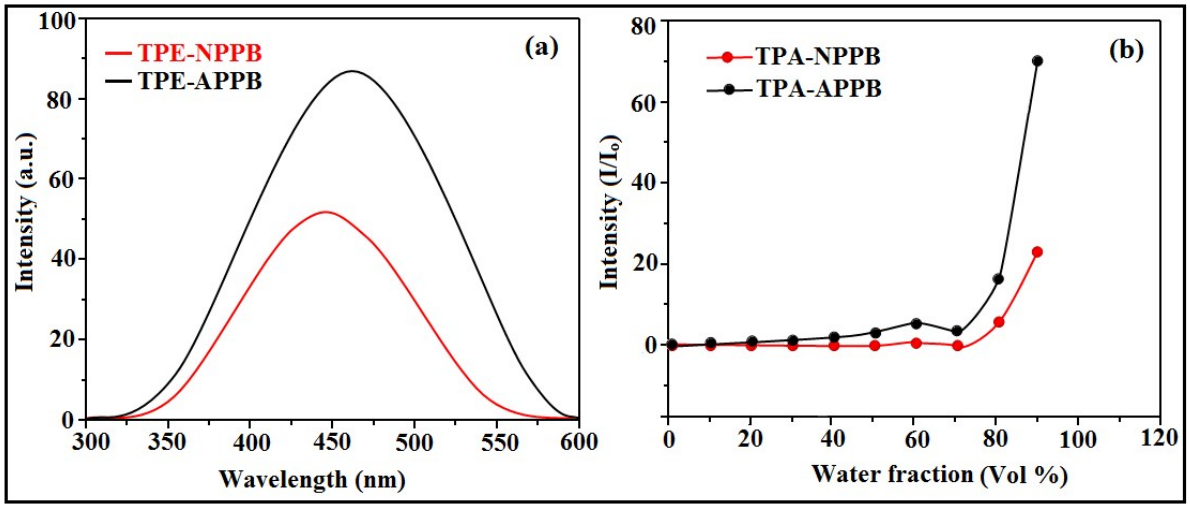
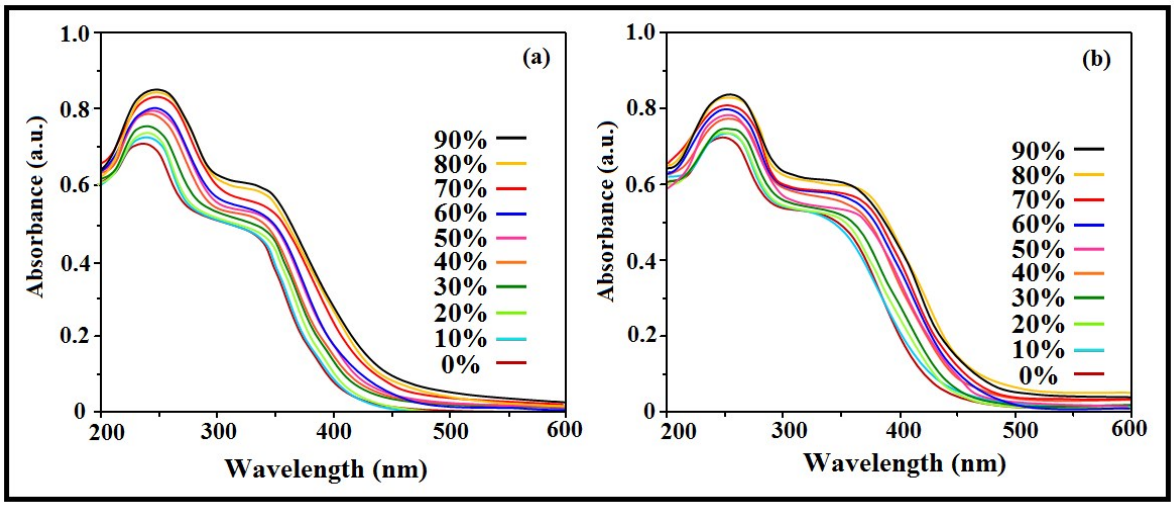


Figure S6. Absorption spectra in THF-water mixtures with different water fractions of (a) TPE-NPPB and (b) TPE-APPB.



SI–II: Tables

Table S1. 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 TPE-NPPB from NTOs.

Energy level	E_S	Oscillator strength (f)	μ	NTO Transitions
1	0.81	0.1344	0.03	$169 \xrightarrow{93\%} 170$
2	2.79	0.4212	4.30	$169 \xrightarrow{44\%} 171$
3	3.04	0.1859	2.97	$169 \xrightarrow{88\%} 181$
4	3.15	0.0177	3.25	$169 \xrightarrow{66\%} 179$
5	3.21	0.0106	3.35	$169 \xrightarrow{74\%} 182$
6	3.23	0.0196	1.44	$169 \xrightarrow{70\%} 183$
7	3.30	0.0189	0.78	$169 \xrightarrow{55\%} 193$
8	3.33	0.0074	2.73	$169 \xrightarrow{90\%} 185$
9	3.39	0.3612	1.44	$167 \xrightarrow{20\%} 170$
10	3.42	0.3836	2.47	$168 \xrightarrow{61\%} 171$

Table S2. 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 TPE-APPB from NTOs.

Energy level	E_S	Oscillator strength (f)	μ	NTO Transitions
1	0.80	0.1647	0.20	$177 \xrightarrow{64\%} 179$
2	1.42	0.1791	4.90	$178 \xrightarrow{82\%} 180$
3	1.92	0.0948	0.76	$178 \xrightarrow{67\%} 181$
4	2.22	0.1420	1.19	$178 \xrightarrow{61\%} 184$
5	2.38	0.5348	5.79	$177 \xrightarrow{45\%} 180$
6	2.54	0.0473	9.69	$178 \xrightarrow{57\%} 179$
7	2.71	0.0046	1.81	$178 \xrightarrow{23\%} 180$
8	2.81	0.0937	1.81	$176 \xrightarrow{24\%} 180$
9	2.86	0.0608	1.83	$177 \xrightarrow{35\%} 190$
10	3.01	0.1950	3.11	$177 \xrightarrow{37\%} 189$

Table S3: Photophysical properties of TPE-NPPB in different solvents.

Solvents	**ε**	**n**	**f (ε,n)**	**λ_{ab} (nm)**	**υ_{ab} (cm^{-1})**	**λ_{flu} (nm)**	**υ_{flu} (cm^{-1})**	**υ_{ss} (cm^{-1})**
Hexane	1.88	1.37	0.0004	329	30395.13	398	25125.62	5269.50
Toluene	2.38	1.49	0.014	330	30303.03	399	25062.65	5240.37
Ethyl ether	4.34	1.35	0.167	328	30487.80	400	25000.00	5487.80
Chloroform	4.81	1.44	0.148	330	30303.03	402	24875.62	5427.40
ethyl acetate	6.09	1.41	0.186	334	29940.11	406	24630.54	5309.57
THF	7.52	1.40	0.209	332	30120.48	403	24813.09	5306.58
DCM	9.08	1.42	0.218	333	30030.03	402	24875.62	5154.40
DMF	36.7	1.42	0.276	334	29940.11	408	24509.80	5430.31
acetonitrile	37.5	1.34	0.305	331	30211.48	404	24752.47`	5459.00

Table S4: Photophysical properties of TPE-APPB in different solvents.

Solvents	**ε**	**n**	**f (ε,n)**	**λ_{ab} (nm)**	**υ_{ab} (cm^{-1})**	**λ_{flu} (nm)**	**υ_{flu} (cm^{-1})**	**υ_{ss} (cm^{-1})**
Hexane	1.88	1.37	0.0004	346	28901.73	406	24630.54	4271.19
Toluene	2.38	1.49	0.014	348	28735.63	408	24509.80	4225.82
Ethyl ether	4.34	1.35	0.167	349	28653.29	412	24271.84	4381.45
Chloroform	4.81	1.44	0.148	350	28571.42	414	24154.58	4416.83
ethyl acetate	6.09	1.41	0.186	349	28653.29	413	24213.07	4440.22
THF	7.52	1.40	0.209	348	28735.63	416	24038.46	4697.17
DCM	9.08	1.42	0.218	351	28490.02	417	23980.81	4509.21
DMF	36.7	1.42	0.276	348	28735.63	414	24154.58	4581.04
acetonitrile	37.5	1.34	0.305	347	28818.44	418	23923.44	4894.99