Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Quantum Chemical Characterization and Design of Host Materials based on Phosphine Oxide-Substituted (Triphenylamine) Fluorene for (deep) Blue Phosphors in OLEDs

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Figures and tables

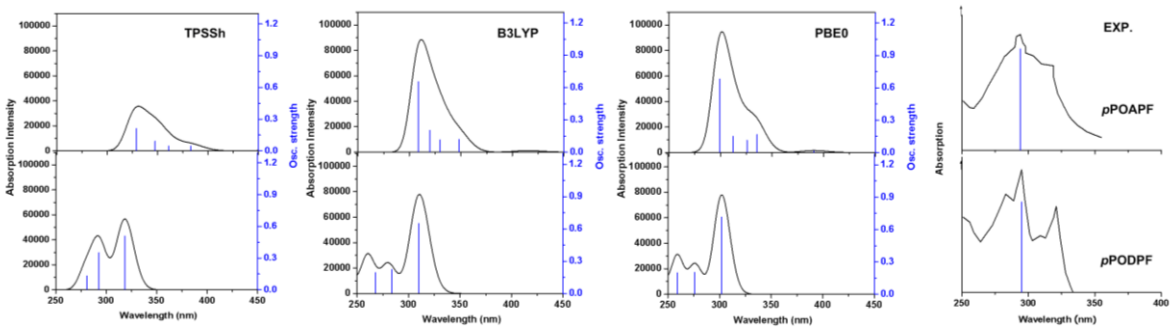

Fig. S1 The simulated absorption spectra of *p*POAPF and *p*PODPF in benzene solution by employing various TDDFT methods with 6-31+G**, together with their corresponding experiment values.[1]

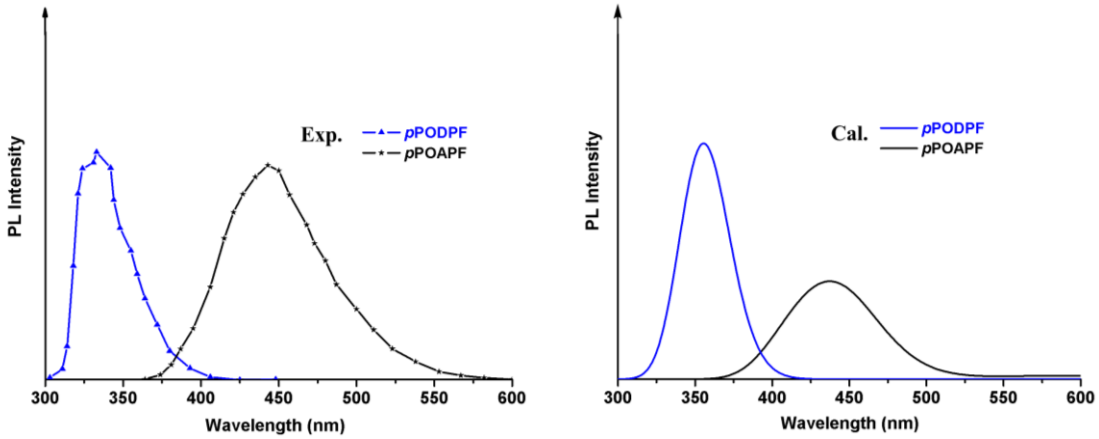

Fig. S2 The simulated emission spectra of *p*POAPF and *p*PODPF in benzene solution by employing TD-PBE0 method with 6-31+G**, together with their corresponding experiment values.[1]

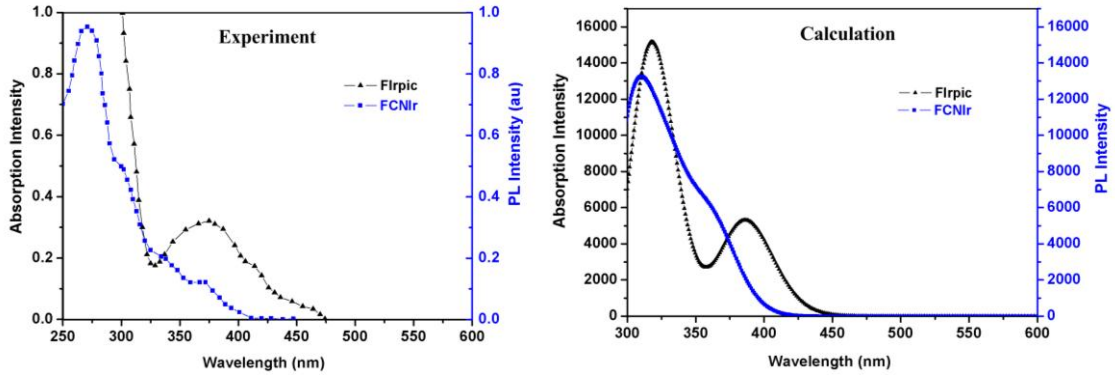

Fig. S3 The simulated absorption spectra of FIrpic and FCNIr in toluene and benzene by employing TD-PBE0 method with 6-31+G**, together with their corresponding experiment values.[2,3]

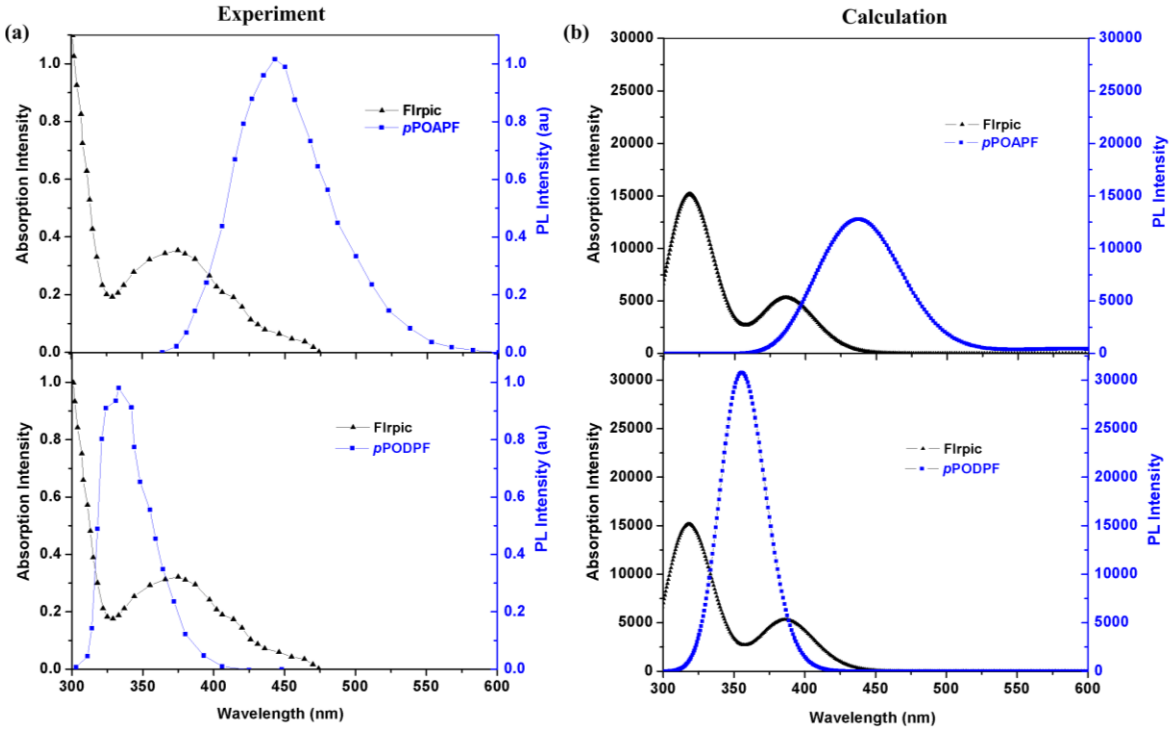

Fig. S4 The simulated emission and absorption spectra from *p*PODPF/*p*POAPF and FIrpic in benzene and toluene solutions, respectively, by employing PBE0 methods with 6-31+G**, together with their corresponding experimental values.[1,2]

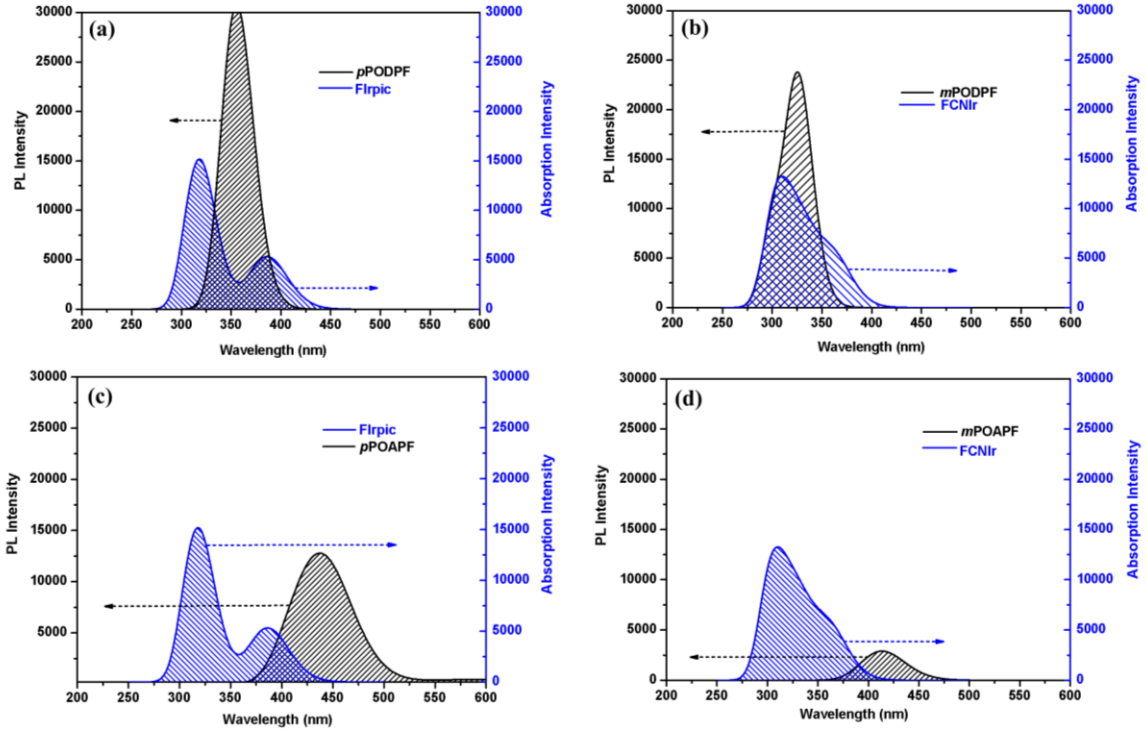

Fig. S9 The host emission and guest absorption spectra in four groups of host-guest systems.

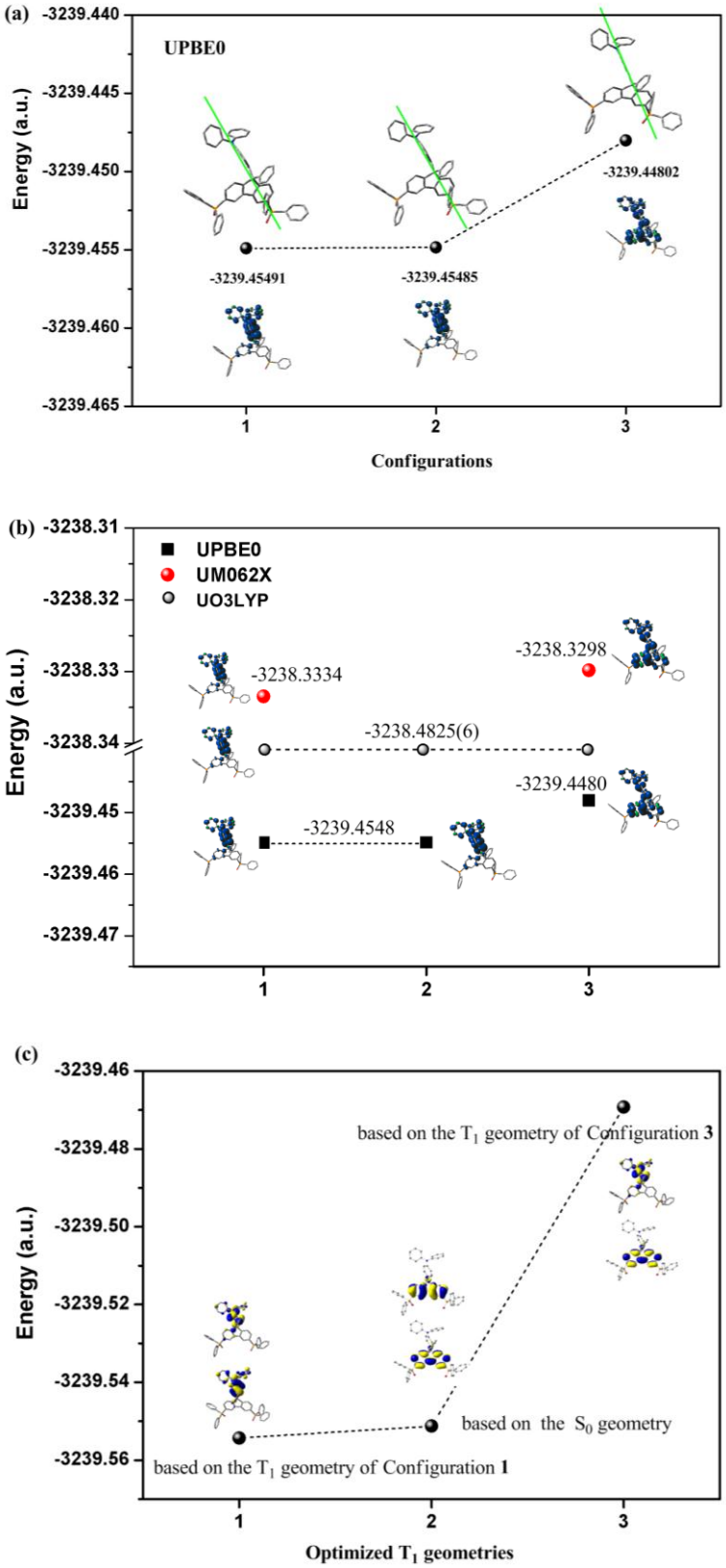

Fig. S10. a) The obtained three T_1 geometries (configurations **1-3**) without imaginary frequency from different initial configurations by optimized calculation using spin-unrestricted PBE0 functional (UPBE0), the corresponding spin density distribution and triplet energies at three T_1 geometries. b) The obtained T_1 geometries without imaginary frequency from different initial configurations by optimized calculation using spin-unrestricted PBE0, O3LYP, and M062X functionals, the

corresponding spin density distribution and triplet energies at the T_1 geometries. c) The energies of three optimized T_1 geometries by TD-PBE0 calculation from configurations **1, 3 (Fig. S10a)** and S_0 geometry (PBE0), respectively. And, hole-electron pairs of T_1 transition orbitals based on the three optimized T_1 geometries.

Table S1 The absorption spectra calculated by TDDFT with 6-31+G** for *p*POAPF and *p*PODPF in benzene solution, together with the available experimental values.

Compounds	Cal.					Exp.
	TDDFT	State (f_{max})	λ(nm)	Config. (CI coeff.)	Assignment	λ(nm)
*p*POAPF	B3LYP	$S_0 \rightarrow S_9$ (0.65)	308	H-1 → L (91%)	$\pi \rightarrow \pi^*$	294[1]
	TPSSh	$S_0 \rightarrow S_{12}$ (0.21)	318	H → L +8 (97%)	$\pi \rightarrow \pi^*$	–
	PBE0	$S_0 \rightarrow S_7$ (0.68)	299	H-1 → L (90%)	$\pi \rightarrow \pi^*$	–
*p*PODPF	B3LYP	$S_0 \rightarrow S_1$ (0.65)	310	H → L (92%)	$\pi \rightarrow \pi^*$	295[1]
	TPSSh	$S_0 \rightarrow S_1$ (0.51)	318	H → L (87%)	$\pi \rightarrow \pi^*$	–
	PBE0	$S_0 \rightarrow S_1$ (0.72)	302	H → L(94%)	$\pi \rightarrow \pi^*$	–

References

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