Electronic Supplementary Information (ESI)

Phenothiazine based blue emitter for light-emitting electrochemical cells

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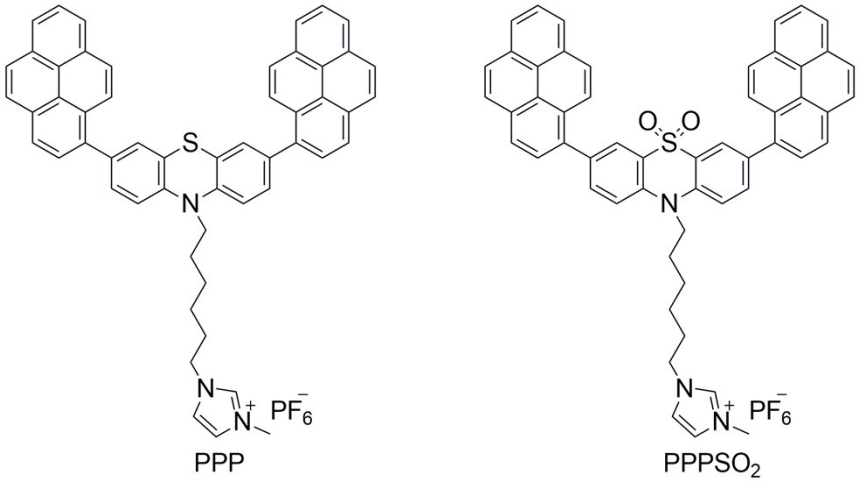

Fig. S1 Structures of PPP and PPPSO2.

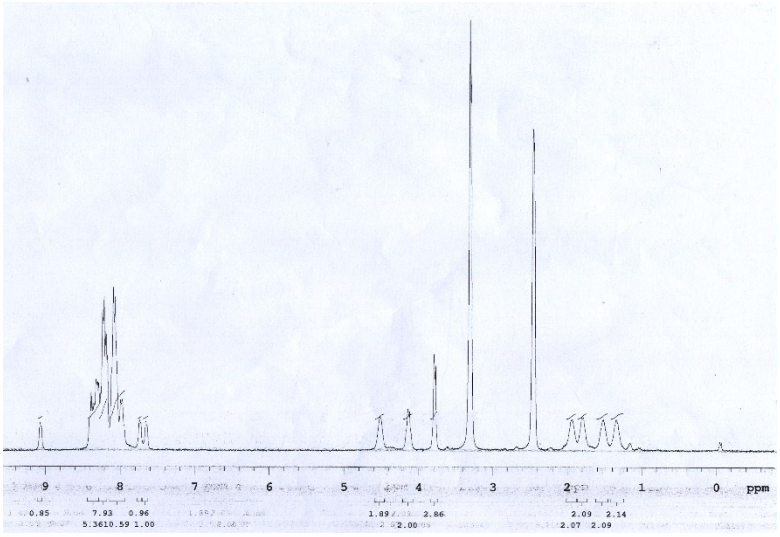

Fig. S2 ^{1}H-NMR spectrum of PPPSO2.

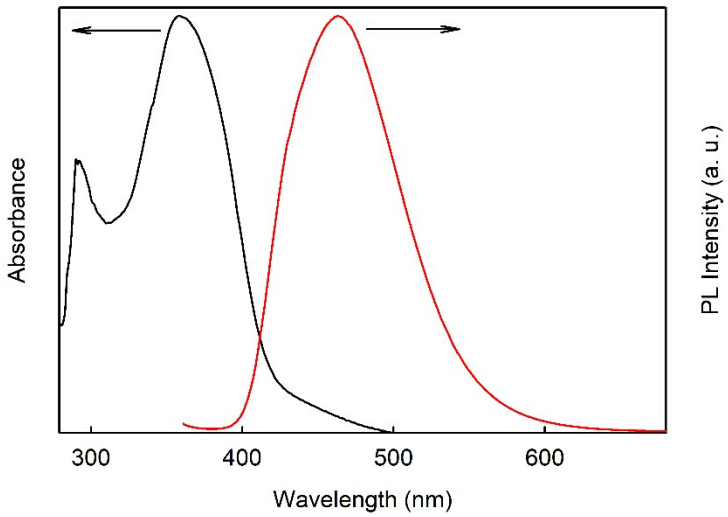

Fig. S3 Thin film absorption and emission spectrum of PPPSO2.

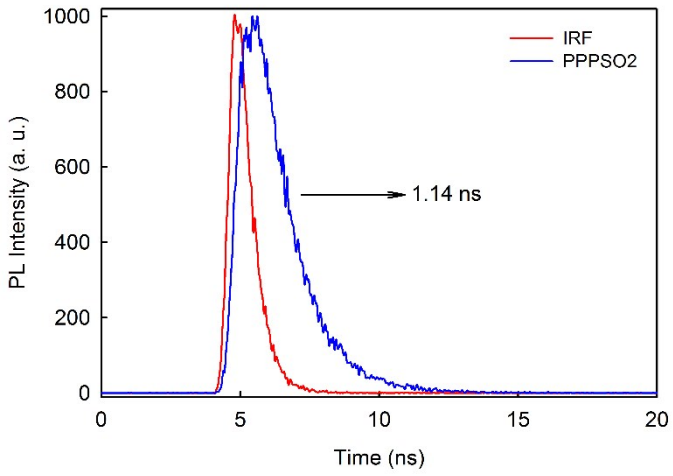

Fig. S4 Transient PL spectra of PPPSO2 in oxygen-free toluene solution.

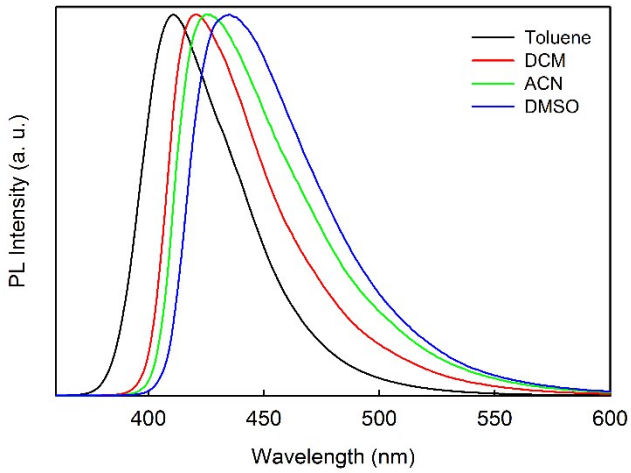

Fig. S5 Emission spectra of PPPSO2 in different solvents.

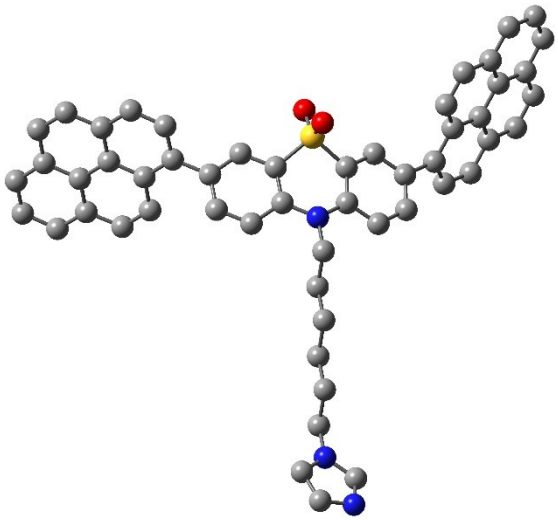

Fig. S6 The DFT optimized ground state geometry of the compound PPPSO2.

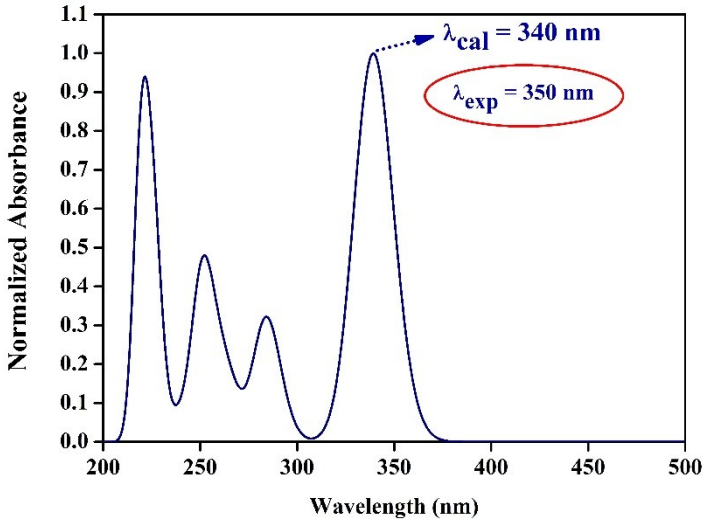

Fig. S7 The UV-visible absorption spectrum of PPPSO2 simulated in dichloromethane.

Table S1. The results of TDDFT calculations.

Transition	λ_{cal} (nm)	*f*	CI Coefficient	Dominant Contribution (%)
$S_0 \rightarrow S_1$	340	1.7652	0.5009	HOMO → LUMO (50)
$S_0 \rightarrow S_2$	331	0.2400	0.4882	HOMO-1 → LUMO (48)
$S_0 \rightarrow S_3$	315	0.0004	0.3070	HOMO-3 → LUMO+1 (19)
$S_0 \rightarrow S_4$	314	0.0006	0.2679	HOMO-5 → LUMO (14)
$S_0 \rightarrow S_5$	289	0.0837	0.4932	HOMO → LUMO+2 (49)

Calculated absorption wavelengths (λ_{cal}), oscillator strengths (***f***), and coefficient of configuration interaction (CI) with the dominant contribution obtained at TD-CAM-B3LYP/6-31G(d) level.