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Electronic Supplementary Information

Phenylcarbazole and Phosphine Oxide/Sulfide Hybrids as Host Materials for Blue Phosphors: Effectively Tuning the Charge Injection Property without Influencing the Triplet Energy

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Figures and tables

Fig. S1 The bond lengths of PhCBZ. The deviations in bond lengths and torsional angle ω of PO-PhCBZs from the unsubstituted PhCBZ in the ground state (S_0) and the lowest triplet state (T_1). The torsional angle ω is defined as an angle between the mean plane of carbazole moiety and the phenyl moiety (see front and side view).

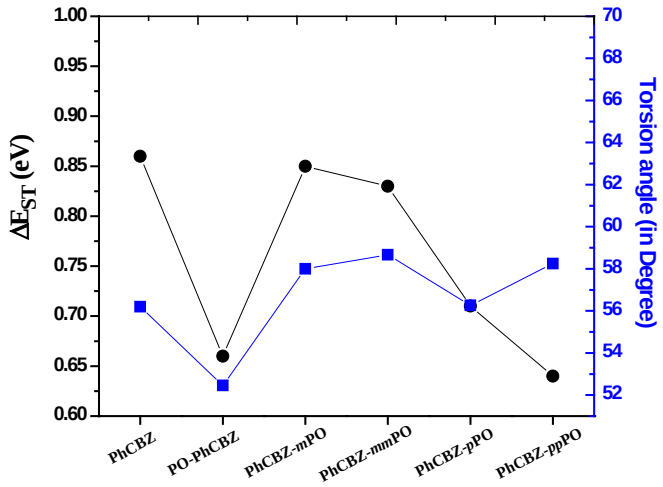


Fig. S2 Evolutions of ΔE_{ST} with respect to torsion angles ω in representative systems.

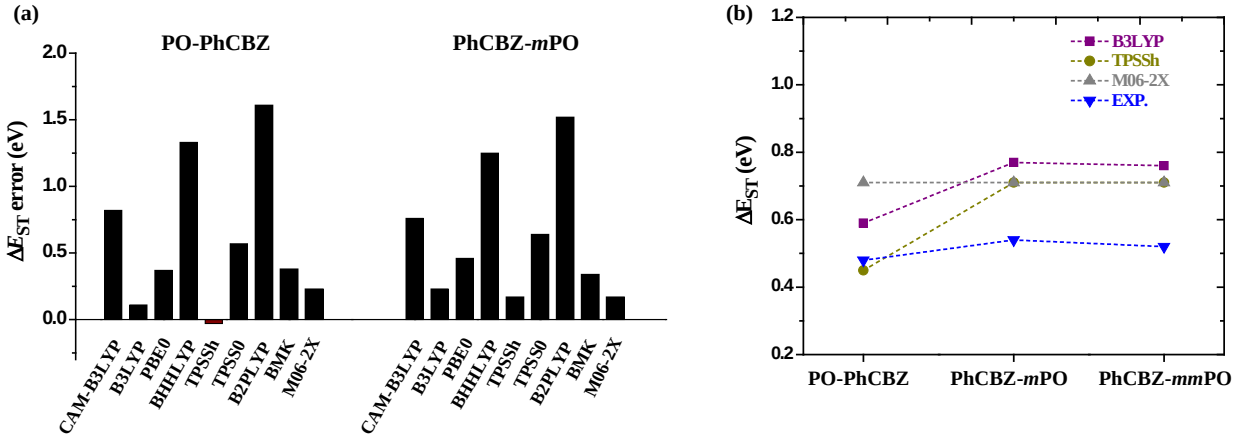


Fig. S3 (a) Evolutions of the ΔE_{ST} errors in PO-PhCBZ and PhCBZ-*m*PO for nine different functionals studied; the wine color represents the underestimated value **(b)** Evolutions of ΔE_{ST} in PO-PhCBZ, PhCBZ-*m*PO, and PhCBZ-*mm*PO for four three functionals and the experiment values.

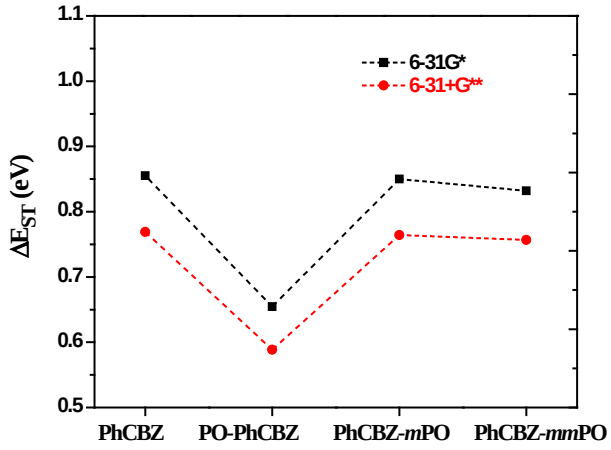


Fig. S4 Evolution of ΔE_{ST} in four systems for B3LYP functional with 6-31G* and 6-31+G** basis sets.

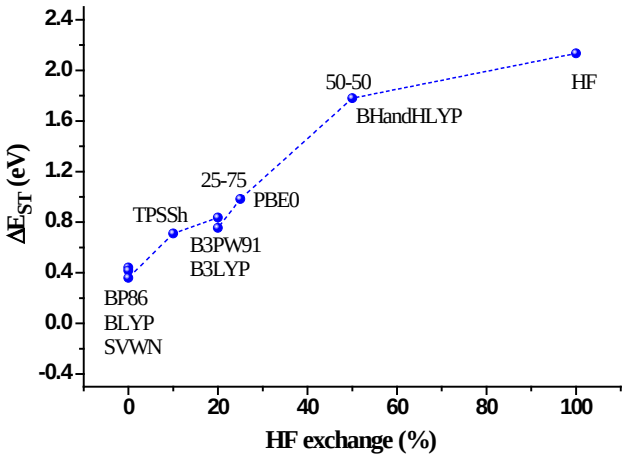


Fig. S5 Evolution of ΔE_{ST} for PhCBZ calculated using different density functionals.

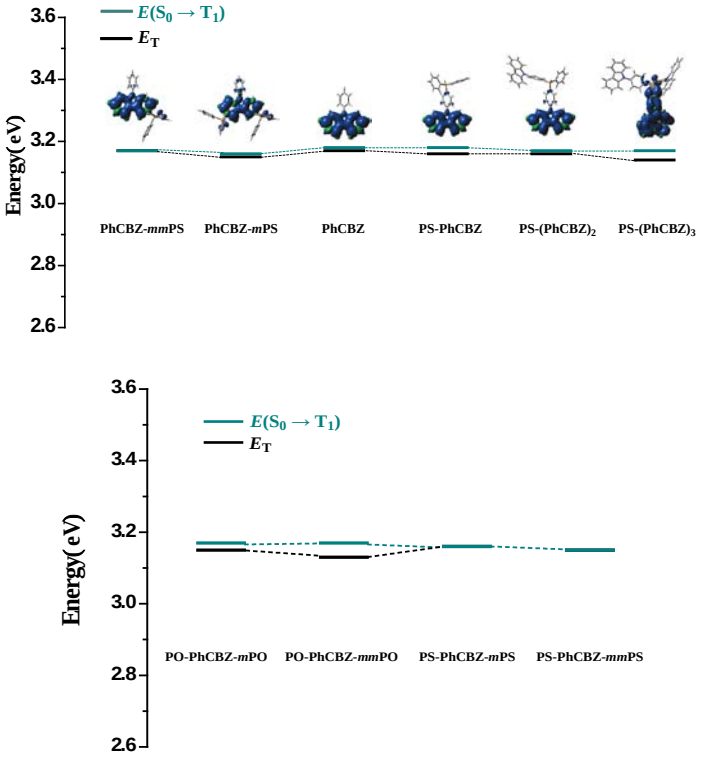


Fig. S6 Spin density (SD) distribution, adiabatic triplet energies (E_T: the energy difference between T_1 and S_0 states) and vertical triplet energies ($E(S_0 \rightarrow T_1)$: vertical excitation energy from S_0 to T_1) for PO(S)-PhCBZs.

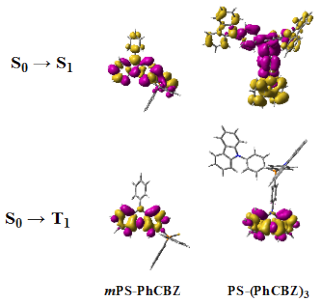
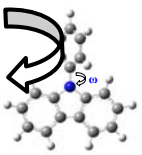


Fig. S7 Change of electron density distribution upon the $S_0 \rightarrow S_1$ and $S_0 \rightarrow T_1$ electronic transition. Yellow and violet colors correspond to a decrease and increase of electron density, respectively.

Table S1 Torsional angles (ω) of optimized geometries in the ground and triplet states

Compounds		PhCBZ	PhCBZ-*m*PO	PhCBZ-*p*PO	PhCBZ-*mm*PO	PhCBZ-*pp*PO	PO-PhCBZ
ω	S_0	56.2	58.00	56.26	58.67	58.25	52.46
	T_1	53.6	55.70	53.25	56.23	54.07	49.34



The torsional angle ω is defined as an angle between the mean plane of carbazole moiety and the phenyl moiety (see front and side view).

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Table S2 Calculated HOMO and LUMO energies, HOMO-LUMO energy gaps *E*(H-L), vertical excitation energies, and triplet energies (energy unit in eV) of PO(S)-PhCBZs

Compounds	HOMO	LUMO	*E*(H-L)	$E(S_0 \rightarrow S_1)$	$E(S_0 \rightarrow T_1)$	ΔE_{ST}	$E_{T(Cal.)}$	$E_{T(Exp.)}$
PO-PhCBZ-*m*PO	-5.68	-1.15	4.53	3.91	3.17	0.74	3.15	3.01
PO-PhCBZ-*mm*PO	-5.82	-1.24	4.58	3.96	3.17	0.79	3.13	3.07
PO-PhCBZ-*p*PO	-5.62	-1.16	4.46	3.83	3.11	0.75	3.07	
PO-PhCBZ-*pp*PO	-5.73	-1.43	4.30	3.72	3.06	0.66	2.98	
PhCBZ-*m*PS	-5.55	-0.98	4.57	3.94	3.17	0.77	3.17	
PhCBZ-*mm*PS	-5.62	-1.18	4.43	3.85	3.16	0.69	3.15	
PS-PhCBZ-*m*PS	-5.64	-1.26	4.38	3.85	3.16	0.69	3.16	
PS-PhCBZ-*mm*PS	-5.65	-1.39	4.26	3.81	3.15	0.66	3.15	
PhCBZ-*p*PS	-5.51	-1.14	4.37	3.77	3.10	0.67	2.97	
PhCBZ-*pp*PS	-5.66	-1.50	4.16	3.61	2.98	0.63	2.85	
PS-PhCBZ-*pp*PS	-5.70	-1.59	4.11	3.56	2.99	0.57	2.86	
PS-PhCBZ	-5.49	-1.11	4.38	3.78	3.18	0.60	3.16	
$PS-(PhCBZ)_2$	-5.52	-1.23	4.29	3.70	3.17	0.52	3.16	
$PS-(PhCBZ)_3$	-5.55	-1.30	4.25	3.67	3.17	0.50	3.14	

Table S3 Main transition type and the vertical excitation energy of lowest singlet and triplet states, and other triplet state possessing the same electronic transition with the S_1 based on S_0-state geometry (energy unit in eV)

Compounds	S_1	T_n	Main Transition type	T_1	Main Transition type
PhCBZ	4.04	$T_2 = 3.35$	HOMO → LUMO	3.18	HOMO–1 → LUMO
PhCBZ-*m*PS	3.94	$T_2 = 3.36$	HOMO → LUMO	3.17	HOMO–3 → LUMO
PhCBZ-*mm*PS	3.85	$T_2 = 3.39$	HOMO → LUMO	3.16	HOMO–5 → LUMO
PS-PhCBZ	3.78	$T_2 = 3.25$	HOMO → LUMO	3.18	HOMO–1 → LUMO+2
$PS-(PhCBZ)_2$	3.70	$T_3 = 3.23$	HOMO → LUMO	3.17	HOMO–2 → LUMO+4
$PS-(PhCBZ)_3$	3.67	$T_3 = 3.21$	HOMO → LUMO	3.17	HOMO–3 → LUMO+6