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Electronic Supplementary Information

### **Bipolar Host Materials for High Efficiency Phosphorescent Organic Light Emitting Diodes: Tuning the HOMO/LUMO Levels without Reducing the Triplet Energy in Linear System**

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### CONTENT

- Optimized geometry and simulated of the HOMO/LUMO levels of S<sub>0</sub> and T<sub>1</sub> state for BCz derivatives (Firgure S1 and Table S1)
- TGA thermograms of BCz derivatives (Firgure S2)
- Energy level diagrams for devices (Firgure S3)
- Power efficiency versus luminescence of devices BA-BC (Firgure S4)
- Power efficiency versus luminescence of devices WA and WB (Firgure S5)
- $\blacksquare$  <sup>1</sup>H, <sup>13</sup>C NMR and MS spectra of all compounds

3D structure	Based on the $\mathbf{S}_{0}$ state		Based on the T <sub>1</sub> state	
	номо	LUMO	номо	LUMO
BCzPh	Speries.	Ants.	Smit	1000
BCzSCN	Morris	i st	State.	
100 A	apres .		Speit	
BCzSPO				

**Firgure S1.** Optimized geometry and spatial distributions of the HOMO and LUMO levels for BCz derivatives.

**Table S1.** Simulated HOMO/LUMO energies of  $S_0$  and  $T_1$  state for BCz derivatives.

Compound	HOMO (eV)	LUMO (eV)	$E_{\rm T}({ m eV})$
BCzPh	4.96	0.67	3.02
BCzSCN	5.21	1.12	3.04
BCzSPO	5.11	0.92	3.02



Figure S2. TGA thermograms of BCz derivatives.



Figure S2. Energy levels of the materials employed in the devices.



Figure S3. Power efficiency versus luminescence curves of devices BA-BC.



Figure S4. Power efficiency versus luminescence curves of devices WA and WB.



400 MHz <sup>1</sup>H NMR spectrum of BCzPh in CDCl<sub>3</sub>









100 MHz <sup>13</sup>C NMR spectrum of BCzPh-Br in CDCl<sub>3</sub>



400 MHz <sup>1</sup>H NMR spectrum of BCzSCN in CDCl<sub>3</sub>



100 MHz  $^{13}\text{C}$  NMR spectrum of BCzSCN in CDCl\_3



<sup>400</sup> MHz <sup>1</sup>H NMR spectrum of BCzSPO in CDCl3



100 MHz <sup>13</sup>C NMR spectrum of BCzSPO in CDCl3

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MS spectrum of BCzPh

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MS spectrum of BCzPh-Br

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MS spectrum of BCzSCN

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MS spectrum of BCzSPO