

***Electronic Supplementary Information for***

Novel carbazole derivatives with *ortho*-linkage strategy for efficient phosphorescent organic light-emitting diodes

Xiang-Yang Liu,<sup>†a</sup> Hui-Ting Ge,<sup>†a</sup> Yue Zhao,<sup>b</sup> Danli Zhao,<sup>a</sup> Jian Fan,<sup>\*,a</sup>, and Liang-Sheng Liao,<sup>\*,a</sup>

<sup>a</sup>*Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM) & Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou 215123, P.R. China.*

<sup>b</sup>*Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing National Laboratory of Microstructures, Nanjing University, Nanjing 210023, China.*

\*E-mail: jianfan@suda.edu.cn; lsliao@suda.edu.cn

†The two authors contribute equally to this paper.

**Fig. S1** The dihedral angles between central benzene and donor/acceptor group.

**Fig. S2** PL spectra of CNPhCz and DCNPhCz in different solvents.

**Fig. S3** Transient photoluminescence (PL) decay curves of CNPhCz and DCNPhCz in toluene (black) and oxygen-free toluene (red) solutions at room temperature.

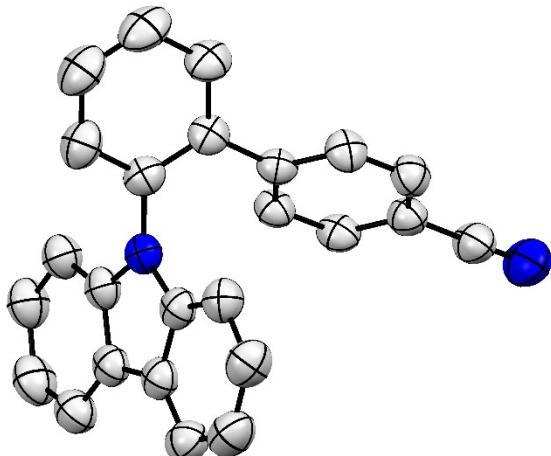
**Fig. S4** Blue and green device structures and representative energy level diagram and structure of the materials.

**Fig. S5**  $^1\text{H}$  NMR spectrum of CNPhCz ( $\text{CDCl}_3$ ).

**Fig. S6**  $^{13}\text{C}$  NMR spectrum of CNPhCz ( $\text{CDCl}_3$ ).

**Fig. S7**  $^1\text{H}$  NMR spectrum of DCNPhCz ( $\text{CDCl}_3$ ).

**Fig. S8**  $^{13}\text{C}$  NMR spectrum of DCNPhCz ( $\text{CDCl}_3$ ).



**Phase data**

<b>Formula sum</b>	C25 H16 N2
<b>Formula weight</b>	344.4 g/mol
<b>Crystal system</b>	monoclinic
<b>Space-group</b>	P 1 21/n 1 (14)
<b>Cell parameters</b>	a=11.544(4) Å b=11.822(4) Å c=16.267(5) Å β=107.419(5)°
<b>Cell ratio</b>	a/b=0.9765 b/c=0.7267 c/a=1.4091
<b>Cell volume</b>	2118.2(12) Å <sup>3</sup>
<b>Z</b>	4
<b>Calc. density</b>	1.07989 g/cm <sup>3</sup>
<b>RAll</b>	0.0874
<b>Pearson code</b>	mP172
<b>Formula type</b>	N2O16P25
<b>Wyckoff sequence</b>	e43

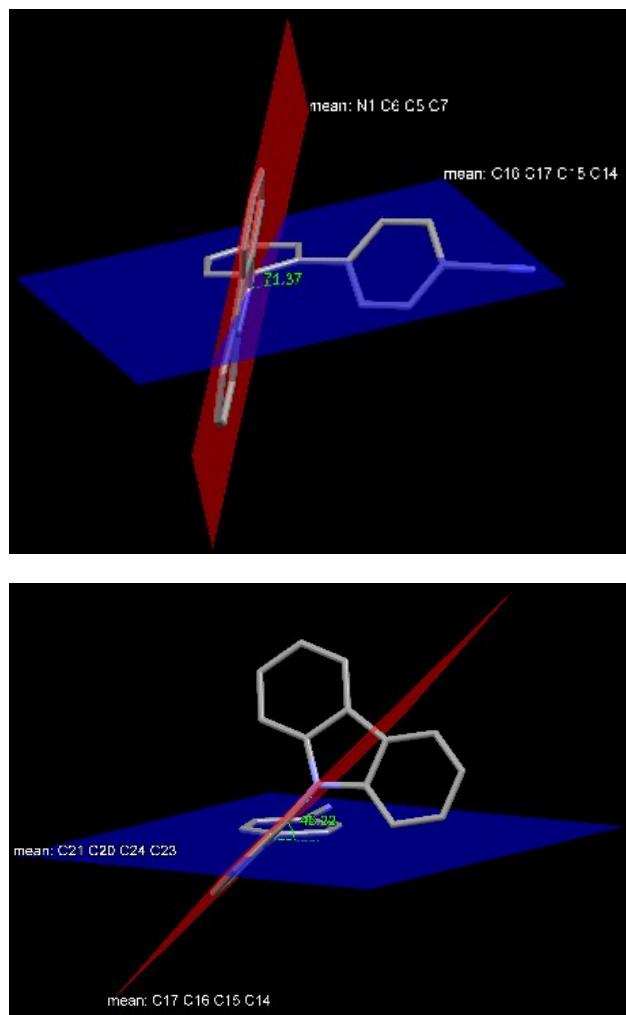


Fig. S1 The dihedral angles between central benzene and donor/acceptor group.

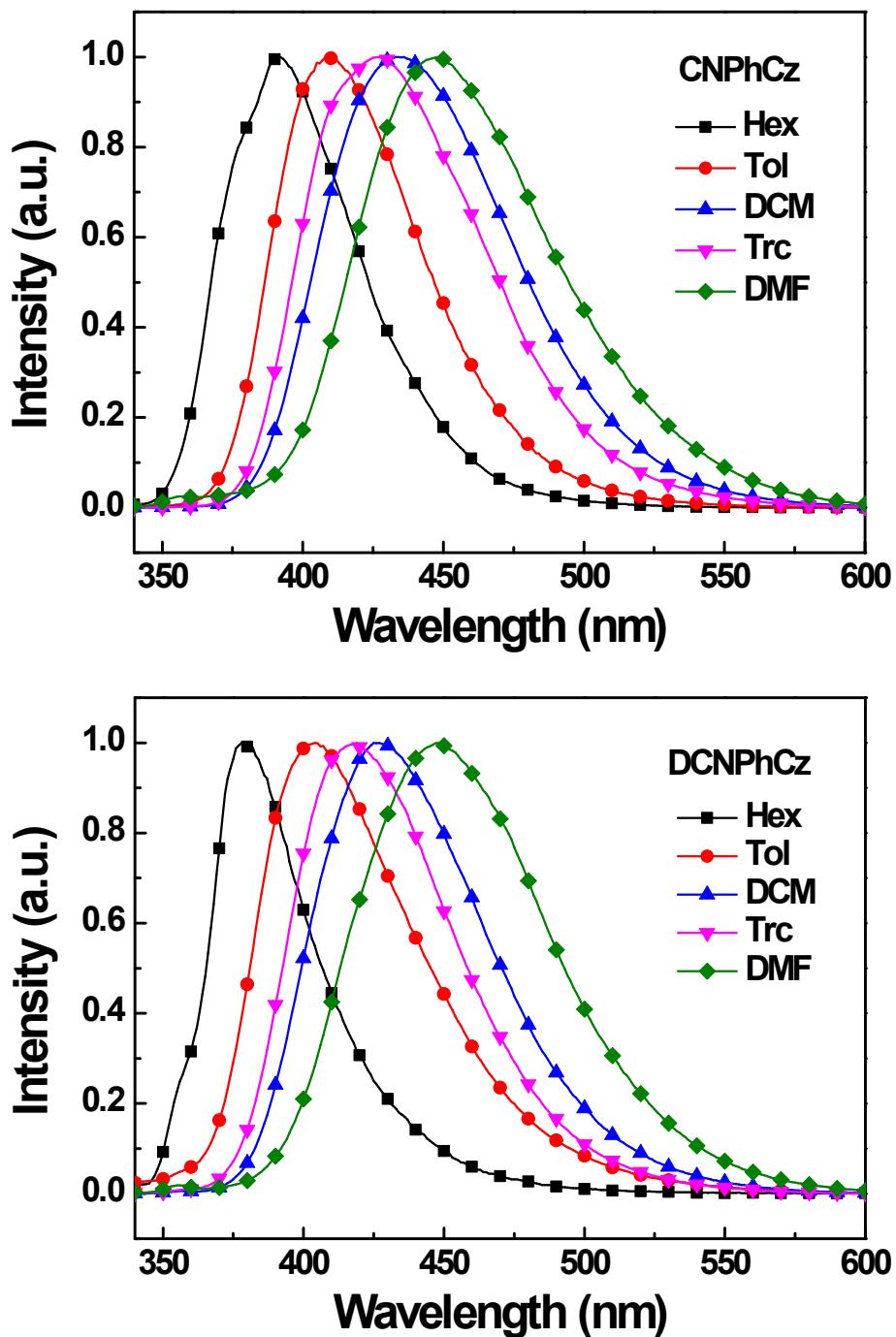


Fig. S2 PL spectra of CNPhCz and DCNPhCz in different solvents.

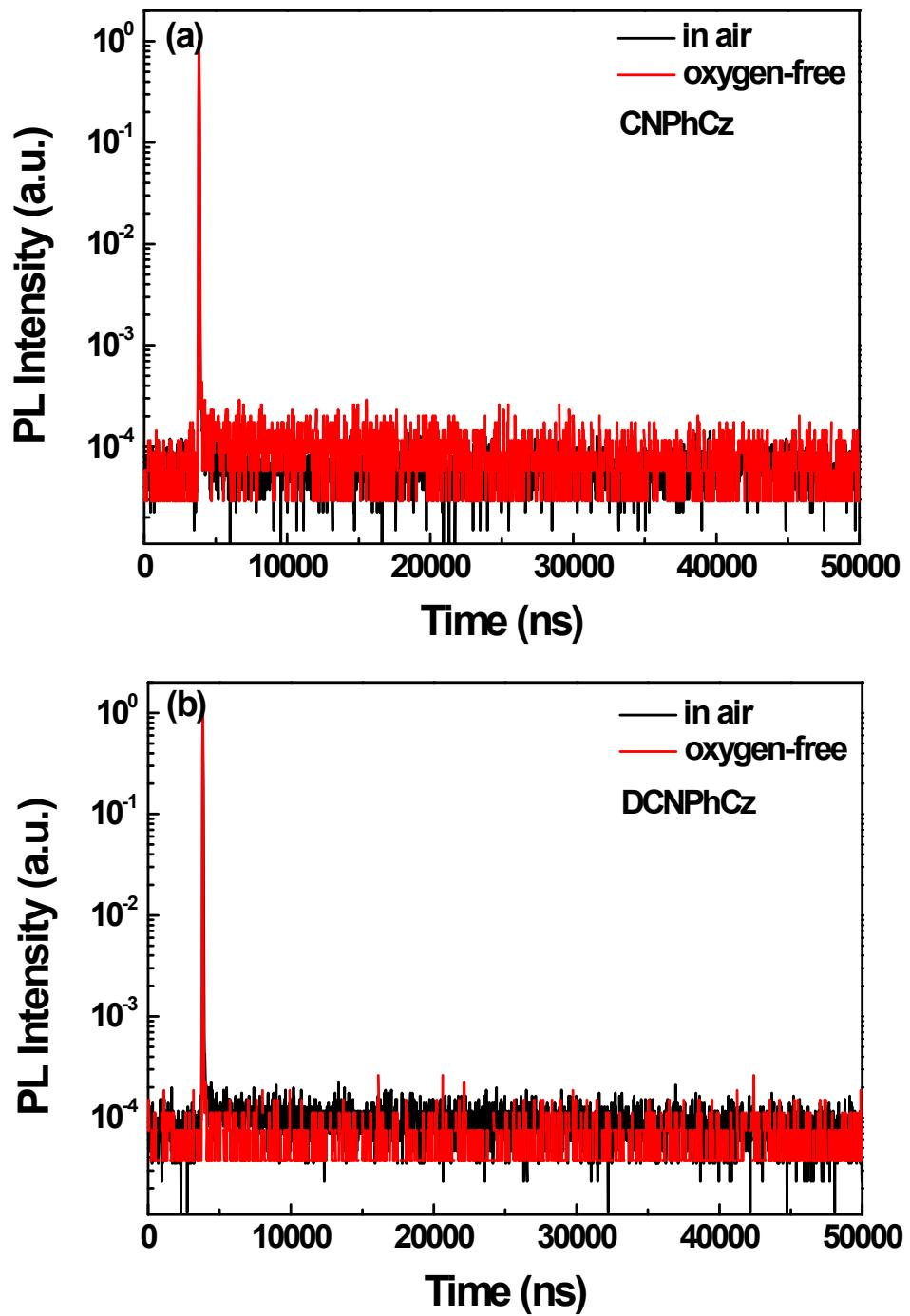


Fig. S3 Transient photoluminescence (PL) decay curves of CNPhCz and DCNPhCz in toluene (black) and oxygen-free toluene (red) solutions at room temperature.

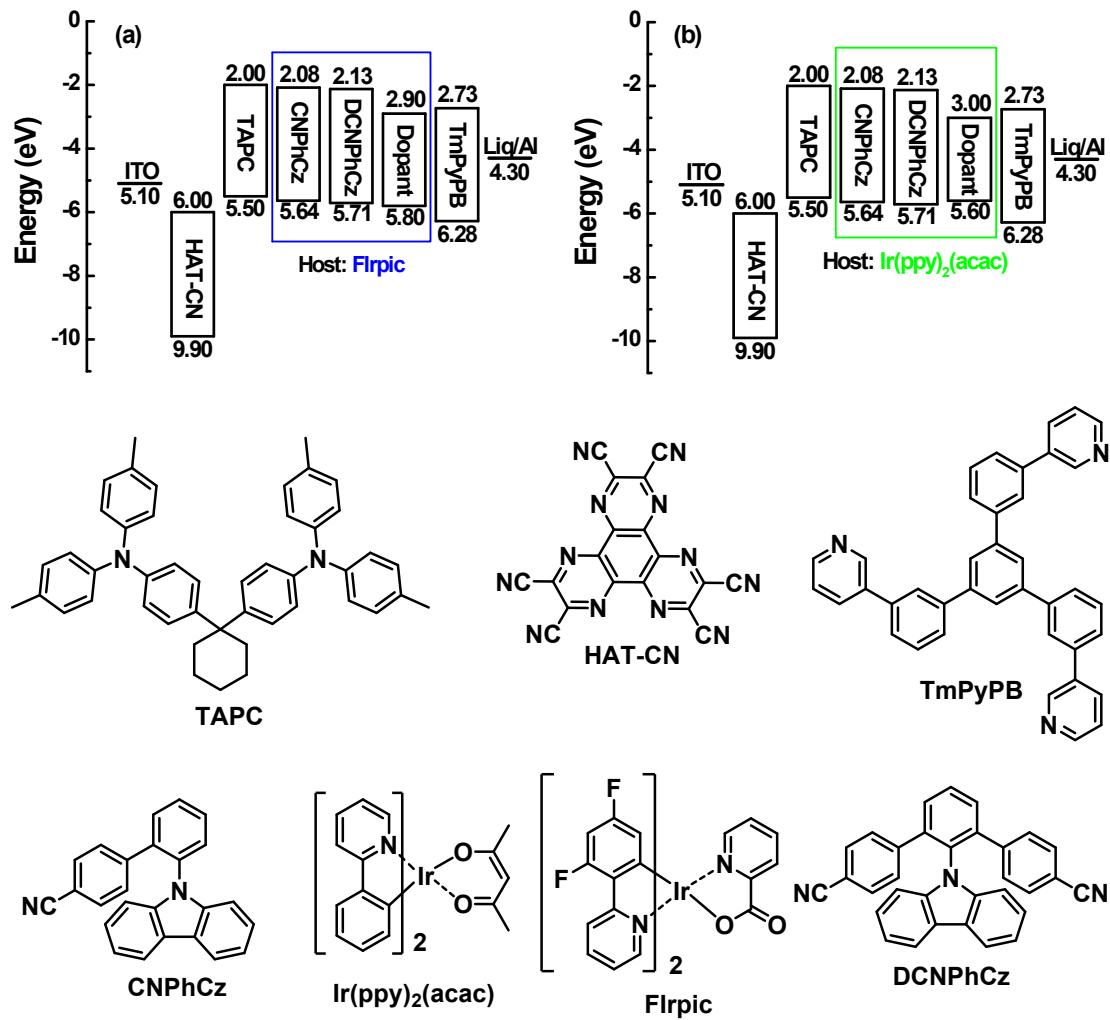


Fig. S4 Blue and green device structures and representative energy level diagram and structure of the materials.

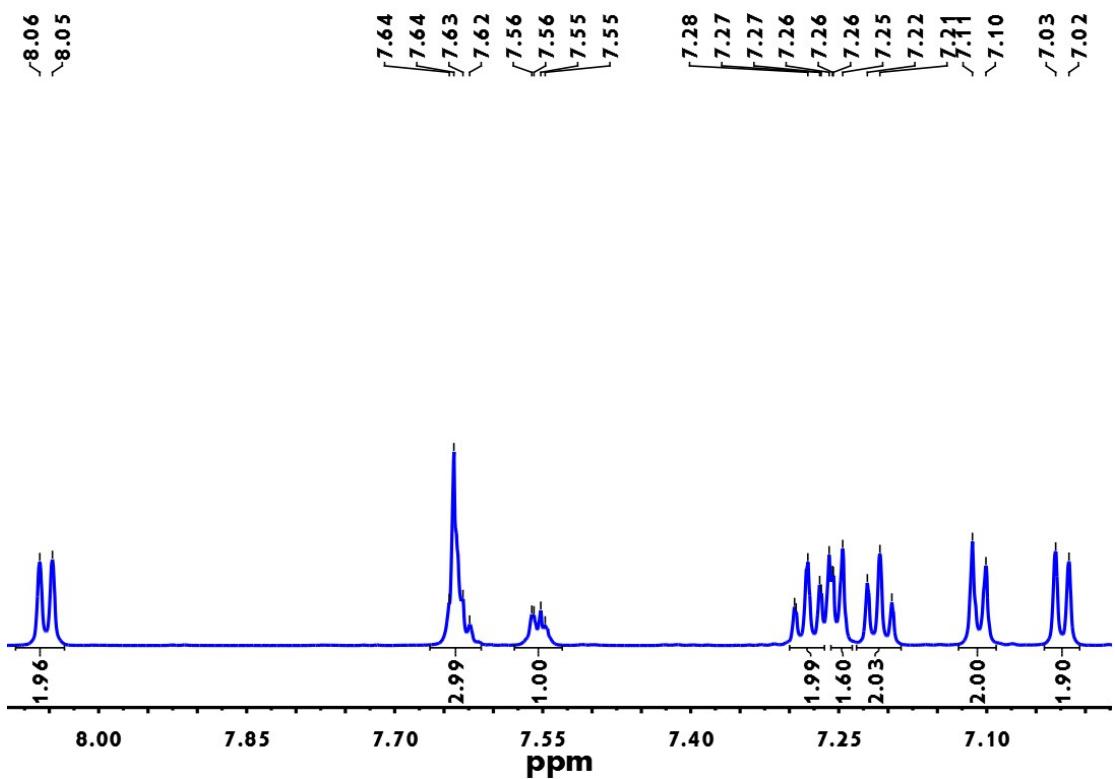


Fig. S5  $^1\text{H}$  NMR spectrum of CNPhCz ( $\text{CDCl}_3$ ).

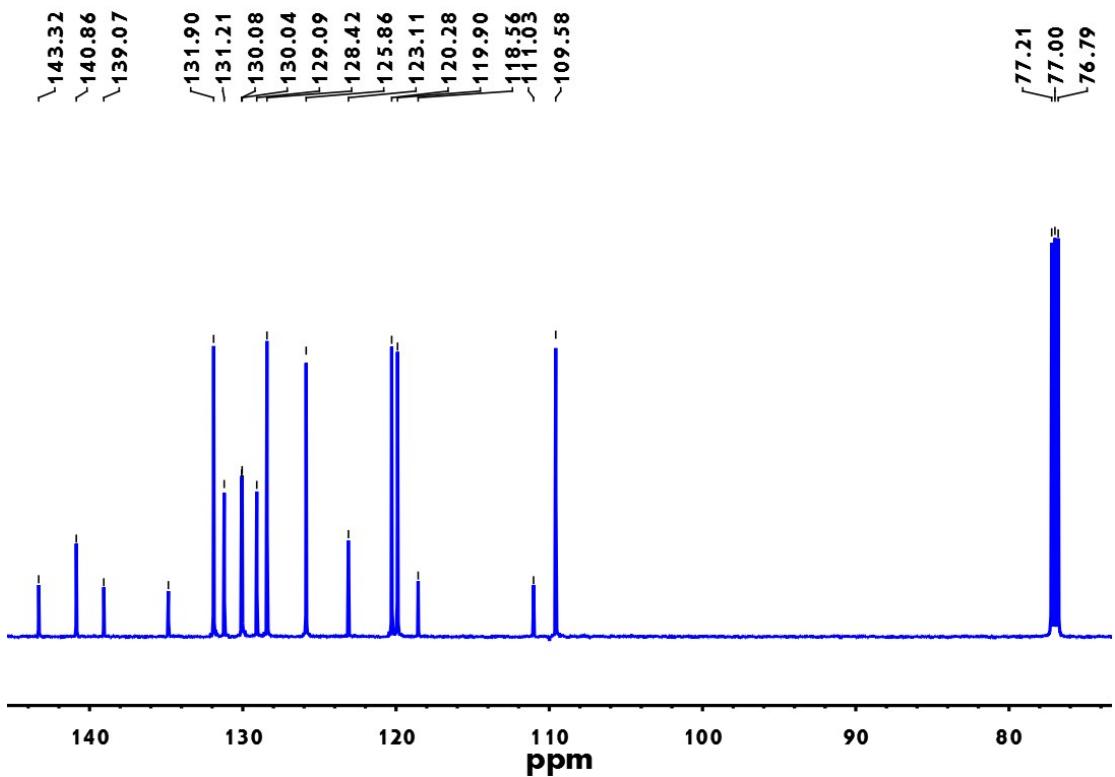


Fig. S6  $^{13}\text{C}$  NMR spectrum of CNPhCz ( $\text{CDCl}_3$ ).

