Supporting information for

# Rational Design of Carbazolyl and Aryl Phosphine Oxide (APO) Based Ambipolar Host Materials for Blue Electrophosphorescence: A Density Functional Theory Study

Dongmei Zhang, Wei Shen, Xiaguang zhang, Huili Sun, Rongxing He, Ming Li*

School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, P. R. China

* Corresponding author:

E-mail: liming@swu.edu.cn; Phone: +86-023-68253023

**Table S1.** The calculated HOMO and LUMO energies (in eV) of DPESPOPhCz (host 2) via directly measuring HOMO/LUMO eigenvalues from the optimized $S_0$ results at the different levels.

| | B3LYP /6-31G* | PBE0 /6-31G* | CAM-B3LYP /6-31G* | B3P86 /6-31G* | B3P86 /6-311G* | exp |
|---|---|---|---|---|---|---|
| HOMO | -5.43 | -5.67 | -6.67 | -6.09 | -6.28 | -6.16 |
| LUMO | -1.24 | -1.12 | 0.12 | -1.88 | -2.05 | -2.49 |

**Table S2.** Calculated absorption spectra of DPESPOPhCz (host 2) by various functionals

| | B3LYP /6-31G* | PBE0 /6-31G* | CAM-B3LYP /6-31G* | B3P86 /6-31G* | B3P86 /6-311G* | exp |
|---|---|---|---|---|---|---|
| λ(nm) | 338 | 323 | 282 | 336 | 335 | 331 |

**Table S3.** Calculated transition natures of the $S_1$ states of studied host molecules based on the $S_0$ geometry by TD-DFT calculations

| Molecule | $E(S_0 \rightarrow S_1)$（eV） | λ(nm) | Transition nature |
|---|---|---|---|
| 1 | 4.05 | 306 | H→ L+1 (93%) |
| 2 | 3.69 | 336 | H→ L (98%) |
| 3 | 3.61 | 343 | H→ L (97%) |
| 4 | 3.71 | 334 | H→ L (84%) |
| 5 | 3.63 | 342 | H→ L (93%) |
| 6 | 3.69 | 336 | H→ L (94%) |
| 7 | 3.60 | 344 | H→ L (94%) |
| 8 | 3.44 | 361 | H→L (93%) |
| 9 | 3.48 | 356 | H→ L (84%) |
| 10 | 3.56 | 348 | H→ L (88%) |

H = HOMO, L = LUMO

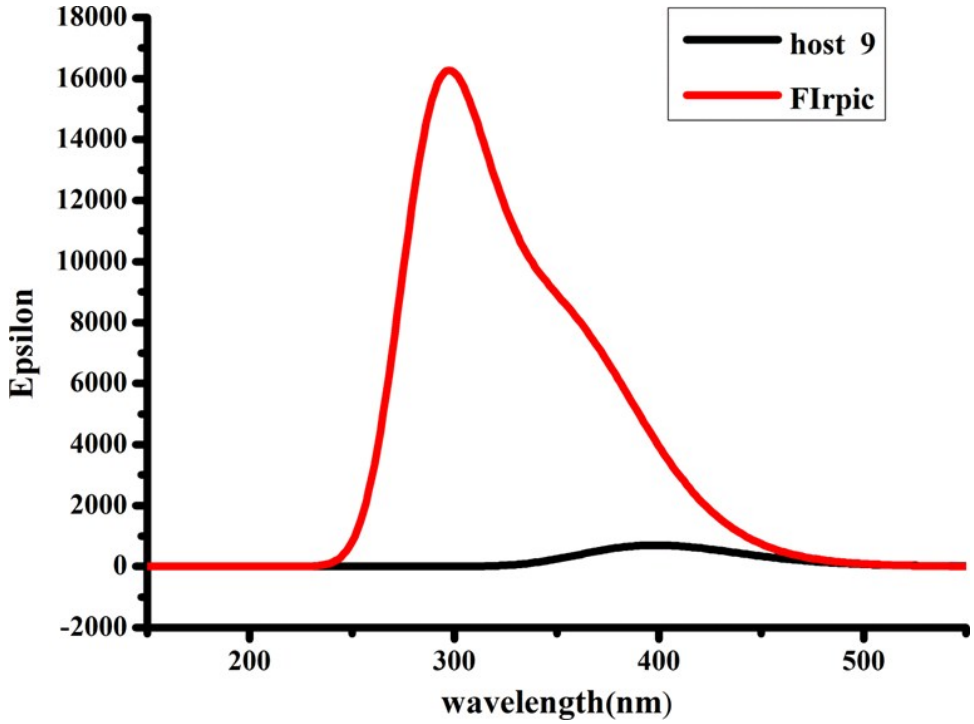


**Figure S1.** Emitter's (FIrpic) absorption spectra and host's emission spectra