Electronic Supplementary Information

Extremely Condensing Triplet States of DPEPO-Type Hosts through Constitutional Isomerization for High-Efficiency Deep-Blue Thermally Activated Delayed Fluorescence Diodes

Jing Zhang,[‡] Dongxue Ding,[‡] Ying Wei,* *Hui Xu**

Key Laboratory of Functional Inorganic Material Chemistry (Ministry of Education) & School of Chemistry and Materials, Heilongjiang University, 74 Xuefu Road, Harbin 150080, P. R. China

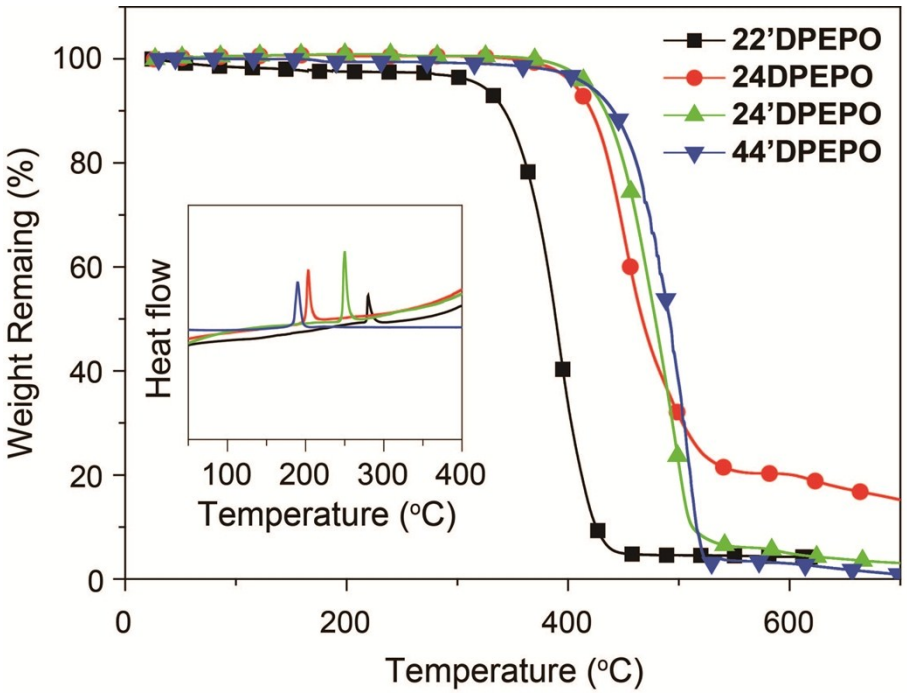

Figure S1. TGA and DSC curves of ***m*DPEPO**.

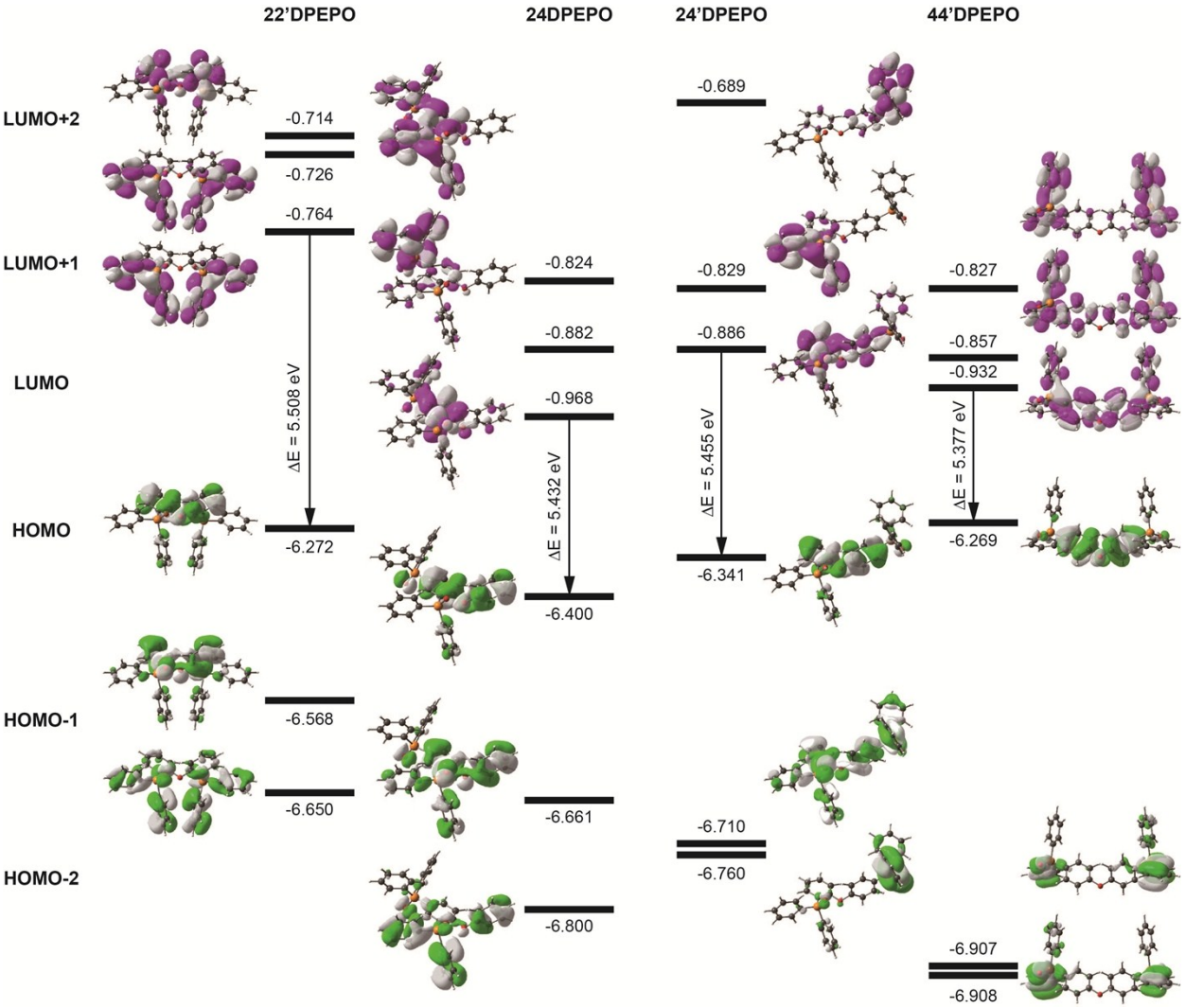

Figure S2. Energy levels and contours of FMOs of ***m*DPEPO**.

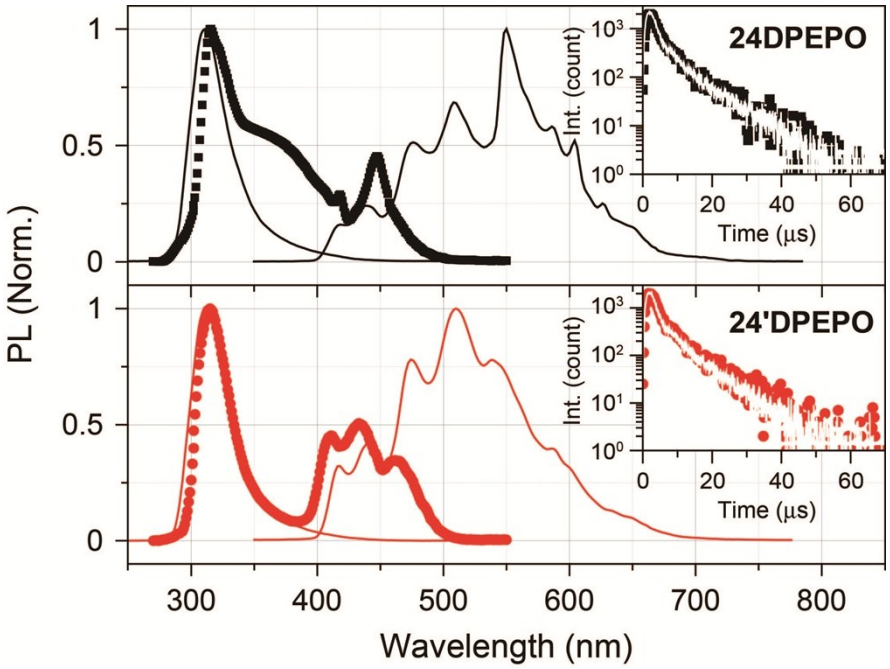

Figure S3. FL and PH in solution (line) and solid state emissions (symbol) of **24DPEPO** and **24'DPEPO**. Insets show the time decay curves of the 0-0 transitions from PH parts in solid state emissions (symbol) and PH spectra in solution (white line).

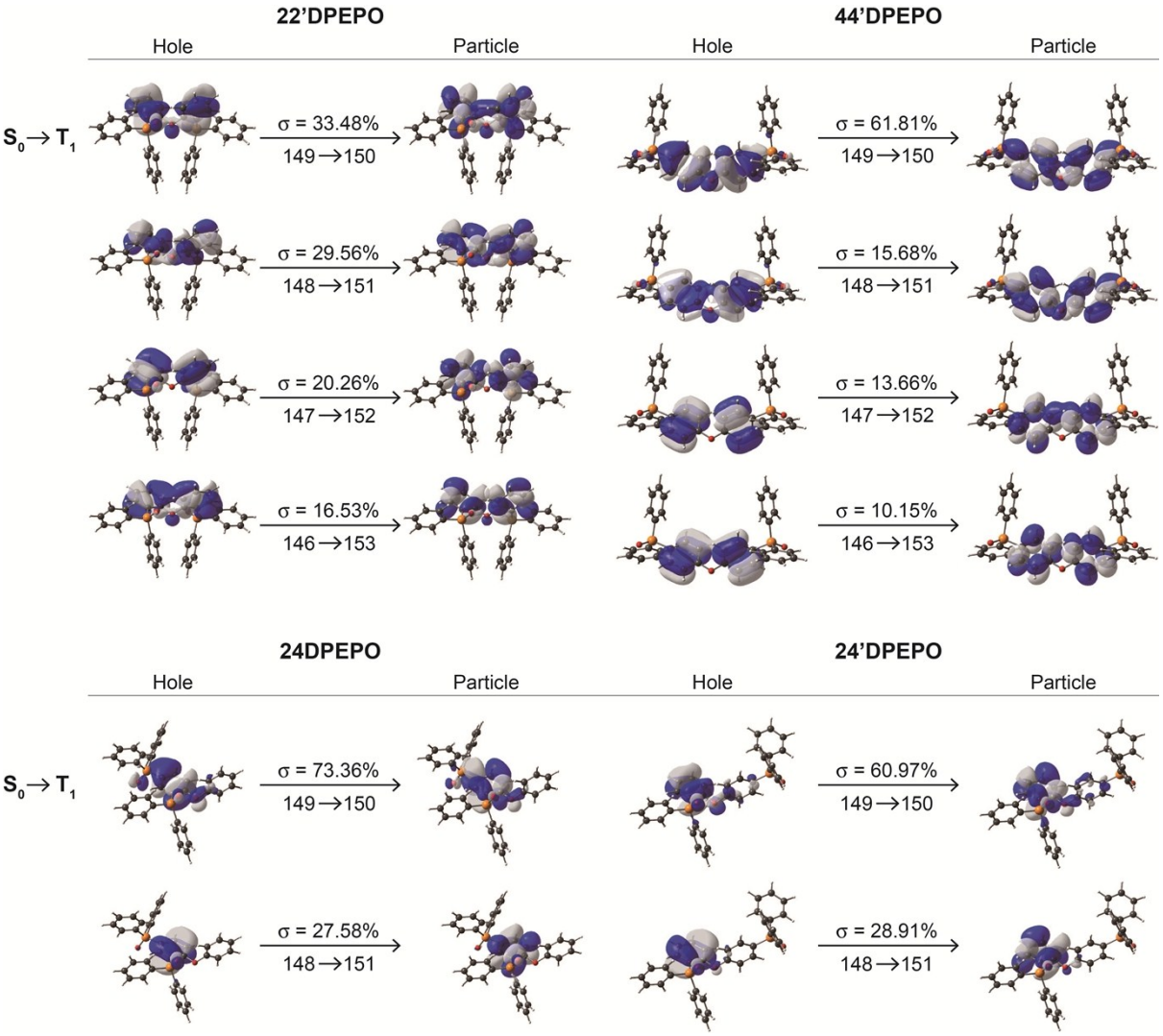

Figure S4. Major Natural transition orbitals (NTO) of $S_0 \rightarrow T_1$ states for ***m*DPEPO**. σ refers to the associated weight.

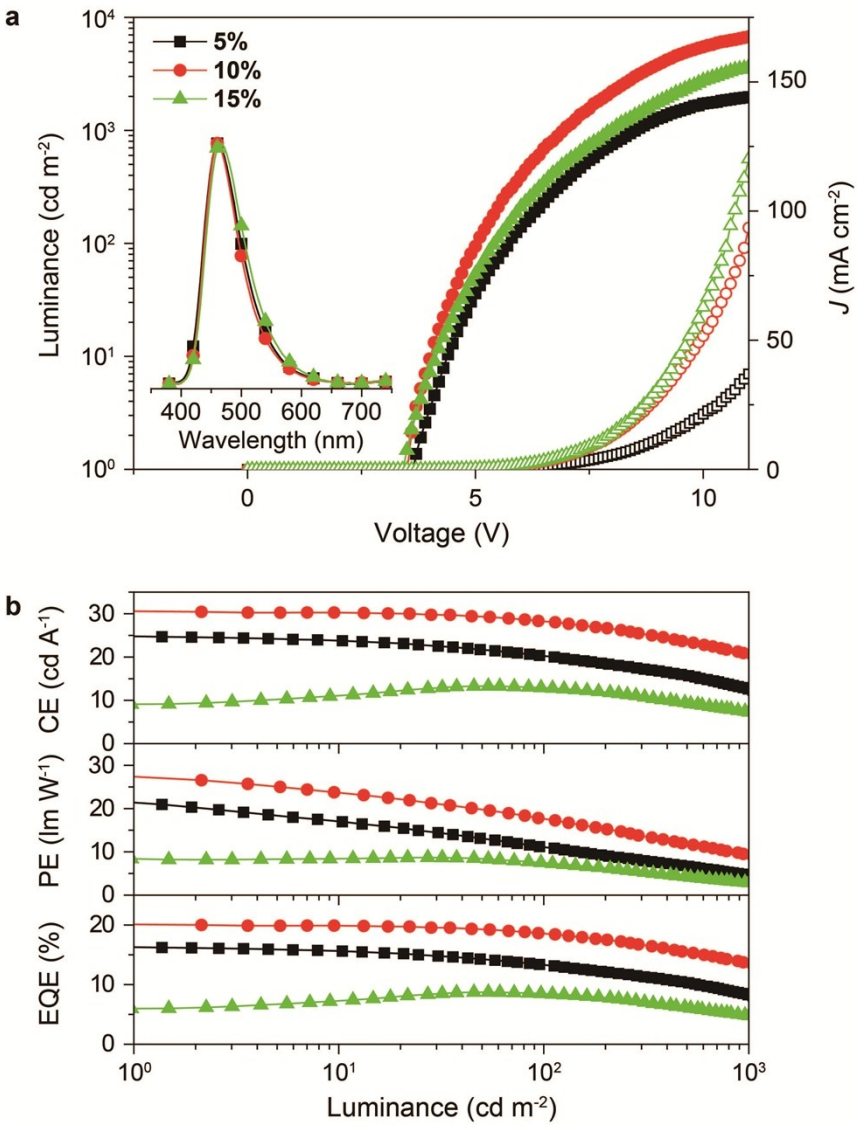

Figure S5. (a) Luminance-*J*-Voltage curves and EL spectra (inset) of **24'DPEPO**-based devices with **DMAC-DPS** doping concentrations of 5, 10 and 15%, respectively; (b) Efficiency *vs.* Luminance curves of the devices.

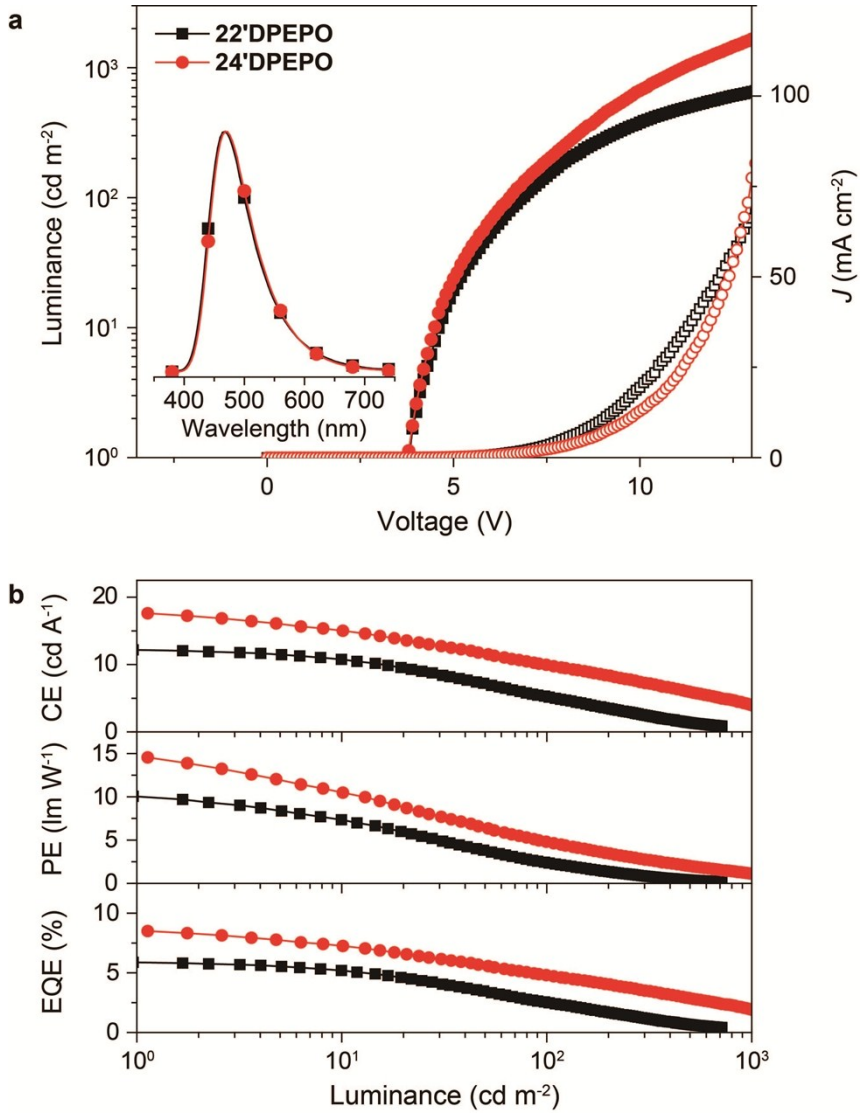

Figure S6. (a) Luminance-*J*-Voltage curves and EL spectra (inset) of **2CzPN**-based devices using **22'DPEPO** and **24'DPEPO** as host, respectively; (b) Efficiency *vs.* Luminance curves of the devices.