Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Ternary Donor-Acceptor Hosts for Highly Efficient Blue Phosphorescence and Thermally Activated Delayed Fluorescence OLEDs

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Content

Thermal Properties

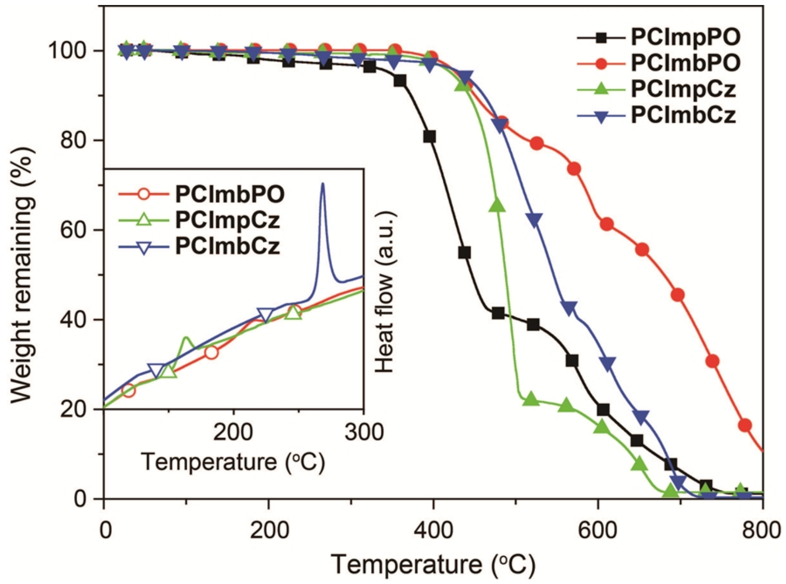


Figure S1. TGA and DSC curves of **PCImG**.

TGA curve of PCImbPO showed two intermediate decomposition stages with weight losses of 24 and 13%, corresponding to two phenyls in DPPO group and one phenyl at 9-position of carbazole group, respectively, which should be ascribed to the large steric hindrance effect between DPPO and N-phenylcarbazole as peripheral groups in PCImbPO.

Solvent Effect on FL Emissions of PCImG

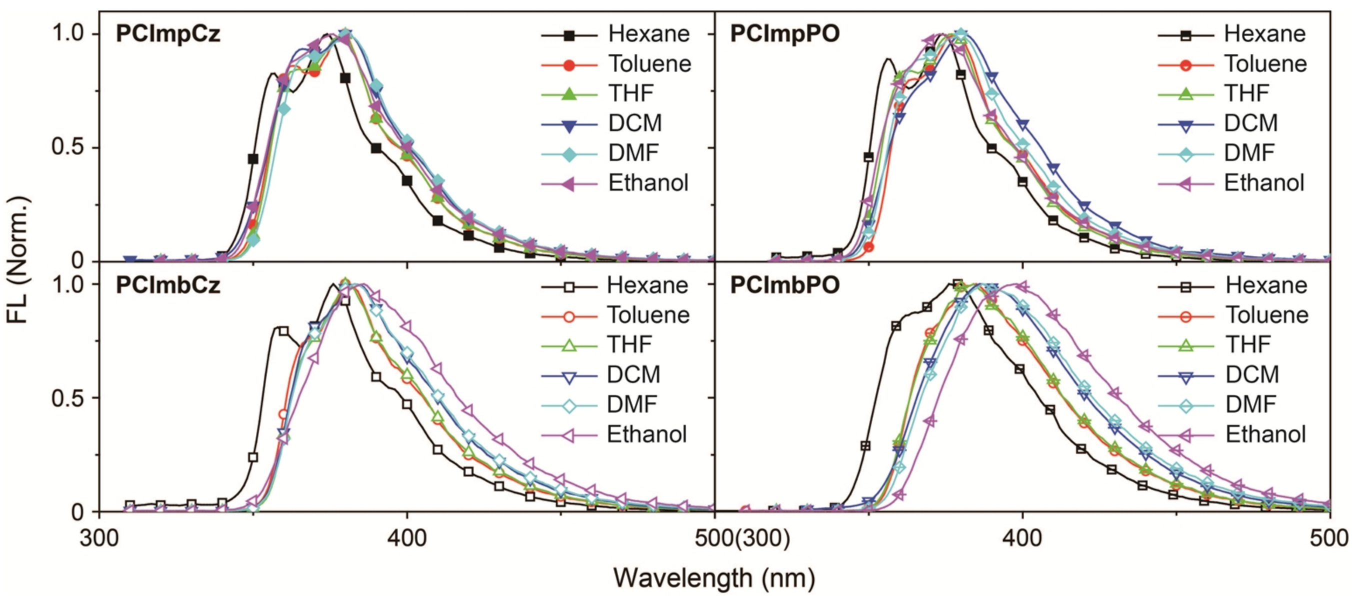


Figure S2. FL spectra of **PCImG** in solvents with different polarities.

Optical Properties in Film

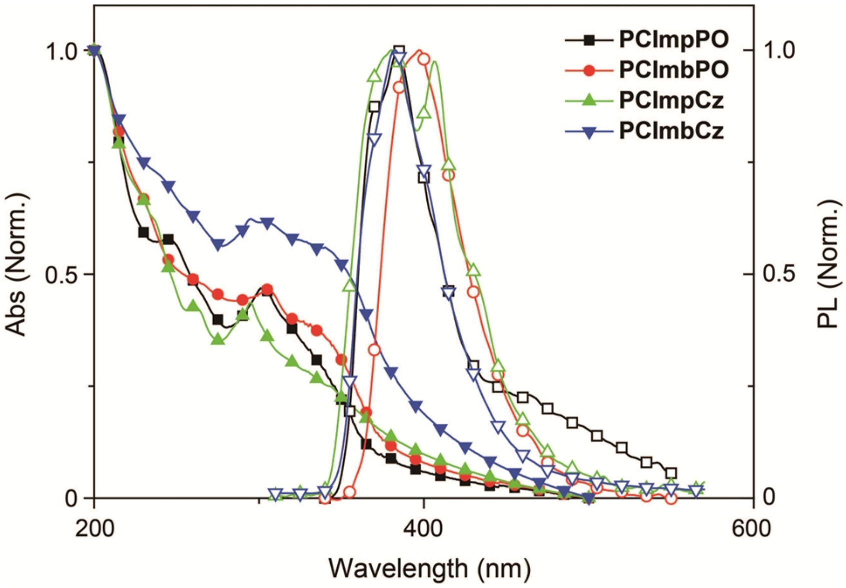


Figure S3. Absorption and PL spectra of **PCImG** in thin film.

Emission and Time-Decay Spectra of Thin Films of FIrpic-Doped PCImG

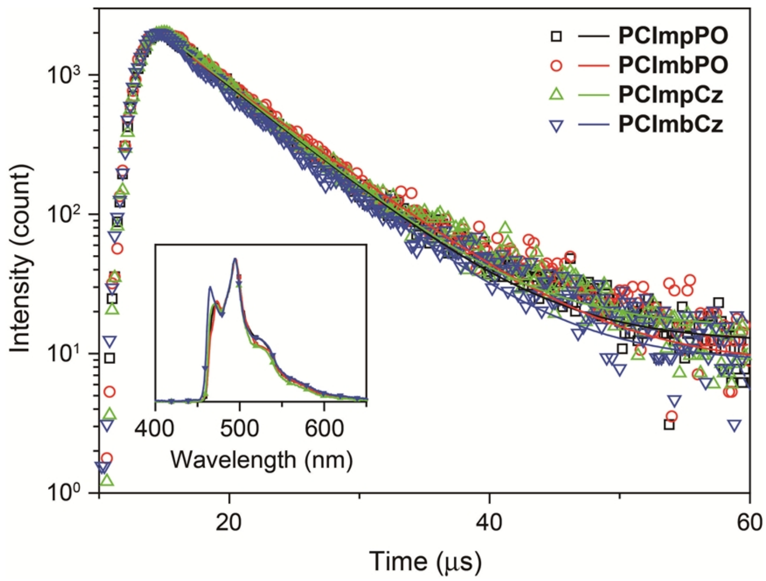


Figure S4. Decay curves and emission spectra (inset) of FIrpic doped (10%) **PCImG** thin films.

The photoluminescence spectra of the doped films consist of three typical FIrpic-originated peaks around 470, 500 and 530 nm, corresponding to its 0-0, 0-1 and 0-2 vibronic bands, respectively.

DFT Calculation Results of PCImG

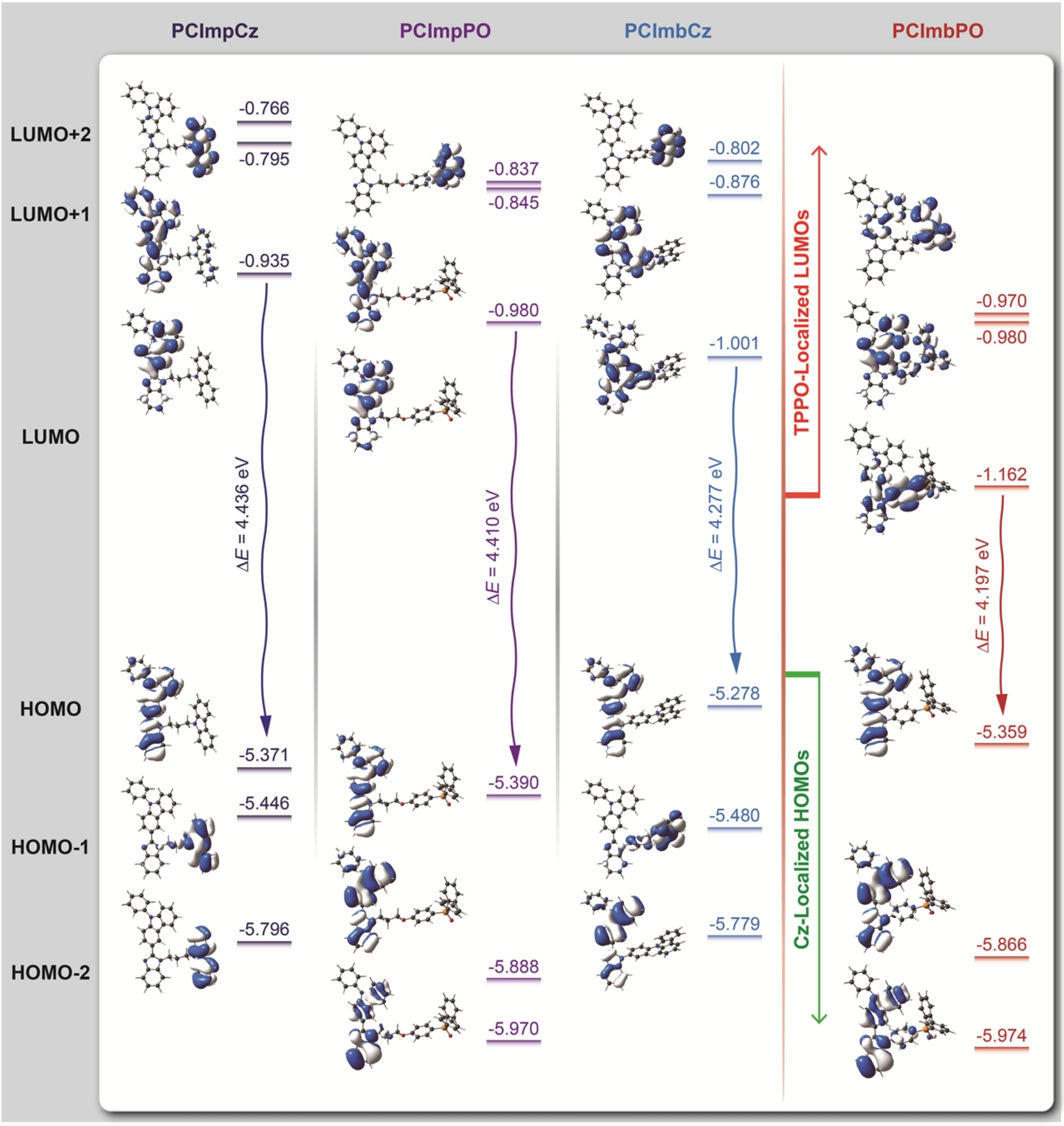


Figure S5. Energy level scheme and contours of frontier molecular orbitals of **PCImG** according to DFT calculation.

DFT Calculation Results of D-A-D and D-A-A type PCImG Analogues

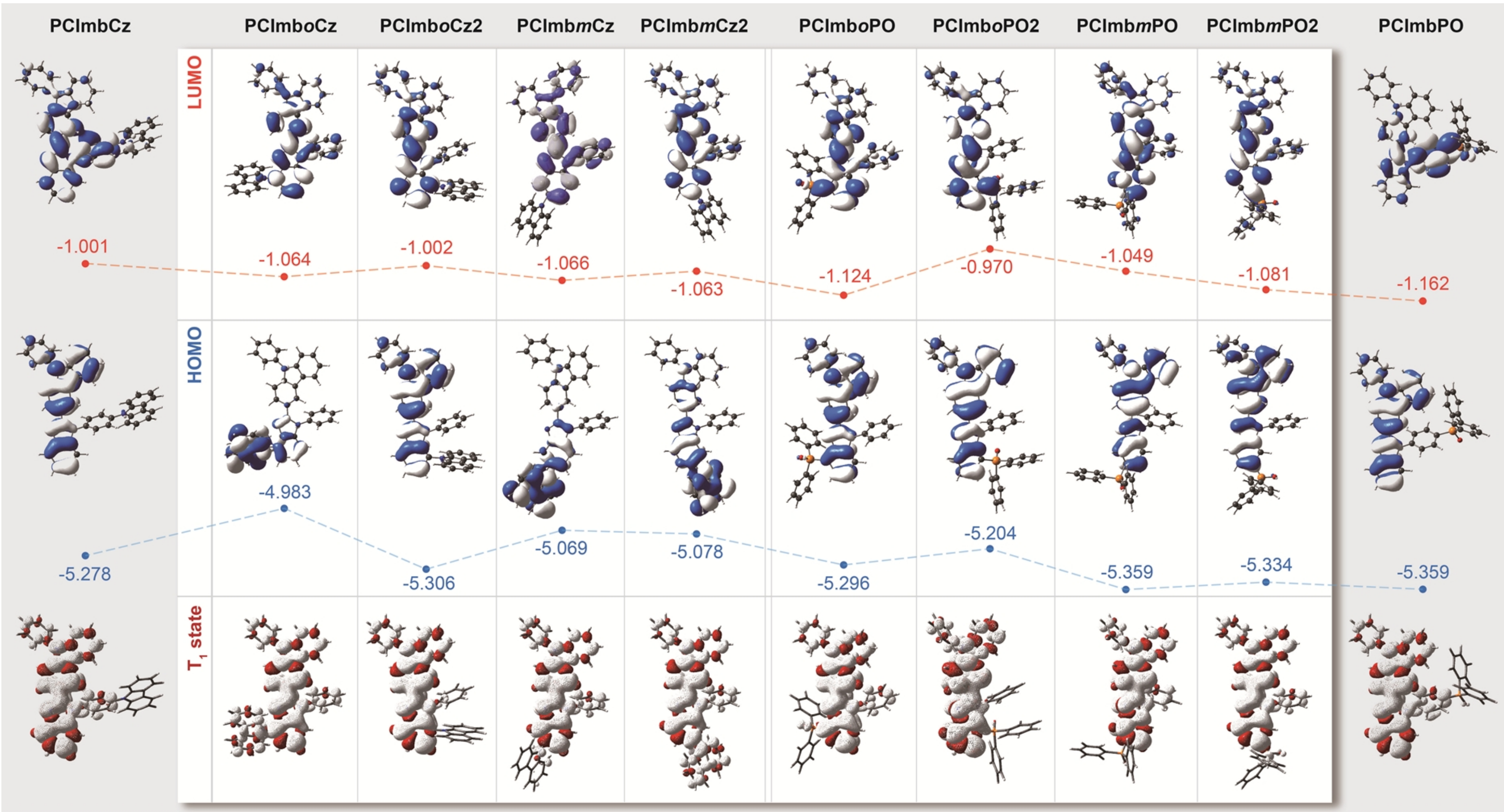
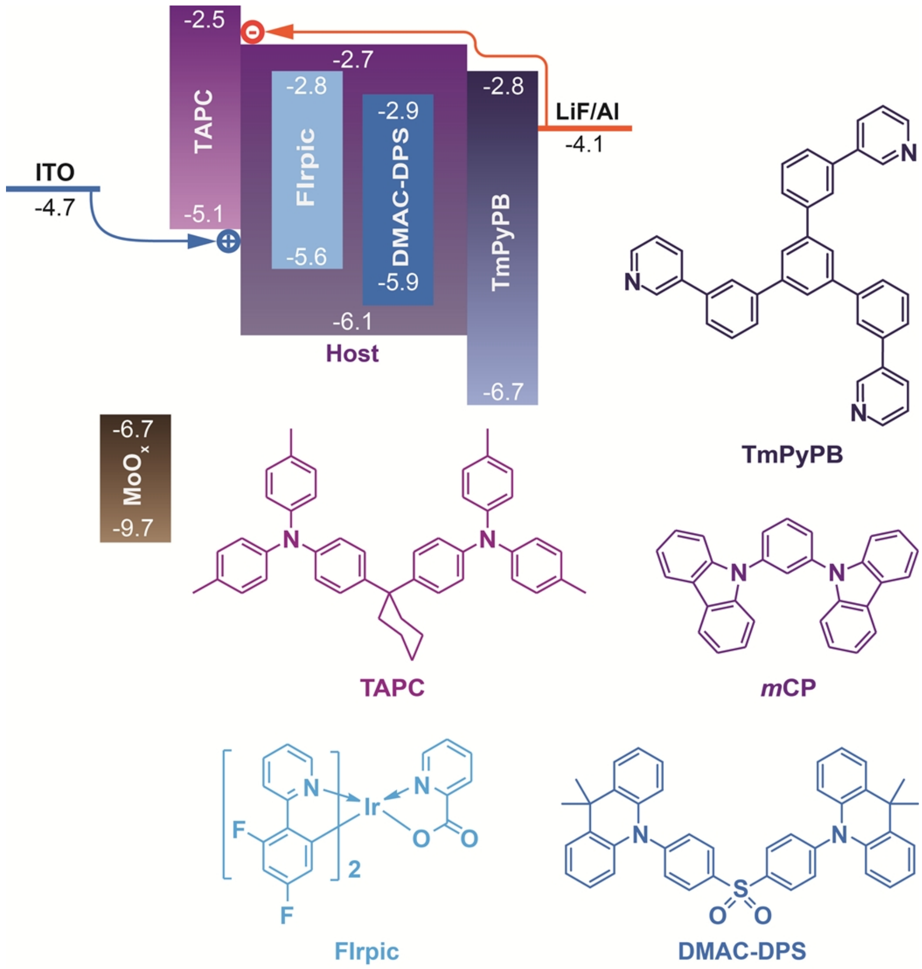


Figure S6. DFT-calculated energy level and contours of FMOs of schemes of D-A-D and D-A-A type **PCImG** analogs.

Device Configuration and Energy Level Diagram



Scheme S1. Energy level diagram of blue PHOLEDs and TADF diodes based on **PCImG** and chemical structures of auxiliary materials.

Since the HOMO energy gap between TAPC and PCImbPO as 1.0 eV is ten times of the LUMO energy gap between TmPyPB and PCImbPO as 0.1 eV, and PCImbPO reveals the feature of electron-transporting predominance with electron-only J remarkably higher than hole-only J of its single-carrier transporting devices, it is rational that as the host matrix in EML, the superiority of PCImbPO in electron injection and transportation would render the charge recombination zone close to the interface between TAPC and EML.

Table S1. EL performance of blue OLEDs based on **PCImG** and *m*CP.

Device	Operating Voltage (V)[a]	Maximum Efficiencies[b]	Efficiency Roll-Offs (%)[c]		
			C.E.	P.E.	E.Q.E.
PA	3.5, <5.5, <7.5	33.7, 30.2, 16.2	10, 20	43, 63	10, 19
PB	3.0, <5.0, <6.5	46.9, 49.1, 22.5	5, 10	43, 58	5, 10
PC	3.0, <5.0, <7.0	17.3, 18.1, 8.3	23, 36	54, 73	23, 36
PD	3.5, <5.0, <7.0	36.4, 38.1, 17.5	8, 19	45, 65	8, 18
PE	3.5, <5.0, <7.0	29.8, 26.7, 14.3	8, 13	36, 53	8, 13
FA	3.7, <5.9, <10.4	12.4, 10.3, 6.1	19, 69	49, 89	18, 69
FB	3.6, <5.1, <7.2	24.2, 21.0, 12.2	6, 28	33, 64	6, 28
FC	3.7, <5.8, <9.7	8.9, 7.2, 4.5	18, 70	44, 88	18, 69
FD	3.6, <5.6, <7.7	18.8, 16.0, 9.4	14, 46	41, 74	14, 46
FE	3.9, <5.6, <8.6	12.2, 9.9, 6.1	12, 52	39, 79	13, 52

[a] In the order of onset, 100 and 1000 cd m^{-2}; [b] in the order of C.E. (cd A^{-1}), P.E. (lm W^{-1}) and E.Q.E. (%); c in the order of 100 and 1000 cd m^{-2}.