Supporting Information

High-performing Bipolar Host Materials for Blue Thermally Activated Delayed Fluorescent Devices with Excellent External Quantum Efficiencies

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Figure S1. UV-vis absorption spectrum of 2CzPN as dopant and PL spectra of host materials.



Figure S2. PL decay curves (a) and PL spectra (b) of mCP, ZDZ, ZDN, and NDN films.



Figure S3. Transient PL decay curves (a, c) and PL spectra (b, d) of host:2CzPN (6 wt%) thin film. *(a) and (b) are delayed PL. (c) and (d) are prompt PL.

Sample	Lifetime		PL λ_{max} (nm)		PLQY (%)		
	delayed	prompt	delayed	prompt	delayed	prompt	Total
mCP: 6% 2CzPN	246.15 ms	14.63 ns	482	485	38.0	51.0	89.0
ZDZ: 6% 2CzPN	228.85 ms	26.37 ns	497	489	40.1	44.0	84.1
ZDN: 6% 2CzPN	208.82 ms	15.76 ns	499	495	48.7	49.5	98.2
NDN: 6% 2CzPN	135.41 ms	19.54 ns	501	498	44.5	43.4	87.9

Table S1. Photophysical properties of host materials doped with 2CzPN

Hole-only devices (HODs) and electron-only devices (EODs)

We fabricated the devices to investigate single-carrier transport behavior. For the purpose, HODs and EODs were fabricated to investigate the current densities in the host materials.

The configuration of HOD was ITO (150 nm)/TAPC (20 nm)/host material (50 nm)/TAPC (20 nm)/Al (100 nm), to enhance hole injection and suppress electron injection. The EOD has the configuration of ITO (150 nm)/TmPyPB (20 nm)/host material (50 nm)/TmPyPB (20 nm)/LiF (1.5 nm)/Al (100 nm), to enhance electron injection and suppress hole injection.



Figure S4. J-V curves of HODs (a) and EODs (b) based on ZDZ, ZDN, and NDN.

The charge-transport capabilities of the three host molecules were investigated using hole- and electron-only devices (HODs and EODs) containing of ZDZ, ZDN, and NDN host materials. Figure S4 shows the current density–voltage curves of the HODs and EODs for the three host materials. The hole-current density against applied voltage plots for ZDZ and ZDN were similar, because of the similar hole affinities of the carbazole moieties.

As expected, when two carboline units were introduced into DBT, the hole-current density decreased, because of the increased electron affinity of the NDN host. The effect of the carboline unit on the electron-current density can be clearly seen in Figure S4. Introduction of a carboline unit into the DBT core gave a much higher electron-current density than that of ZDZ. In particular, we postulate that the hole- and electron-current densities of ZDN are both suitable for blue TADF emitting layers. The higher current density of ZDN in terms of both the HOD and EOD is achieved by the combined effects of lower-energy barriers against the TAPC and TmPyPB layers, facilitating both hole and electron injection and promotion of the electron-transport characteristics by carboline. The charge balance in the ZDN-based TADF-OLED is expected to give a high EQE.



Figure S5. Energy level diagram of blue TADF-OLED device fabricated in this study.