Supporting Information

Solution-Processed Thermally Activated Delayed Fluorescence Organic Light-Emitting Diodes Using New Polymeric Emitter Containing Non-conjugated Cyclohexane Units

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KEYWORDS: cyclohexane unit, organic light emitting diode, thermally activated delayed fluorescence, polymeric emitter, solution process.

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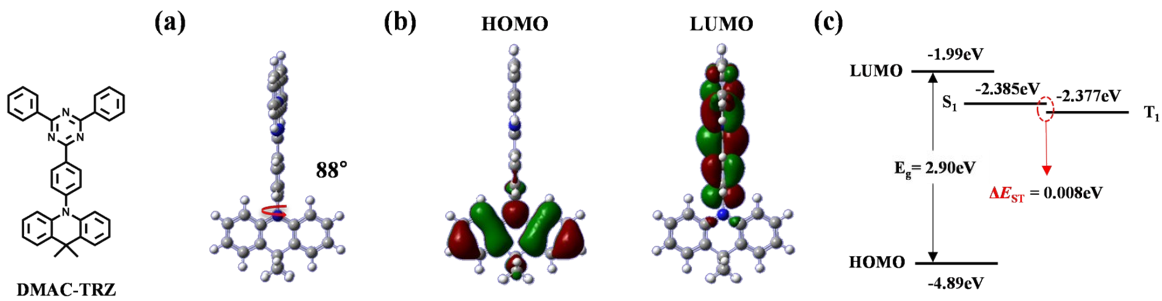

Fig. S1 (a) Optimized geometry, (b) HOMO and LUMO spatial distribution, and (c) energy level diagram for DMAC-TRZ calculated by DFT (B3LYP/6-31G) using Gaussian 09W.

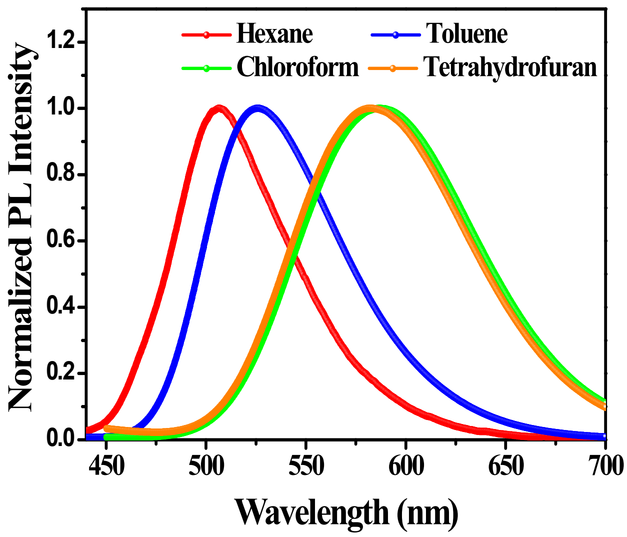

Fig. S2 Photoluminescence (PL) spectra of **P(DMTRZ-Cp)** in solvents with different polarities.

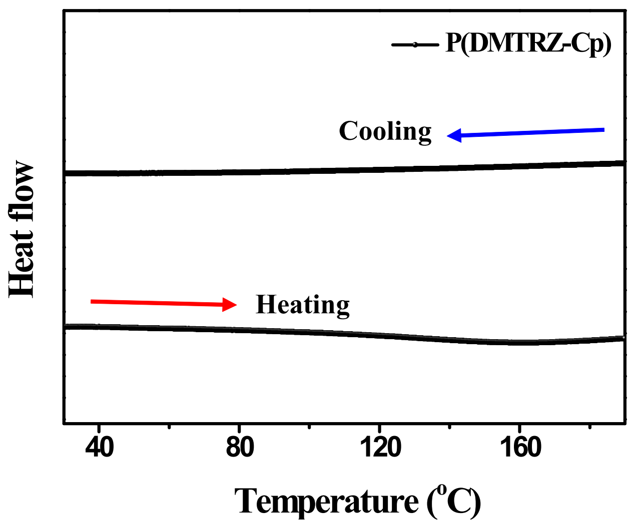

Fig. S3 Differential scanning calorimetry curve for **P(DMTRZ-Cp).**

Table S1 Photophysical properties of the **P(DMTRZ-Cp)**-doped with mCP.

Polymer Emitter	τ_p [a] (ns)	τ_d [a] (μs)	Φ_p / Φ_d / Φ_{PL} Solution [b]	Film [b]	k_p [c] (s^{-1})	k_d [d] (s^{-1})	k_r^S [e] (s^{-1})	k_{ISC} [f] (s^{-1})	k_{RISC} [g] (s^{-1})	k_{nr}^T [h] (s^{-1})
P(DMTRZ-Cp)	12.2	1.8	0.21/0.32 /0.53	0.49/0.48 /0.97	8.22x10^7	5.56x10^5	4.03x10^7	4.19x10^7	1.07x10^6	3.20x10^4

[a] PL lifetimes of the prompt (τ_p) and delayed (τ_d) decay components (film). [b] Absolute photoluminescence quantum yield using an integrating sphere in the solution and film states without degassing (prompt, Φ_P) and under nitrogen (delayed: Φ_d, total: Φ_{PL}). [c] Prompt fluorescence decay rate constant. [d] Delayed fluorescence decay lifetime. [e] The radiative decay rate constant of the singlet excited state. [f] The rate constant for intersystem crossing (ISC) from the singlet excited state to the triplet excited state. [g] The rate constant for reverse intersystem crossing (RISC) from the triplet excited state to the singlet excited state. [h] The non-radiative (nr) decay rate constant of the triplet excited state.

To further understand the fundamental mechanism of the TADF polymeric emitter, the kinetic parameters of the polymeric emitter-doped film in mCP were determined from the experimental data (**Table S1**). The prompt (Φ_p) and delayed (Φ_d) fluorescence quantum yields were determined by the ratio of emission area in the transient PL spectra based on total photoluminescence quantum yield (Φ_{PL}). Prompt (τ_p) and delayed (τ_d) fluorescence lifetimes are obtained by fitting the transient PL curve. Through this values, prompt (k_p) and delayed (k_d) fluorescence decay rate constants (where $k_p = 1/\tau_p$ and $k_d = 1/\tau_d$) were obtained. The radiative decay rate constants of the singlet excited state (k_r^S), the rate constant for intersystem crossing (k_{ISC} , $S_1 \rightarrow T_1$), the rate constant for reverse intersystem crossing (k_{RISC} , $T_1 \rightarrow S_1$) were calculated using the following equations.

$$k_r^S = k_p \cdot \Phi_p \qquad (1)$$

$$k_{ISC} = k_p \cdot (1-\Phi_p) \qquad (2)$$

$$k_{RISC} = (k_p \cdot k_d / k_{ISC}) \cdot (\Phi_d / \Phi_p) \qquad (3)$$

From the equations (1)-(3), the non-radiative (nr) decay rate constant of the triplet excited state (k_{nr}^{T}) can be obtained.

$$k_{nr}^{T} = k_{d} - k_{RISC} \cdot \Phi_{p} \qquad (4)$$

This value was based on the assumption that the non-radiative decay rate constant of the singlet excited state (k_{nr}^{S}) is zero at 300 K.[1, 2]

All the kinetic parameters including PL characteristics are summarized in **Table S2** and it demonstrate that the **P(DMTRZ-Cp)** polymeric emitter-doped film with mCP shows comparable rate constant values.[1, 3-10]

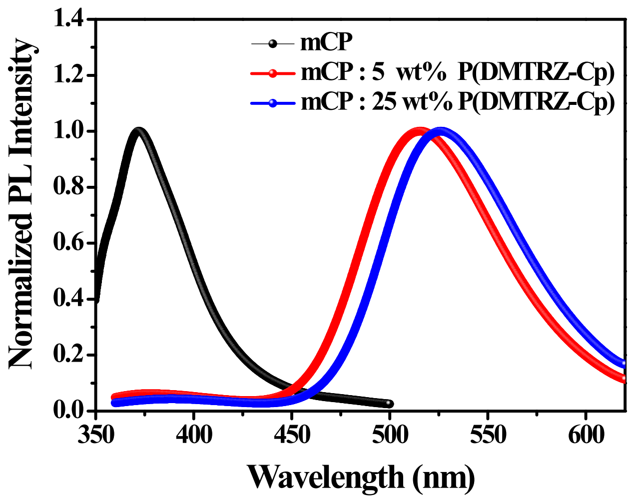

Fig. S4 PL spectra of the mCP film and **P(DMTRZ-Cp):** mCP blend film (5 wt% and 25 wt%).

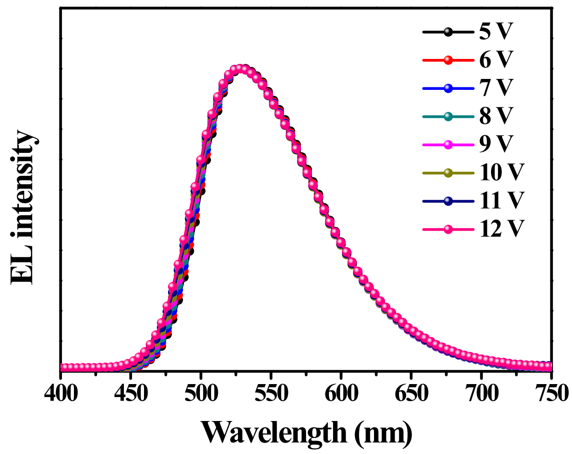

Fig. S5 Normalized electroluminescence (EL) spectra of devices based on **P(DMTRZ-Cp)** (25 wt%) as functions of different applied voltages.

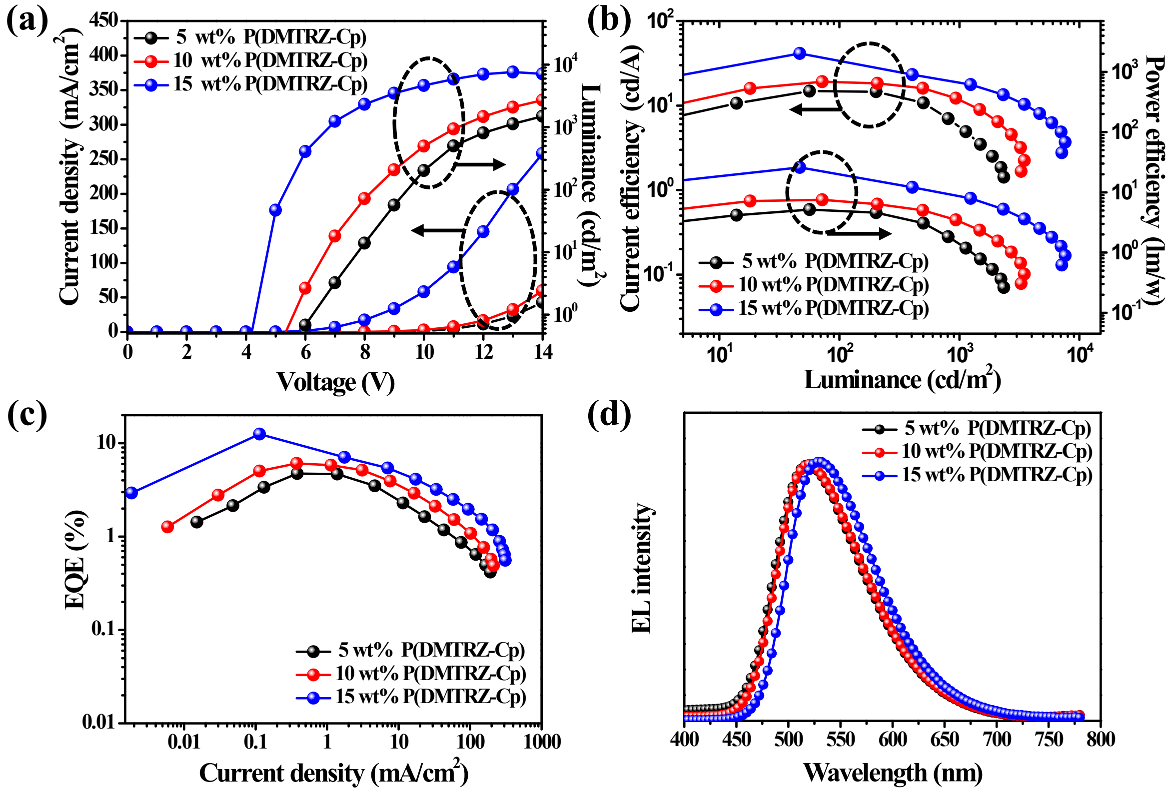

Fig. S6 (a) Current density-voltage-luminance (*J*-*V*-*L*) curves, (b) current efficiency-luminance-power efficiency curves, (c) external quantum efficiency (EQE)-current density (η_{ext}-*J*) curves and (d) electroluminescence (EL) spectra at 1000 cd/m^2 of TADF-OLEDs fabricated using the new **P(DMTRZ-Cp)** polymer emitter at different concentrations (5, 10, 15 wt%).

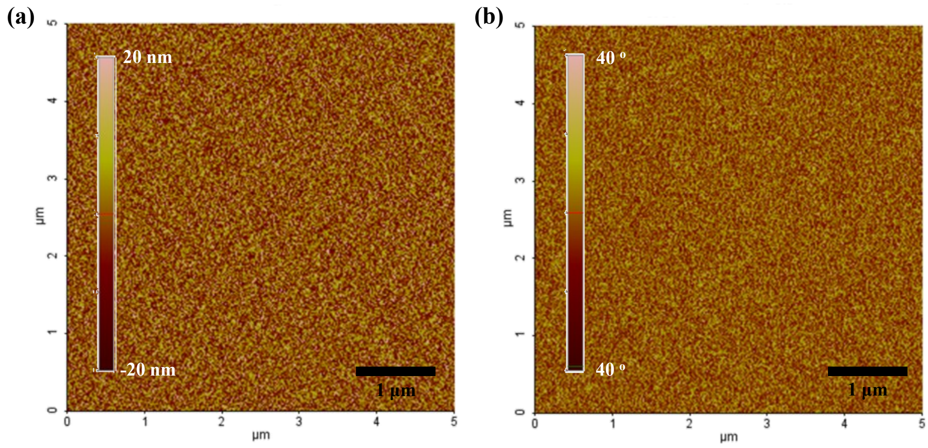

Fig. S7 AFM (a) height and (b) phase images of mCP:P(DMTRZ-Cp) (25 wt%) blended film.

To investigate the surface homogeneity of the emitting layer, an AFM image of a blend film (mCP: **P(DMTRZ-Cp)** (25 wt%)) was measured. High uniformity and smoothness were expected to be sufficient to act as a light emitting layer.

Notes and references

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