Supporting Information

Exciton dynamics of an aggregation-induced delayed fluorescence emitter in non-doped OLEDs and its application as host for high efficiency red phosphorescent OLEDs

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Figure S1. (a) Current density-voltage characteristics of the fabricated OLEDs with different CP-BP-PXZ doping concentrations in mCBP. (b) Current efficiency–luminance-current density characteristics of the fabricated OLEDs with different CP-BP-PXZ doping concentrations in mCBP.

Figure S2. EQE characteristics of the two non-doped OLEDs with different emitters of neat mCBP and CP-BP-PXZ.
**Figure S3.** Normalized electroluminescence spectra of the resulting OLEDs with different CP-BP-PXZ doping concentrations in mCBP.

**Figure S4.** MEL responses of the non-doped OLED based on CP-BP-PXZ under different applied currents.
**Figure S5.** Absorption spectrum of Ir(dmdppr-dmp)₂(divm) and emission spectrum of CP-BP-PXZ.

**Figure S6.** (a) EQE - luminance characteristics of the resulting red phosphorescent OLEDs based on CP-BP-PXZ and mCBP as host. The insert is the chemical structure of mCBP and Ir(dmdppr-dmp)₂(divm). (b) Lifetime comparison of the resulting red phosphorescent OLEDs based on CP-BP-PXZ and mCBP as host at the initial luminance of 500 cd/m².
Table S1. Summary of EL performances of the OLEDs with different CP-BP-PXZ doping concentrations in mCBP host.

<table>
<thead>
<tr>
<th>Doping Concentration</th>
<th>V_{on} (V)</th>
<th>L_{Max} (cd/m²)</th>
<th>CE (cd/A)</th>
<th>PE (lm/W)</th>
<th>EQE/EQE^a (%)</th>
<th>k_{STA} (cm³/s)</th>
<th>k_{TTA} (cm³/s)</th>
<th>CIE^b</th>
</tr>
</thead>
<tbody>
<tr>
<td>10wt%</td>
<td>3</td>
<td>42674</td>
<td>47.76</td>
<td>48.50</td>
<td>16.24/13.98</td>
<td>1.52*10⁻¹³</td>
<td>6.49*10⁻¹⁴</td>
<td>(0.31,0.51)</td>
</tr>
<tr>
<td>20wt%</td>
<td>2.7</td>
<td>51536</td>
<td>45.55</td>
<td>44.31</td>
<td>15.30/14.10</td>
<td>1.00*10⁻¹⁵</td>
<td>3.24*10⁻¹⁴</td>
<td>(0.33,0.53)</td>
</tr>
<tr>
<td>50wt%</td>
<td>2.5</td>
<td>46699</td>
<td>41.98</td>
<td>42.56</td>
<td>13.83/12.95</td>
<td>3.59*10⁻¹⁵</td>
<td>3.67*10⁻¹⁴</td>
<td>(0.37,0.54)</td>
</tr>
<tr>
<td>80wt%</td>
<td>2.5</td>
<td>50069</td>
<td>40.06</td>
<td>42.58</td>
<td>13.23/12.59</td>
<td>2.06*10⁻¹⁴</td>
<td>2.69*10⁻¹⁴</td>
<td>(0.39,0.54)</td>
</tr>
<tr>
<td>neat</td>
<td>2.4</td>
<td>54830</td>
<td>40.31</td>
<td>47.28</td>
<td>13.31/12.80</td>
<td>2.42*10⁻¹⁴</td>
<td>3.45*10⁻¹⁴</td>
<td>(0.39,0.54)</td>
</tr>
</tbody>
</table>

^a.EQE at 1000cd/m²; b.the CIE coordinates at 6 V

Table S2. Calculations of the rate constants of CP-BP-PXZ doped mCBP host with different doping concentrations.

<table>
<thead>
<tr>
<th>Doping Concentration(wt%)</th>
<th>τ_p(\text{ns})</th>
<th>τ_d(\text{μs})</th>
<th>k_s^r(10^7\text{s}^{-1})</th>
<th>k_{ISC}(10^7\text{s}^{-1})</th>
<th>k_{RISC}(10^6\text{s}^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>10wt%</td>
<td>20.8</td>
<td>1.49</td>
<td>2.71</td>
<td>2.09</td>
<td>1.18</td>
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<tr>
<td>20wt%</td>
<td>25</td>
<td>1.07</td>
<td>1.28</td>
<td>3.25</td>
<td>3.29</td>
</tr>
<tr>
<td>50wt%</td>
<td>25</td>
<td>1.04</td>
<td>1.24</td>
<td>2.75</td>
<td>3.06</td>
</tr>
<tr>
<td>80wt%</td>
<td>25</td>
<td>0.93</td>
<td>1.37</td>
<td>2.62</td>
<td>3.09</td>
</tr>
<tr>
<td>Neat</td>
<td>26</td>
<td>0.87</td>
<td>1.41</td>
<td>2.43</td>
<td>3.13</td>
</tr>
</tbody>
</table>
The photophysical parameters are calculated by the following functions\(^1,2\):

\[
\begin{align*}
  k_F &= \frac{\Phi_{\text{prompt}}}{\tau_{\text{prompt}}} \\
  k_p &= \frac{1}{\tau_{\text{prompt}}}; \quad k_d = \frac{1}{\tau_{\text{delayed}}} \\
  k_P &= k_F + k_{\text{ISC}} \\
  k_P k_d &= k_F k_{\text{RISC}} \\
  k_{\text{ISC}} &= k_p - k_F = k_p (1 - \Phi_{\text{prompt}}) \\
  k_{\text{RISC}} &= (k_pk_d)/(k_p - k_{\text{ISC}})
\end{align*}
\]

The carrier kinetics

As hole and electron transport and recombination on CP-BP-PXZ in non-doped OLED, the free carriers can be described as following equations\(^3\)

\[
\begin{align*}
  \frac{dn_h}{dt} &= \frac{jh}{eL_h} - \gamma n^2 \\
  \frac{dn_e}{dt} &= \frac{je}{eL_e} - \gamma n^2
\end{align*}
\]
where the $\gamma$ is the bimolecular recombination coefficient, $j_h$ and $j_e$ are the hole and electron injection currents flowing through the transport layers($L_h$ and $L_e$), respectively. Under the steady-state condition, $L_h = L_e = 40$nm for device, $j_h = j_e = j$, and $n_0$ can be attained as following

$$n_0 = (2j/e\gamma L)^{1/2}$$

The electrons and holes in the recombination zone are free and equal to each other($n_h = n_e = n$), after turn off pulse, the charge decay can be express as

$$\frac{1}{n} = \frac{1}{n_0} + \gamma t$$

Taken into account EL yield, $\Phi_{EL} = \Phi_{PL} P_S \gamma n(t)^2$, $\Phi_{PL}$ is PLQY, $P_S$ is the function that excitons generated. The EL decay can be described as

$$\frac{1}{\sqrt{\Phi_{EL}(t)}} = \frac{1}{\sqrt{\Phi_{PL} P_S \gamma n_0^2}} + \frac{\gamma}{\sqrt{\Phi_{PL} P_S}} t$$

and $\gamma$ can be calculated as

$$\gamma = \left(\frac{\gamma \Phi_{PL} P_S}{\Phi_{PL} P_S n_0^2} \right)^{0.5} eL/j$$

$$= \left(\frac{\gamma \Phi_{PL} P_S}{\Phi_{PL} P_S n_0^2} \right)^{-2} eL/j$$

Reference

