Supporting Information

Vitrimer enhanced carbazole-based organic room-temperature phosphorescent materials

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Experimental Section

Materials and instruments: All reagents were purchased from Energy Chemical or Macklin Biochemical Co., Ltd depending on the supply availability and used without further purification. ¹H NMR and ¹³C NMR spectra were recorded on a AVANCE III 500 BRUKER instrument. High-resolution mass spectra were measured by Bruker solanX 70 FT-MS. CHN elemental analysis results obtained with Elementar UNICUBE. UV-Vis spectra were recorded by a JASCO V570 spectrophotometer. Fourier transform infrared (FTIR) spectra were acquired on Perkin Elmer Frontier or Thermo Scientific Nicolet iS50. Fluorescence spectra were measured using a F-280 fluorescence spectrophotometer in darkness and under ambient conditions. Phosphorescence spectra were measured by a Hitachi F-4600 fluorescence spectrophotometer in the dark and under ambient conditions. Phosphorescence lifetime, fluorescence quantum yield and phosphorescence quantum yield were measured by the Edinburgh Instruments FLS-980 or Edinburgh Instruments FLS-1000 photoluminescence spectrometer in darkness and under ambient conditions. Differential scanning calorimetry curves were obtained by TA Instruments DSC25 in an argon atmosphere. Photos were taken by Sony DSC-RX100M6 or Xiaomi MI 10 Ultra.

Computational methods

The DFT and TDDFT calculations were performed using Gaussian16 at the PBE0/6-311g(d,p) level with the D3(BJ) empirical dispersion correction.

Characterizations

TPACZ: ¹H-NMR (500 MHz, DMSO-d6) δ 11.29 (s, 1H), 8.16 (d, J = 8.1 Hz, 1H), 8.14 – 8.09 (m, 1H), 7.73 – 7.67 (m, 3H), 7.52 – 7.42 (m, 2H), 7.42 – 7.31 (m, 5H), 7.16 (ddd, J = 8.0, 7.1, 1.0 Hz, 1H),
7.13 – 7.05 (m, 8H). $^1$H-NMR (126 MHz, DMSO-d$_6$) δ 147.61, 146.87, 140.88, 140.71, 137.72, 135.74, 130.08, 128.39, 125.97, 124.50, 124.09, 123.61, 122.69, 121.95, 121.05, 120.63, 119.12, 117.92, 111.40, 108.73. HRMS(MALDI): [M$^+$] calcd 410.18, found 410.17987. CHN elemental analysis: predicted C, 87.77%; H, 5.40%; N, 6.82%; measured C, 87.91%; H, 5.39%; N, 6.71%.

Fig. S1 $^1$H-NMR spectrum of TPACZ in DMSO-d$_6$

$^{13}$C-NMR (126 MHz, DMSO-d$_6$) δ 147.61, 146.87, 140.88, 140.71, 137.72, 135.74, 130.08, 128.39, 125.97, 124.50, 124.09, 123.61, 122.69, 121.95, 121.05, 120.63, 119.12, 117.92, 111.40, 108.73. HRMS(MALDI): [M$^+$] calcd 410.18, found 410.17987. CHN elemental analysis: predicted C, 87.77%; H, 5.40%; N, 6.82%; measured C, 87.91%; H, 5.39%; N, 6.71%.

Fig. S2 $^{13}$C-NMR spectrum of TPACZ in DMSO-d$_6$
**DMACZ:** $^1$H-NMR (500 MHz, DMSO-d$_6$) $^1$H NMR (500 MHz, DMSO-d$_6$) δ 11.20 (s, 1H), 8.09 (dd, $J = 10.0, 7.8$ Hz, 2H), 7.61 (d, $J = 8.9$ Hz, 3H), 7.47 (d, $J = 8.0$ Hz, 1H), 7.45 – 7.32 (m, 2H), 7.15 (t, $J = 7.4$ Hz, 1H), 6.88 – 6.82 (m, 2H), 2.96 (s, 6H). $^{13}$C NMR (126 MHz, DMSO-d$_6$) δ 150.16, 141.05, 140.57, 138.61, 129.26, 127.86, 125.65, 122.66, 121.19, 120.90, 120.42, 119.00, 117.56, 113.25, 111.29, 107.94, 39.66. HRMS(MALDI): [M$^+$] calcd 286.15 found 286.14679. CHN elemental analysis: predicted C, 83.88%; H, 6.34%; N, 9.78%; measured C, 84.01%; H, 6.31%; N, 9.68%.

**Fig. S3** HRMS-MALDI of TPACZ

**Fig. S4** $^1$H-NMR spectrum of DMACZ in DMSO-d$_6$
Vitrimer Films: In contrast to the uncured DEGBA, the characteristic peak of the epoxy group at 916 cm$^{-1}$ disappears from the Vitrimer films, proving that the epoxy resin has been fully cured.

Fig. S5 $^{13}$C-NMR spectrum of DMACZ in DMSO-d$_6$

Fig. S6 HRMS-MALDI of TPACZ
Fig. S7 FTIR spectra of Vitrimer films and uncured DGEBA, TPACZ doped at 0.2 mol%.

Fig. S8 Phosphorescence decay curves of TPACZ-Vitrimer at different doping concentrations.
Table S1 Phosphorescent lifetime at different doping concentrations.

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<th>0.2mol%</th>
<th>0.6mol%</th>
<th>1.0mol%</th>
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<td>TPACZ</td>
<td>1015.0ms</td>
<td>934.8ms</td>
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<td>839.2ms</td>
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<td>DMACZ</td>
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<td>1464.2ms</td>
<td>973.8ms</td>
<td>1223.8ms</td>
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</tbody>
</table>

Fig. S9 Phosphorescence decay curves of DMACZ-Vitrimer at different doping concentrations.

Fig. S10 Fluorescence decay curves of two molecules at a doping concentration of 0.2 mol%.
Fig. S11 DSC curves of Vitrimer with different curing agents.

Fig. S12 Phosphorescence spectra and phosphorescence decay curves of TPACZ in different matrixes.
References


