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. ^{1}H NMR and ^{13}C 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[1] at the PBE0[2]/6-311g(d,p)[3] level with the D3(BJ) empirical dispersion correction[4].

Characterizations

TPACZ: ^{1}H-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). ^{13}C-NMR (126 MHz, DMSO-d6) 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%.
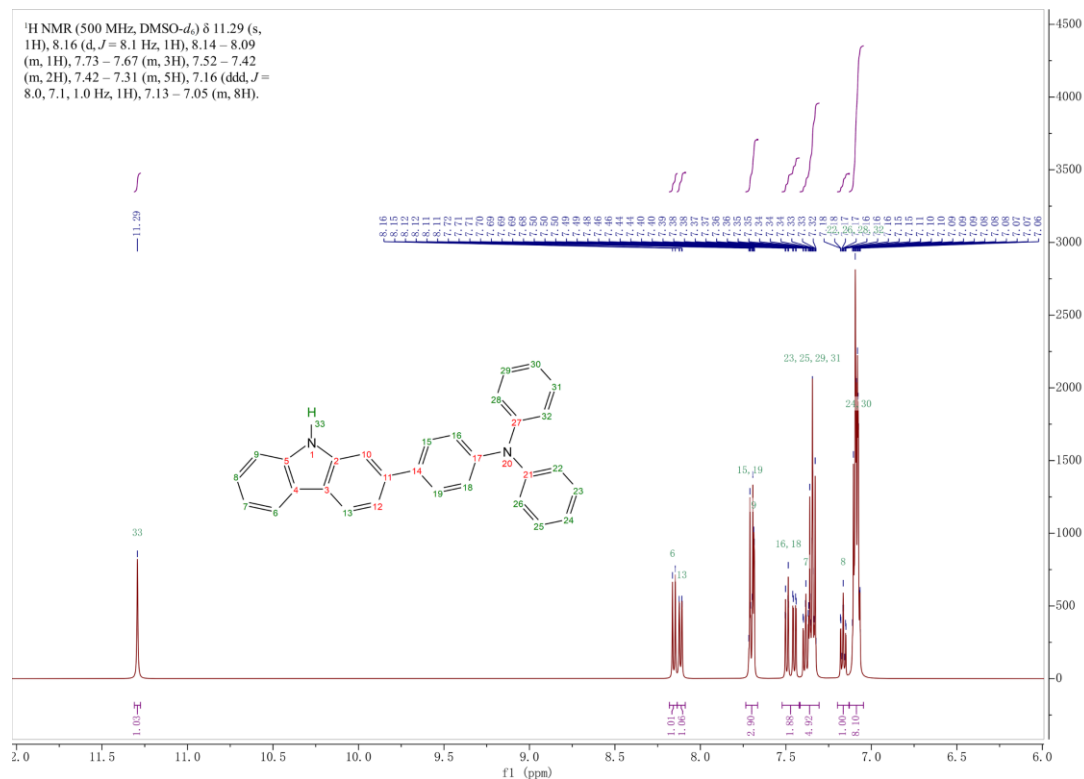
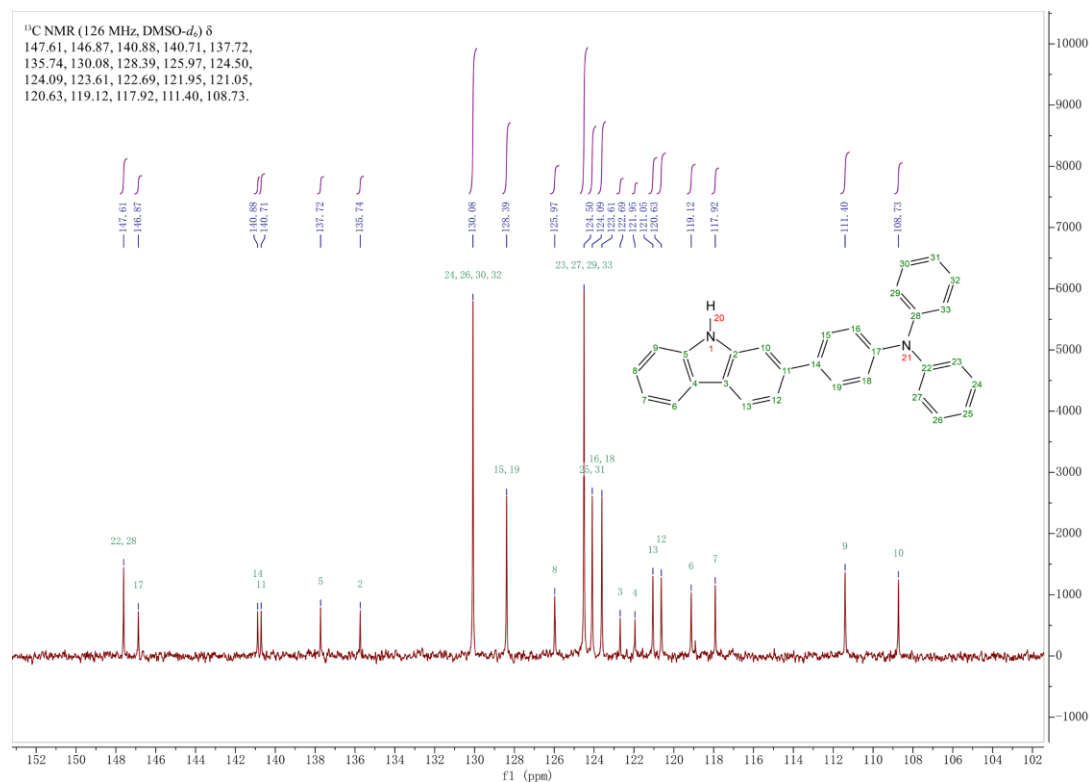

Fig. S1 ^{1}H-NMR spectrum of TPACZ in DMSO-d$_6$
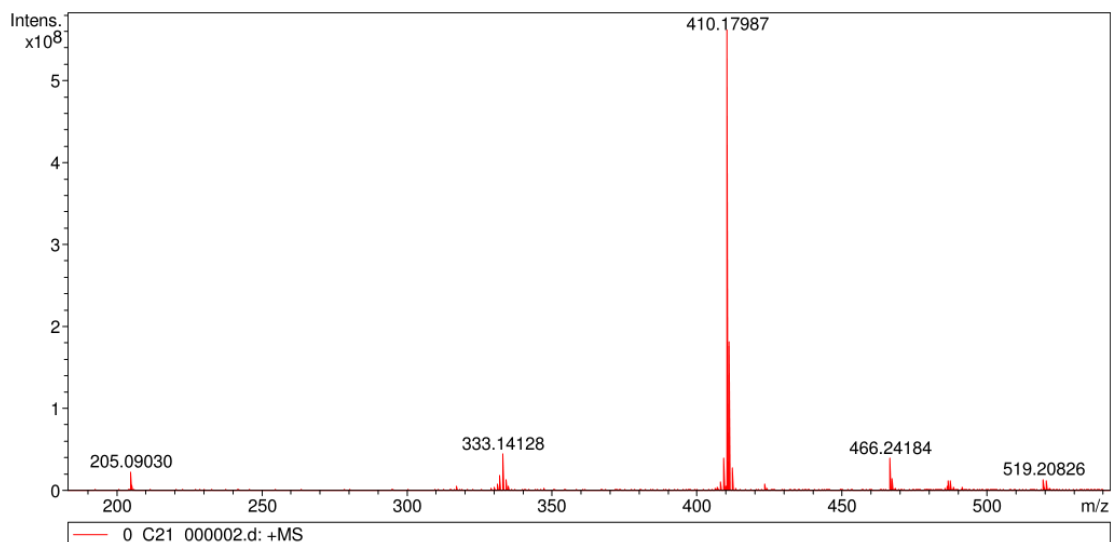

Fig. S2 ^{13}C-NMR spectrum of TPACZ in DMSO-d$_6$

Fig. S3 HRMS-MALDI of TPACZ

DMACZ: ^{1}H-NMR(500 MHz, DMSO-d6) ^{1}H NMR (500 MHz, DMSO-d6) 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-d6) δ 150.16, 141.05, 140.57, 138.61, 129.26, 127.86, 125.65, 122.86, 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%.
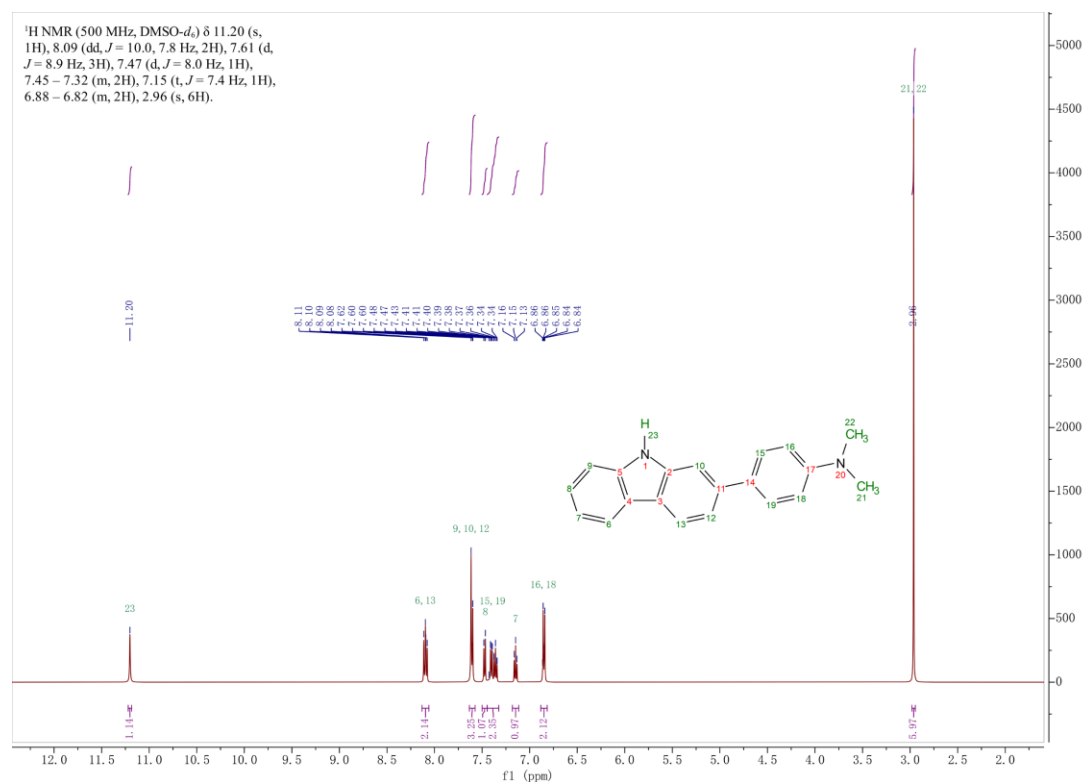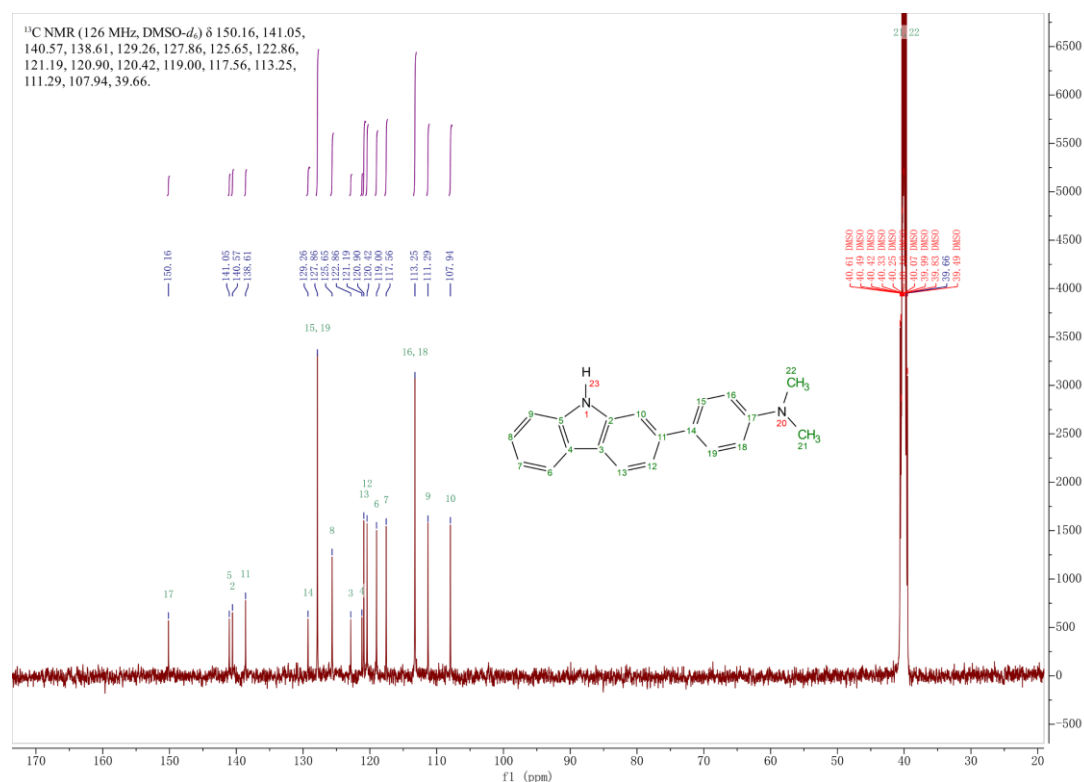

Fig. S4 ^{1}H-NMR spectrum of DMACZ in DMSO-d$_6$
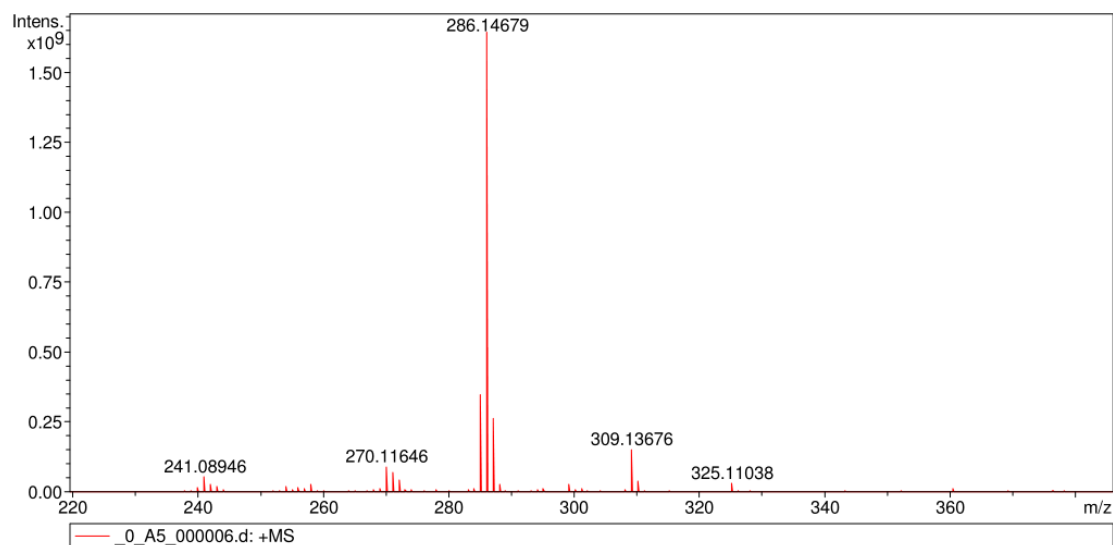
Fig. S5 ^{13}C-NMR spectrum of DMACZ in DMSO-d_6

Fig. S6 HRMS-MALDI of TPACZ

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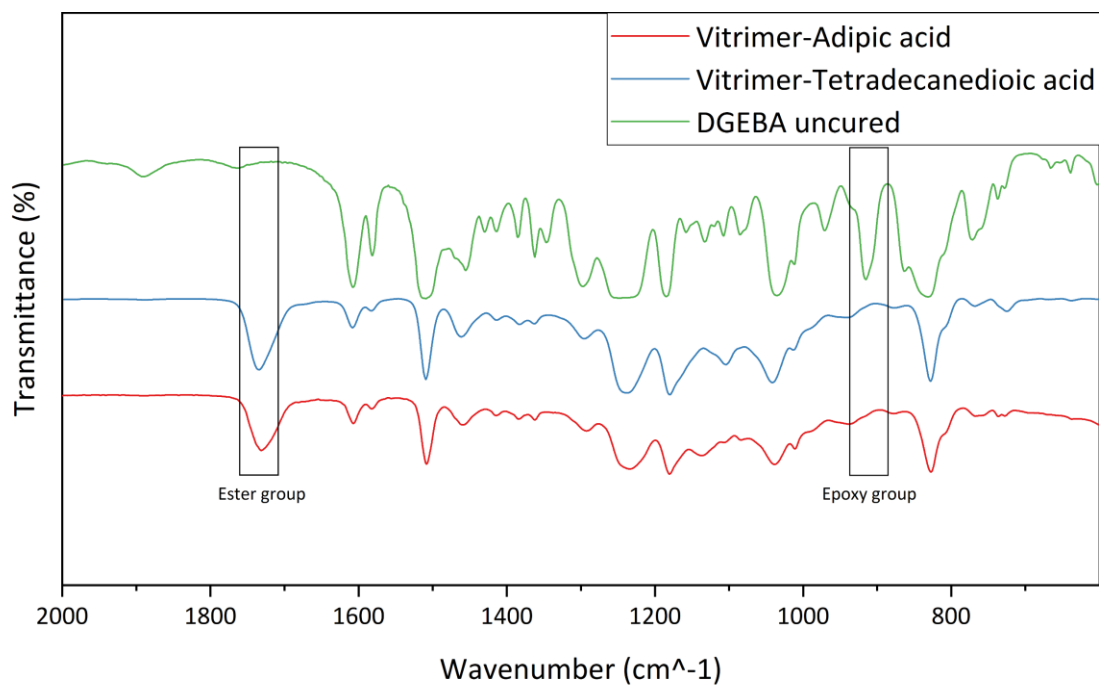
Fig. S7 FTIR spectra of Vitrimer films and uncured DGEBA, TPACZ doped at 0.2 mol%.
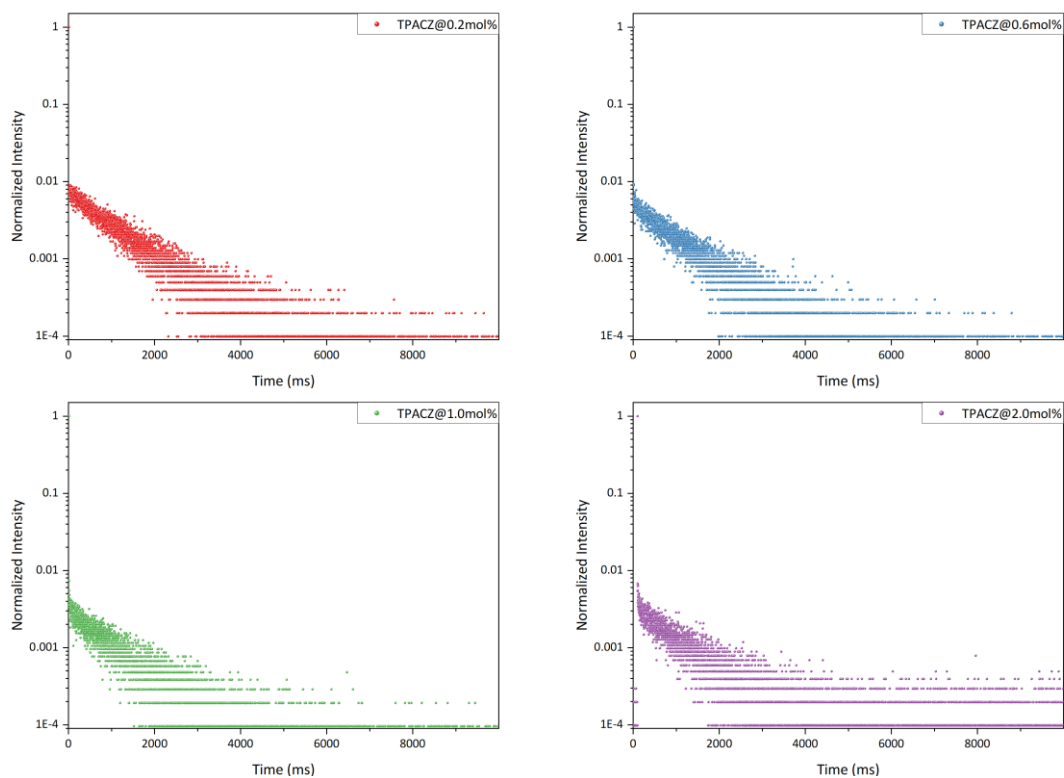

Fig. S8 Phosphorescence decay curves of TPACZ-Vitrimer at different doping concentrations.
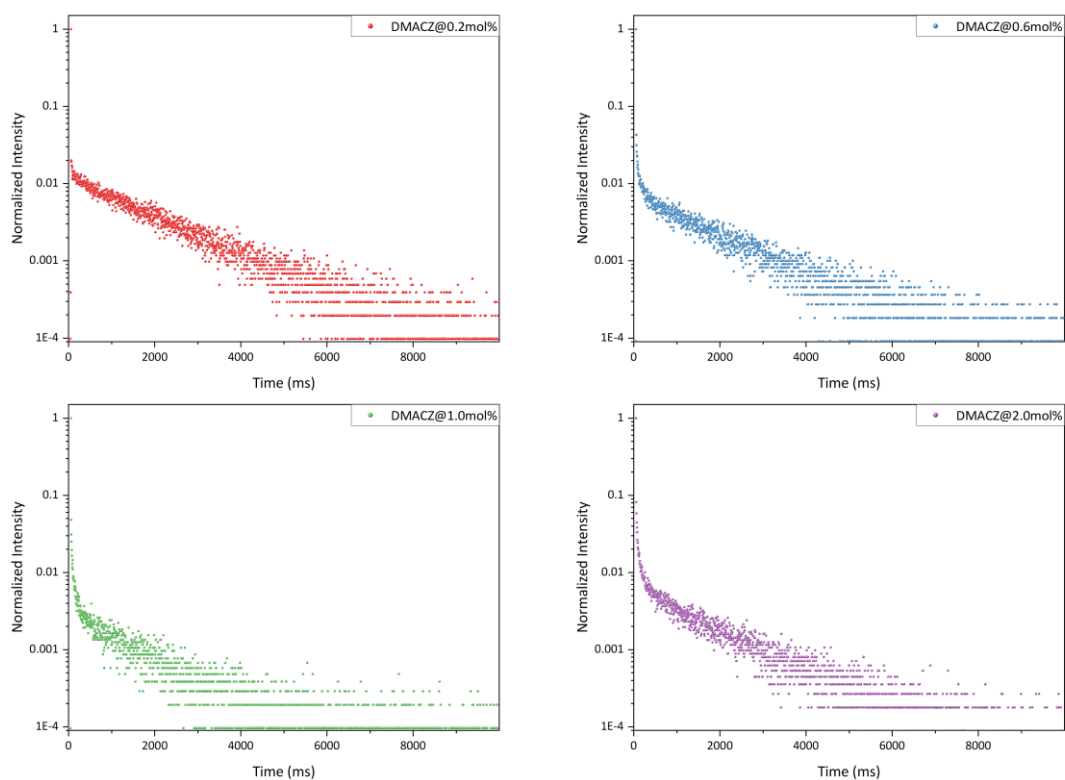
Fig. S9 Phosphorescence decay curves of DMACZ-Vitrimer at different doping concentrations.
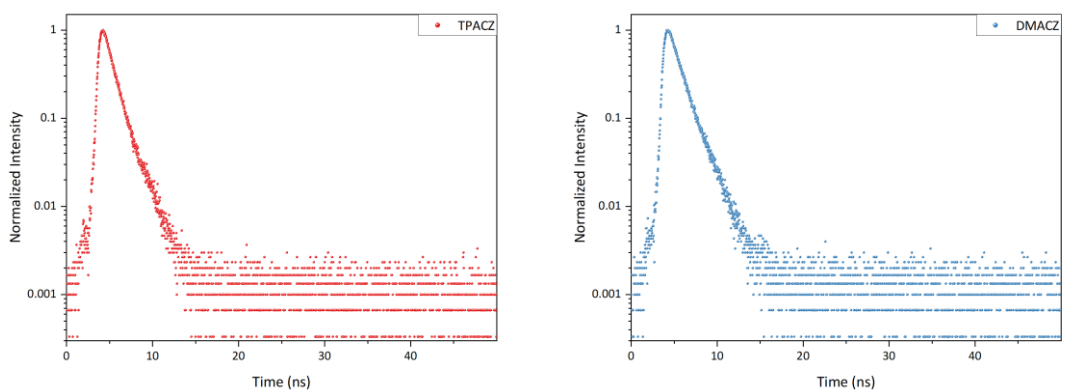

Fig. S10 Fluorescence decay curves of two molecules at a doping concentration of 0.2 mol%.

	0.2mol%	0.6mol%	1.0mol%	2.0mol%
TPACZ	1015.0ms	934.8ms	847.6ms	839.2ms
DMACZ	1689.1ms	1464.2ms	973.8ms	1223.8ms

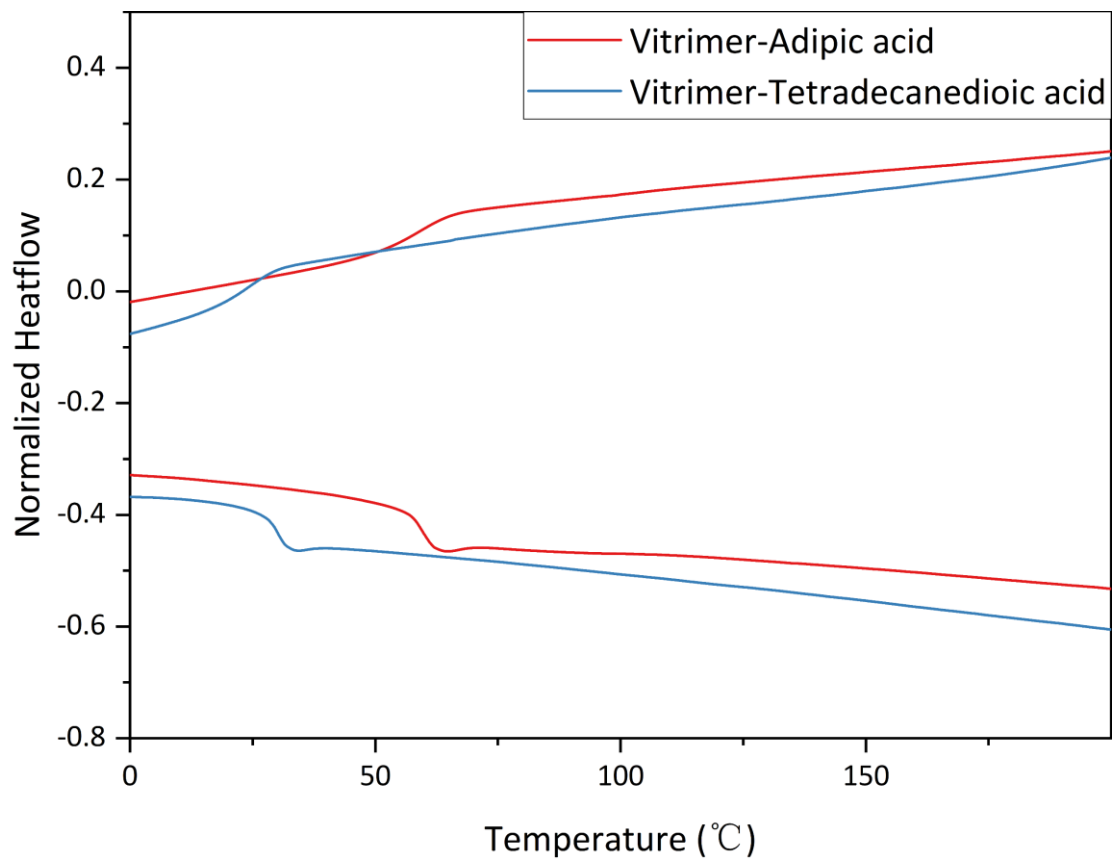Table S1 Phosphorescent lifetime at different doping concentrations.

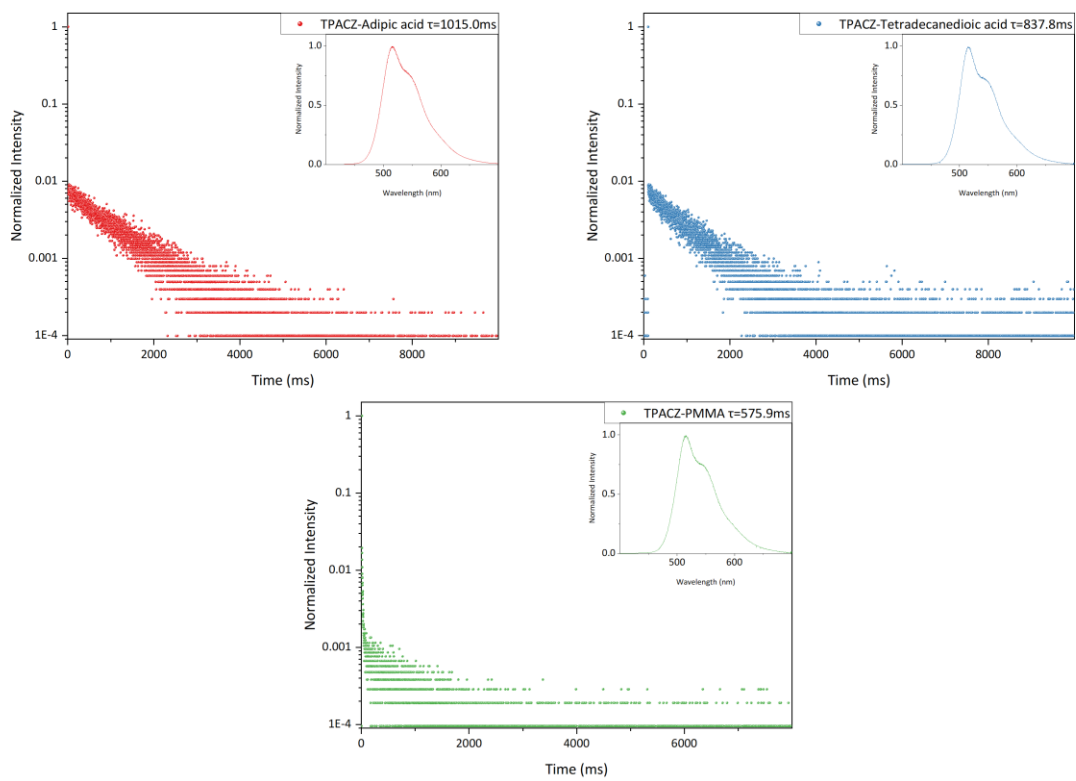Fig. S11 DSC curves of Vitrimer with different curing agents.

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

References

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