

## AIE (AIEE) and Mechanofluorochromic Performances of TPE-methoxylates: Effects of Single Molecular Conformations

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## Characterizations of diaryl methanones (1-4)

4,4'-Dihydroxybenzophenone (**1**) was synthesized according to the procedure described in literature.<sup>[1]</sup> <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 10.27 (s, 2H), 7.60 (d, *J* = 8.7 Hz, 4H), 6.87 (d, *J* = 8.7 Hz, 4H).

4, 4'-Dimethoxybenzophenone (**2**) was obtained by methoxylation of **1**. <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.71 (d, *J* = 8.9 Hz, 4H), 7.08 (d, *J* = 8.9 Hz, 4H), 3.85 (s, 6H).

3, 3', 4, 4'-Tetrahydroxybenzophenone (**3**) was synthesized according to the procedure described in the previous literature.<sup>[1]</sup> <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 9.72 (s, 2H), 9.34 (s, 2H), 7.16 (d, *J* = 2.1 Hz, 2H), 7.05 (dd, *J* = 8.2, 2.1 Hz, 2H), 6.82 (d, *J* = 8.2 Hz, 2H).

3, 3', 4, 4'-Tetramethoxybenzophenone (**4**) was obtained by methoxylation of **3**. <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>) δ (ppm): 7.32 (m, 4H), 7.12–7.06 (m, 2H), 3.86 (s, 6H), 3.81 (s, 6H).

## Characterizations of TMOE, TDMOE and TPE

Tetra(4-methoxyphenyl)ethylene (**TMOE**)

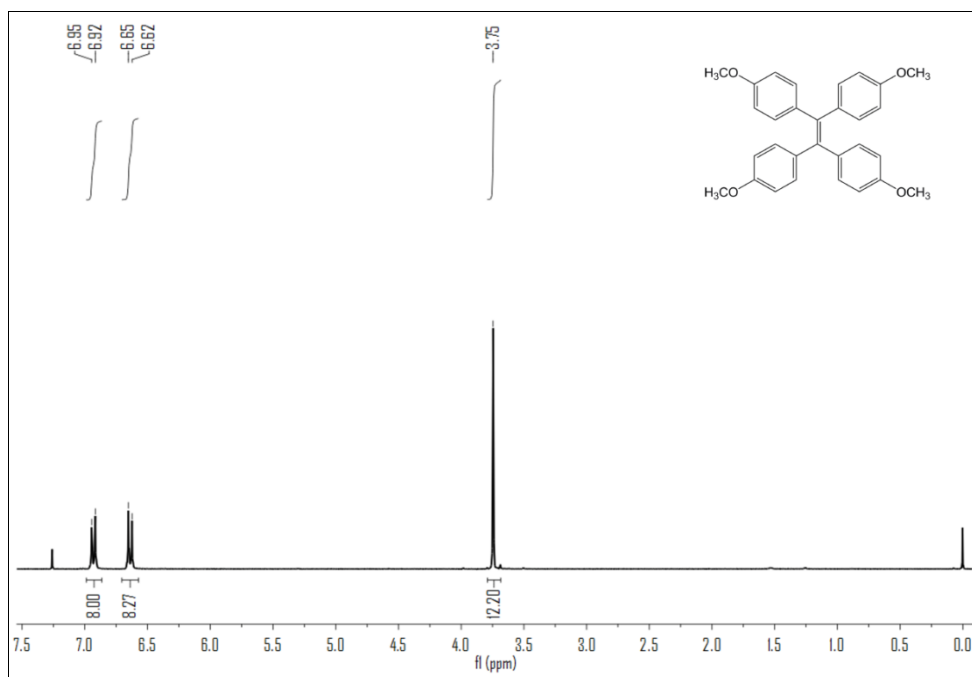
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ (ppm): 6.93 (d, *J* = 8.7 Hz, 8H), 6.64 (d, *J* = 8.7 Hz, 8H), 3.74 (s, 12H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 157.79, 138.38, 136.91, 132.55, 113.03, 55.09.

Tetra(3, 4-dimethoxyphenyl)ethylene (**TDMOE**)

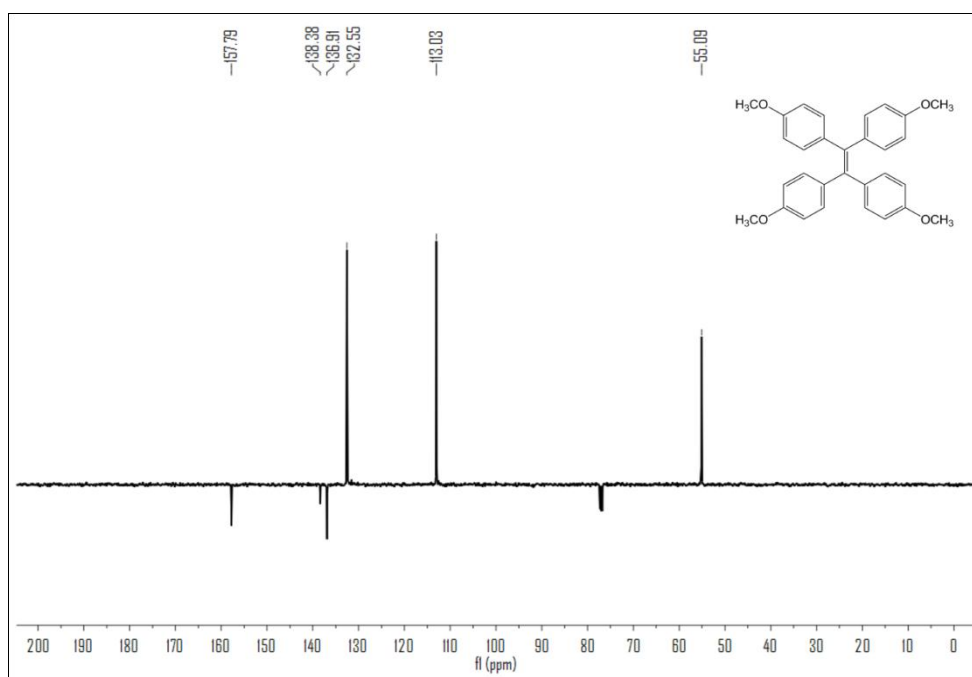
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ (ppm): 6.66–6.58 (m, 12H), 3.83 (s, 12H), 3.55 (s, 12H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 148.04, 147.49, 139.02, 136.78, 123.91, 114.90, 110.35, 55.75, 55.69.

Tetraphenylethene (**TPE**)

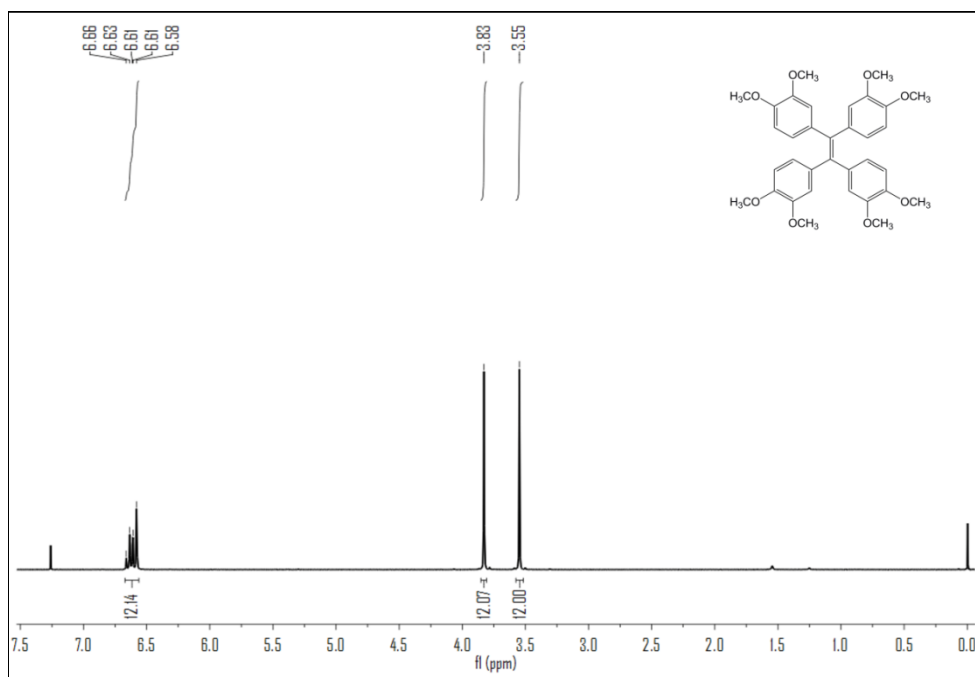
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 7.17–6.95 (m, 20H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 143.75, 140.99, 131.36, 127.67, 126.44.



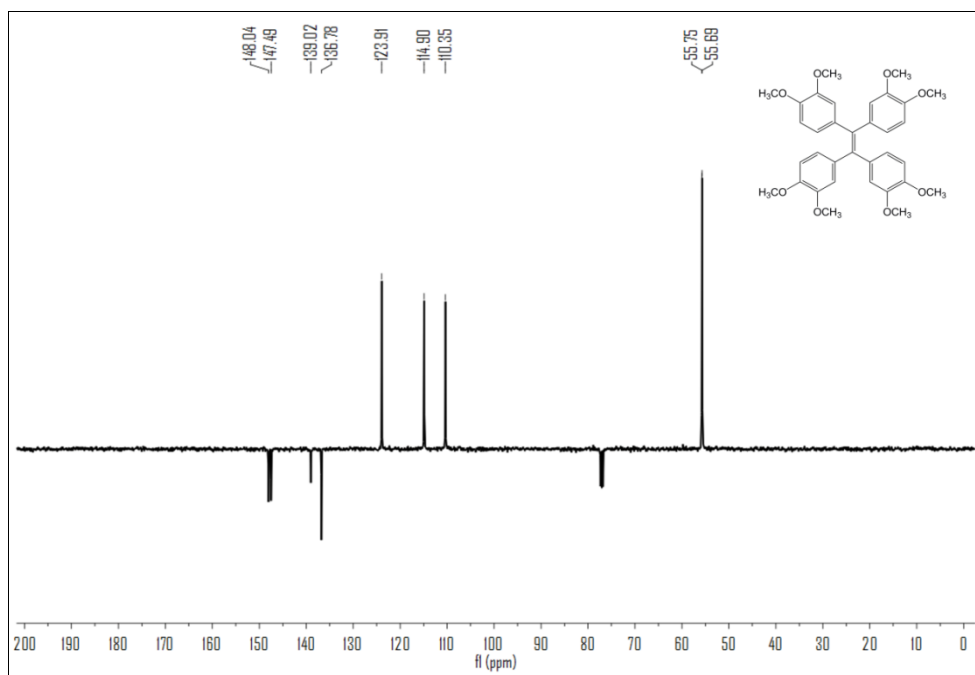
**Fig. S1** <sup>1</sup>H NMR spectrum of TMOE in CDCl<sub>3</sub> solution.



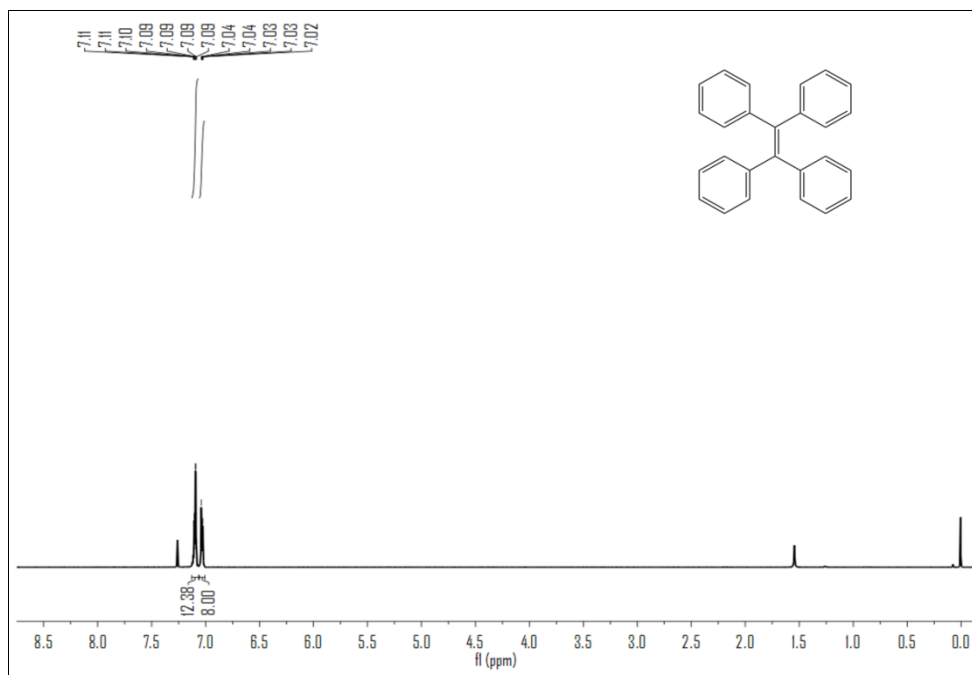
**Fig. S2** <sup>13</sup>C NMR spectrum of TMOE in CDCl<sub>3</sub> solution.



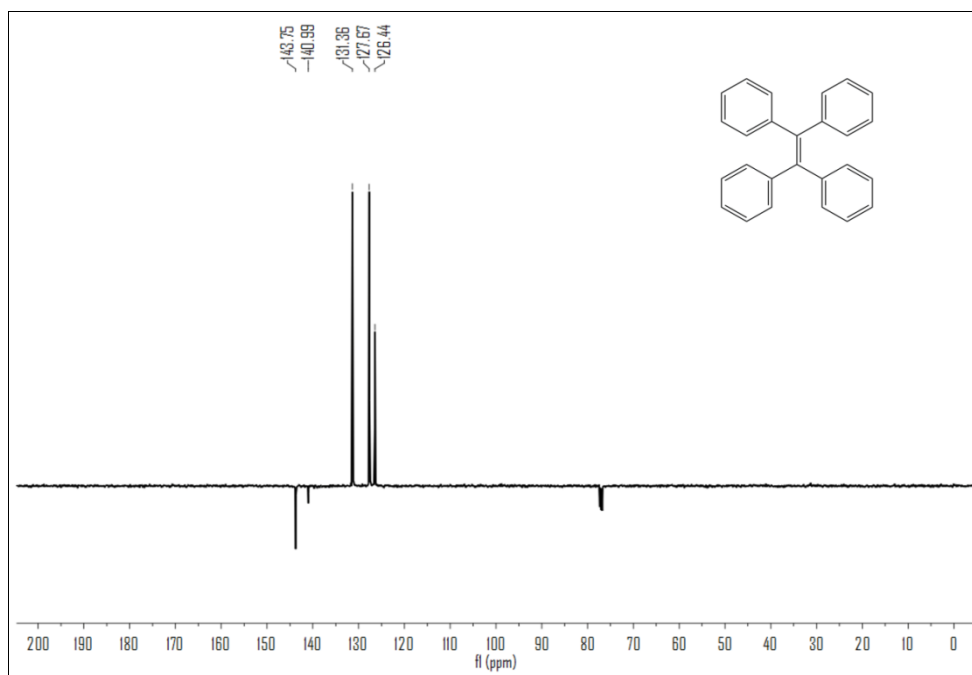
**Fig. S3**  $^1\text{H}$  NMR spectrum of TDMOE in  $\text{CDCl}_3$  solution.



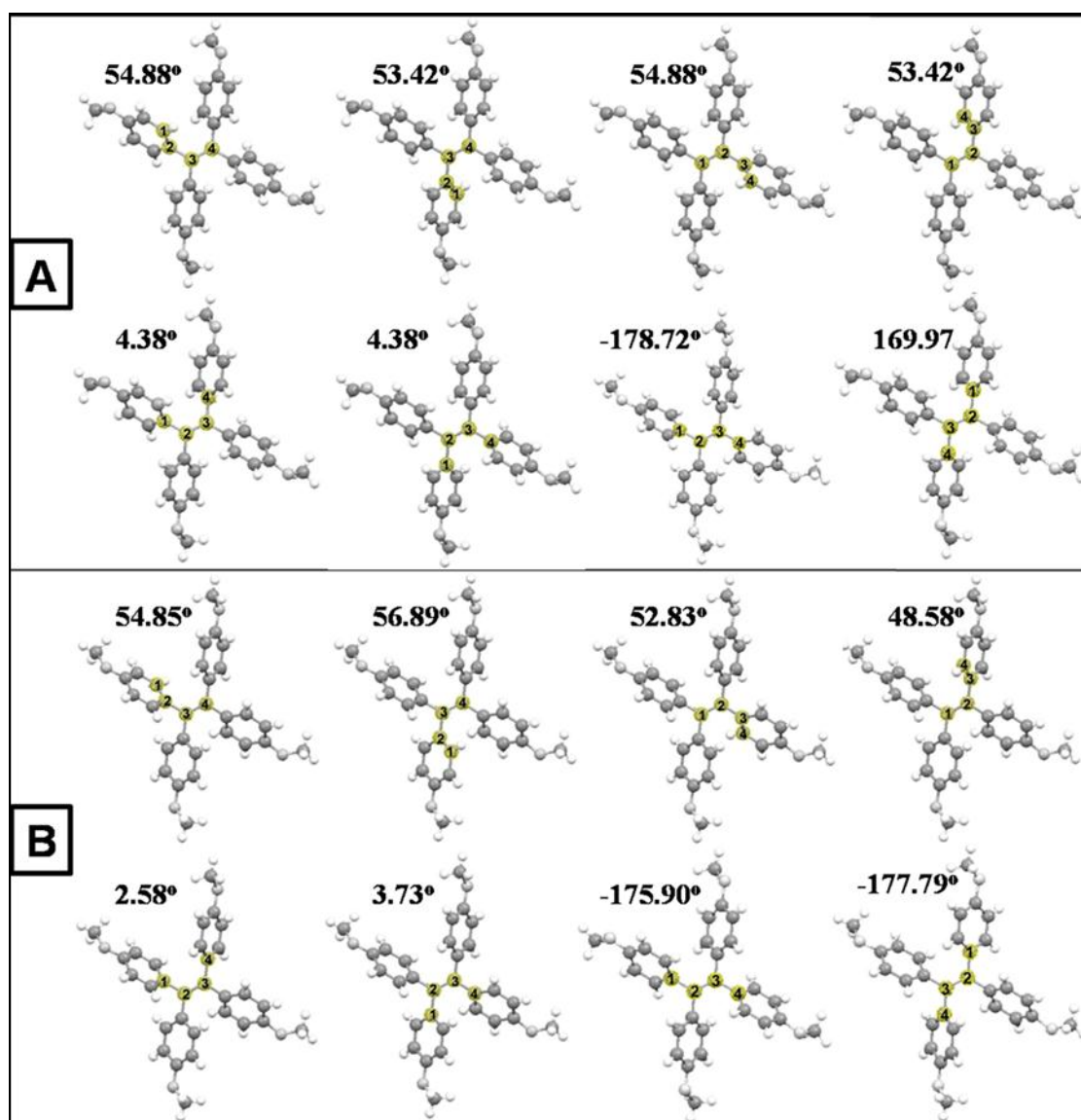
**Fig. S4**  $^{13}\text{C}$  NMR spectrum of TDMOE in  $\text{CDCl}_3$  solution.



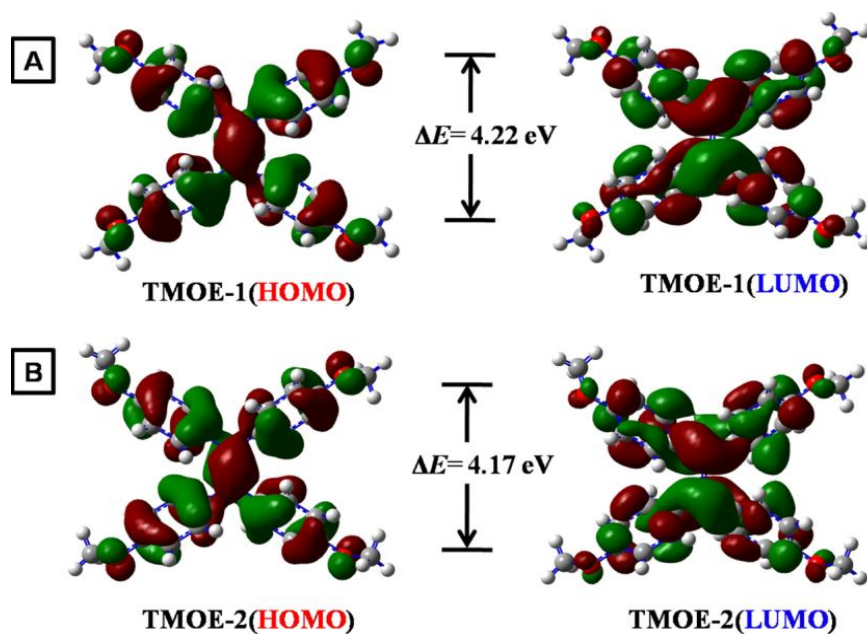
**Fig. S5** <sup>1</sup>H NMR spectrum of TPE in CDCl<sub>3</sub> solution.



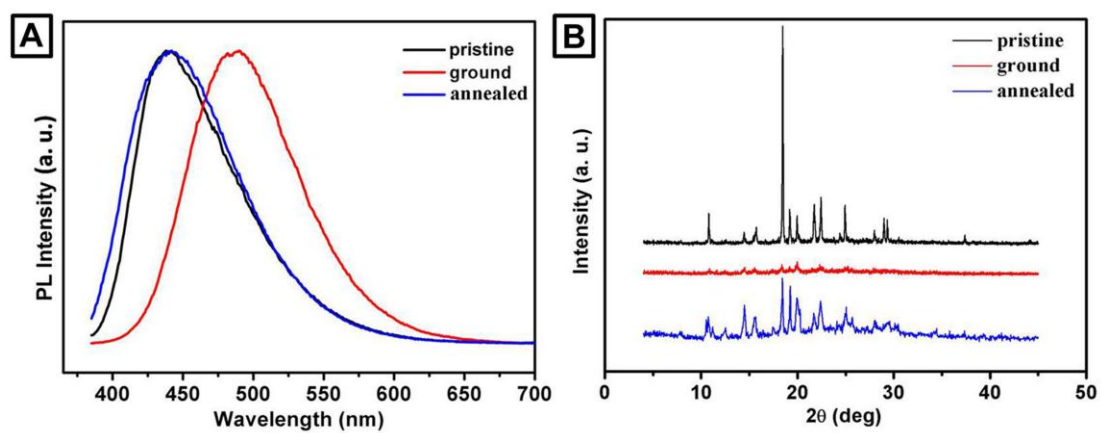
**Fig. S6** <sup>13</sup>C NMR spectrum of TPE in CDCl<sub>3</sub> solution.



**Fig. S7** Torsion angle data in (A) TMOE-1 and (B) TMOE-2 crystals.

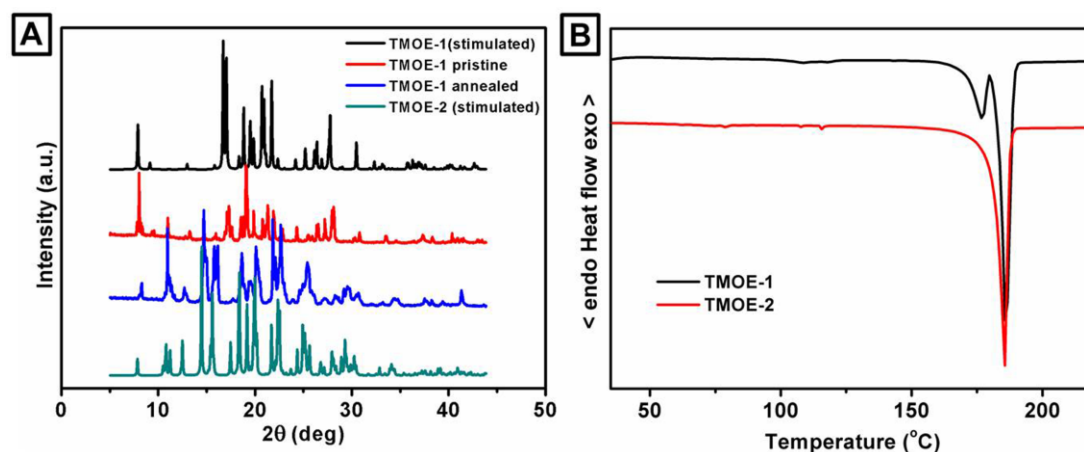


**Fig. S8** Calculated HOMO-LUMO bandgaps of TMOE in (A) TMOE-1 and (B) TMOE-2 crystals using B3LYP/6-31+g(d, p) basis set.

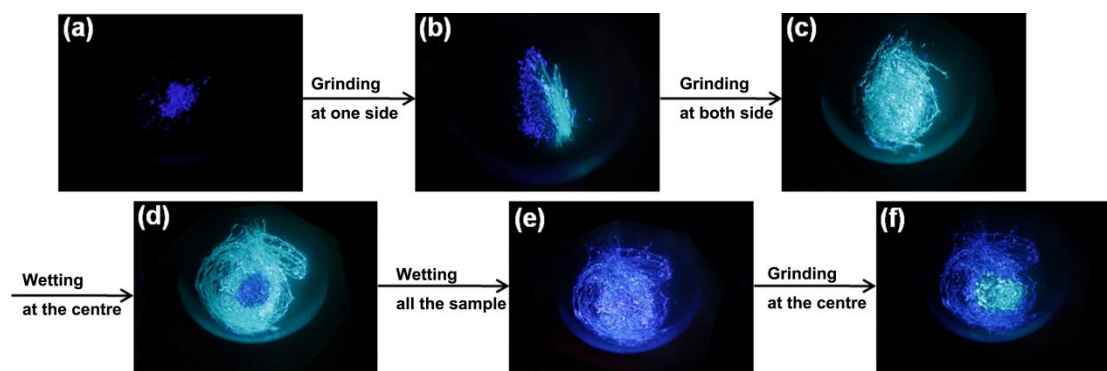


**Fig. S9** PL spectra (A) and XRD patterns (B) of TMOE-2: pristine, ground and annealed sample (150°C for 1 min).

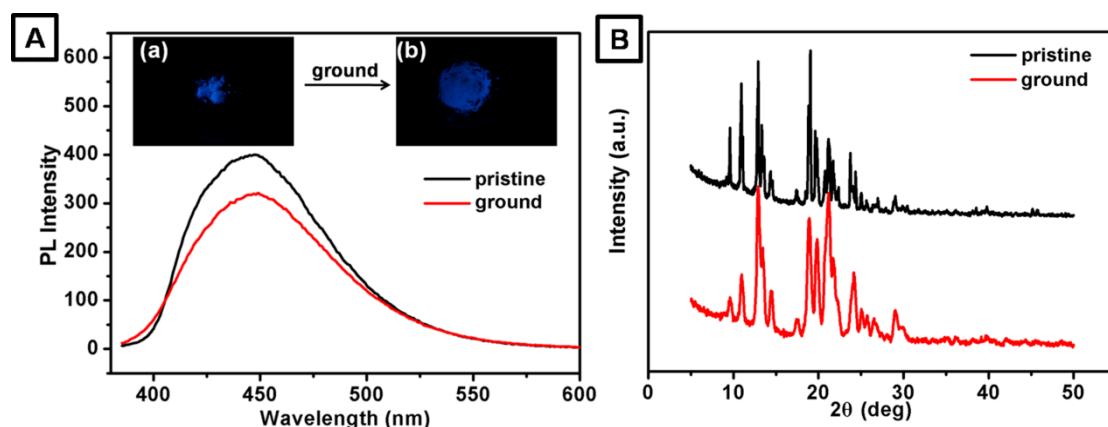




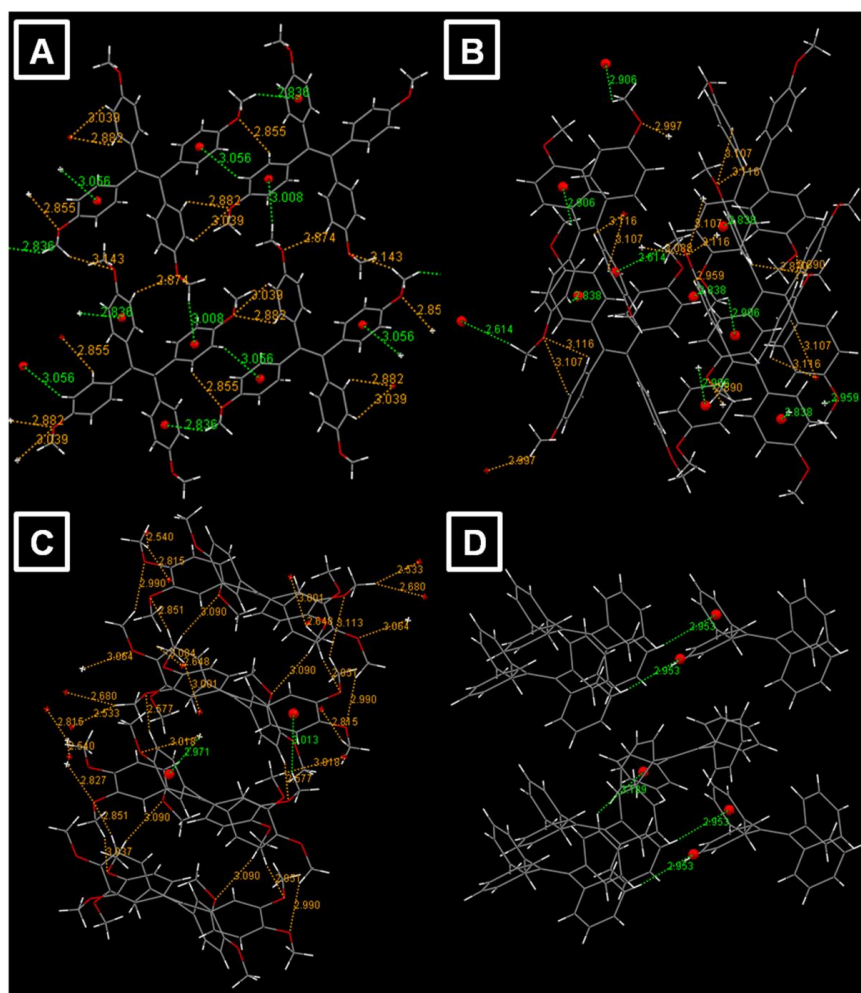
**Fig. S10** (A) Powder X-ray diffraction patterns of TMOE-1 before and after annealing at 176°C for 10 min, and the XRD patterns of TMOE-1 and TMOE-2 stimulated from their single crystal. (B) DSC curves of TMOE-1 and TMOE-2 crystals.



**Fig. S11** Real object illustration of the reversible mechanofluorochromic properties of TMOE with grinding and wetting with ethanol. The pictures were taken under 365 nm UV light irradiation. (a) TMOE-1 pristine crystals; (b) partially ground sample at one side; (c) entirely ground sample; (d) partially recovered sample by wetting with ethanol at the centre ; (e) entirely recovered sample by wetting with ethanol; (f) partially ground sample at the center from the recovered sample.



**Fig. S12** (A) PL spectra of TPE crystals before and after grinding. Inset: corresponding digital photos taken under 365 nm UV light irradiation. (B) Powder X-ray diffraction patterns of TPE crystals before and after grinding.



**Fig. S13** Analysis of the weak interactions in single crystal structures of (A) TMOE-1, (B) TMOE-2, (C) TDMOE and (D) TPE. C-H... $\pi$  (green line) and C-H...O (orange line).

**Reference:**

1. L. N. Stanley, *US Pat.*, 3 073 866, 1963.