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

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Electronic Supplementary Information (ESI\textdagger)
Figure S10. (A) Powder X-ray diffraction patterns of TMOE-1 before and after annealing at 176 °C, 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..............................................................................................................................................9

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Characterizations of diaryl methanones (1-4)

4,4'-Dihydroxybenzophenone (1) was synthesized according to the procedure described in literature.[1] $^1$H NMR (300 MHz, DMSO-$d_6$) 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. $^1$H NMR (300 MHz, DMSO-$d_6$) 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.[1] $^1$H NMR (300 MHz, DMSO-$d_6$) 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. $^1$H NMR (300 MHz, DMSO-$d_6$) 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)
$^1$H NMR (300 MHz, CDCl$_3$) δ (ppm): 6.93 (d, $J = 8.7$ Hz, 8H), 6.64 (d, $J = 8.7$ Hz, 8H), 3.74 (s, 12H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ (ppm): 157.79, 138.38, 136.91, 132.55, 113.03, 55.09.

Tetra(3, 4-dimethoxyphenyl)ethylene (TDMOE)
$^1$H NMR (300 MHz, CDCl$_3$) δ (ppm): 6.66–6.58 (m, 12H), 3.83 (s, 12H), 3.55 (s, 12H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ (ppm): 148.04, 147.49, 139.02, 136.78, 123.91, 114.90, 110.35, 55.75, 55.69.

Tetraphenylethene (TPE)
$^1$H NMR (500 MHz, CDCl$_3$) δ (ppm): 7.17–6.95 (m, 20H). $^{13}$C NMR (125 MHz, CDCl$_3$) δ (ppm): 143.75, 140.99, 131.36, 127.67, 126.44.
Fig. S1 $^1$H NMR spectrum of TMOE in CDCl$_3$ solution.

Fig. S2 $^{13}$C NMR spectrum of TMOE in CDCl$_3$ solution.
**Fig. S3** $^1$H NMR spectrum of TDMOE in CDCl$_3$ solution.

**Fig. S4** $^{13}$C NMR spectrum of TDMOE in CDCl$_3$ solution.
Fig. S5 \(^1\)H NMR spectrum of TPE in CDCl\(_3\) solution.

Fig. S6 \(^{13}\)C NMR spectrum of TPE in CDCl\(_3\) 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 mecanofluorochromic 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···π (green line) and C-H···O (orange line).

Reference: