Supporting Information

Tuning Photochromism of Indeno-Fused 2H-Naphthopyrans by Steric Spiro cyclic Groups

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1. Synthesis of compounds NPs

5-hydroxy-7H-benzo[c]fluoren-7-one (1) and 1,1-bis(4-methoxyphenyl)-2-propyn-1-ol were prepared according to the procedures in the literature.1,2

Synthesis of 5-methoxy-benzofluoren-7(H)-one (2)

A mixture of 5-hydroxy-7H-benzo[c]fluoren-7-one (2.60 g, 10.65 mmol), K₂CO₃ (5.84 g, 42.223 mmol) and CH₃I (2.25 g, 15.84 mmol) in acetonitrile (30 mL) was stirred at room temperature for 4 h. The reaction mixture was poured into H₂O (100 mL) and extracted with ethyl acetate (50 mL × 3). The organic extracts were combined, washed with brine and water, dried with anhydrous MgSO₄, filtered, and the solvent was then removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 20:1) as an eluent affording 5-methoxy-benzofluoren-7(H)-one (2) as a reddish-brown solid (2.43 g, 9.34 mmol) in 88% yield. m.p 142.6 - 143.8°C.

^1H NMR (400 MHz, Chloroform-d) δ 8.32 (d, J = 8.3 Hz, 1H), 8.27 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 7.5 Hz, 1H), 7.61 – 7.50 (m, 3H), 7.42 (t, J = 7.5 Hz, 1H), 7.18 (t, J = 7.4 Hz, 1H), 7.03 (s, 1H), 4.03 (s, 3H).

^13C NMR (101 MHz, Chloroform-d) δ 194.84, 156.78, 145.52, 135.16, 134.50, 134.48, 132.47, 129.53, 129.28, 128.09, 127.46, 127.44, 124.49, 123.82, 123.72, 122.22, 98.05, 77.38, 77.06, 76.74, 55.91.

Synthesis of 5-methoxy-7-(1,2,2-triphenylvinyl)-7H-benzo[c]fluoren-7-ol (3)

To a flame-dried 250 mL Schlenk flask, bromotriphenylethylene (1.90 g, 5.76 mmol), magnesium powder (158.74 mg, 6.53 mmol), small amounts of I₂ (9.75 mg, 38.42 µmol) and dry THF (80 mL) were added under argon atmosphere. The mixture was stirred for 5 hours at 60°C, then cooled to 0°C. Subsequently, 5-methoxy-benzofluoren-7(H)-one (2) (1.0 g, 3.84 mmol) was slowly added using a syringe and the mixture was heated to reflux. After allowing it to react overnight and cool to room temperature, a solution of ammonium chloride was added and the mixture was extracted with ethyl acetate (50 mL × 3). The organic extracts were combined and washed with brine and water, then dried with anhydrous MgSO₄, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 50:1) as an eluent affording 5-methoxy-7-(1,2,2-triphenylvinyl)-7H-benzo[c]fluoren-7-ol (3) as a pale-yellow solid (365 mg, 0.689 mmol) in 18% yield. m.p. 183.5 - 184.5 °C.
^1H NMR (400 MHz, DMSO-d_6) δ 8.32 – 8.22 (m, 2H), 7.78 – 7.74 (m, 1H), 7.74 – 7.70 (m, 1H), 7.61 – 7.56 (m, 1H), 7.53 – 7.47 (m, 1H), 7.30 – 7.22 (m, 5H), 7.05 (t, J = 7.4 Hz, 2H), 7.00 – 6.95 (m, 1H), 6.94 – 6.85 (m, 4H), 6.84 – 6.79 (m, 1H), 6.65 – 6.59 (m, 1H), 6.54 (t, J = 7.2 Hz, 2H), 6.44 (d, J = 7.4 Hz, 2H), 5.42 (s, 1H).

^13C NMR (101 MHz, DMSO-d_6) δ 155.86, 152.65, 151.16, 144.61, 143.16, 142.49, 141.76, 141.44, 140.59, 132.14, 129.73, 129.57, 128.59, 128.35, 127.71, 127.64, 127.25, 126.85, 126.70, 126.09, 126.05, 125.70, 125.66, 125.30, 125.17, 124.60, 124.16, 122.95, 122.04, 101.94, 82.94, 56.31, 40.64, 40.43, 40.22, 40.01, 39.80, 39.59, 39.38.

HRMS (ESI) calcd. for C_{38}H_{28}O_{2} [M+Na]^+ 539.1982; found 539.1984.

Synthesis of 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden] (4)

Under an argon atmosphere, anhydrous SnCl\textsubscript{2} (175 mg, 0.39 mmol) was added into a solution of 5-methoxy-7-(1,2,2-triphenylvinyl)-7H-benzo[c]fluoren-7-ol (3) (0.46 mmol) in dry CH\textsubscript{2}Cl\textsubscript{2} (20 mL). The mixture was stirred for 3 h at room temperature. The reaction mixture was extracted by ethyl acetate twice (50 mL × 2). The organic extracts were combined, washed with brine and water, dried with anhydrous MgSO\textsubscript{4}, filtered, and the solvent was then removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 50:1) as an eluent affording 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden] (4) was obtained as a pale-yellow solid (144 mg, 0.29 mmol) in 85% yield. m.p. 186.5 - 187.5 °C

^1H NMR (400 MHz, Chloroform-d) δ 8.71 (d, J = 8.4 Hz, 1H), 8.34 (dd, J = 8.4, 1.3 Hz, 1H), 8.25 (d, J = 7.8 Hz, 1H), 7.73 – 7.64 (m, 1H), 7.57 – 7.49 (m, 3H), 7.48 – 7.32 (m, 5H), 7.30 – 7.22 (m, 1H), 7.15 – 7.05 (m, 2H), 7.03 – 6.97 (m, 1H), 6.88 – 6.81 (m, 1H), 6.79 – 6.71 (m, 2H), 6.67 – 6.58 (m, 3H), 6.47 (s, 1H), 3.82 (s, 3H).

^13C NMR (101 MHz, Chloroform-d) δ 156.18, 148.56, 146.27, 145.90, 145.52, 145.49, 143.65, 143.41, 135.54, 134.98, 130.41, 129.92, 129.78, 128.75, 128.68, 127.86, 127.69, 127.66, 127.38, 127.22, 126.93, 126.48, 126.15, 125.76, 124.88, 123.66, 123.35, 123.26, 122.55, 122.11, 120.82, 99.89, 77.44, 77.33, 77.13, 76.81, 70.86, 55.79.

HRMS (ESI) calcd. for C_{38}H_{28}O_{2} [M+Na]^+ 521.1876; found 521.1878.

Synthesis of 2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden]-5-ol (5)

Under an argon atmosphere, 30 mL of dry dichloroethane was added to a dry Schlenk flask (100 mL), followed by the appropriate stoichiometric amount of 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden] (4) (260 mg, 0.52 mmol). A solution of boron
S4 tribromide (653 mg, 2.16 mmol) was then added in an ice bath. The reaction was allowed to proceed for 5 hours at room temperature, followed by the addition of water at 0 °C. The reaction mixture was extracted by ethyl acetate twice (50 mL × 2). The organic extracts were combined, washed with brine and water, dried with anhydrous MgSO₄, filtered, and the solvent was then removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 50:1) as an eluent affording 2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden]-5-ol (5) was obtained as a white solid (220 mg, 0.29 mmol) in 87% yield. m.p. 197.5 - 198.6 °C

1H NMR (400 MHz, Chloroform-d) δ 8.77 (d, J = 8.5 Hz, 1H), 8.30 (d, J = 8.2 Hz, 2H), 7.72 (t, J = 7.7 Hz, 1H), 7.60 – 7.53 (m, 3H), 7.51 – 7.37 (m, 5H), 7.32 – 7.27 (m, 1H), 7.19 – 7.11 (m, 2H), 7.06 – 6.99 (m, 1H), 6.90 – 6.84 (m, 1H), 6.83 – 6.76 (m, 2H), 6.72 – 6.59 (m, 3H), 6.51 (s, 1H).

13C NMR (101 MHz, Chloroform-d) δ 152.02, 148.49, 146.03, 145.48, 145.22, 143.56, 143.42, 135.51, 134.84, 130.60, 130.30, 129.70, 128.77, 128.65, 127.90, 127.69, 127.64, 127.45, 127.26, 126.94, 126.45, 125.88, 124.87, 123.80, 123.39, 123.11, 122.52, 122.10, 120.77, 104.57, 77.42, 77.10, 76.78, 70.45.

HRMS (ESI) calcd. for C₃₇H₂₄O [M+Na]⁺ 507.1719; found 507.1723

The synthesis of compounds NP-a:

A solution of 2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden]-5-ol (5) (3.8 mmol), 1,1-diphenylprop-2-yn-1-ol 5a (0.11 g, 0.52 mmol), and two drops of dodecylbenzenesulfonic acid in dry toluene (8 mL) was stirred at 40 °C for 3 h. After cooling down to room temperature, the reaction mixture was extracted by ethyl acetate twice (50 mL × 2). The organic extracts were combined, washed with brine and water, dried with anhydrous MgSO₄, filtered, and the solvent was then removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 50:1) as an eluent affording NP-a as a pale-yellow solid in 43%. m.p. 183.5 - 184.6 °C

1H NMR (400 MHz, Chloroform-d) δ 8.70 (d, J = 8.5 Hz, 1H), 8.46 (d, J = 8.4 Hz, 1H), 8.24 (d, J = 7.8 Hz, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.56 (d, J = 7.2 Hz, 4H), 7.48 (t, J = 7.4 Hz, 2H), 7.44 – 7.28 (m, 8H), 7.17 – 7.07 (m, 3H), 6.90 (t, J = 7.4 Hz, 1H), 6.83 (d, J = 8.5 Hz, 2H), 6.78 – 6.68 (m, 5H), 6.59 (d, J = 7.7 Hz, 2H), 6.43 (d, J = 9.8 Hz, 1H), 5.91 (d, J = 9.8 Hz, 1H), 3.80 (s, 3H), 3.75 (s, 3H).

13C NMR (101 MHz, Chloroform-d) δ 157.72, 147.05, 146.75, 145.40, 145.25, 144.07, 142.05, 141.66, 138.89, 136.00, 135.22, 134.36, 133.68, 129.72, 128.84, 128.44, 127.99, 127.65, 127.63, 127.29, 127.26, 126.61, 126.55, 126.48, 126.24, 126.01, 125.71, 125.51, 124.75, 124.52, 124.00, 122.68, 122.27, 121.56, 121.36, 121.18, 120.04, 119.07, 113.13, 112.30, 81.38, 69.31, 54.17, 54.09.

HRMS (ESI) calcd. for C₅₂H₃₄O₃ [M+Na]⁺ 757.2713; found 757.2718.

Synthesis of 5-methoxyspiro[benzo[c]fluorene-7,13'-inden][1,2-l]phenantherene (6)

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To a flame-dried 50 mL round-bottom flask, Potassium iodide (4.10 mmol) and 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-indenene] (4) (0.802 mmol and cyclohexane (20 mL) were added under air atmosphere. The solution was irradiated with a UV lamp (365 nm, 500 mW) for 4 hours. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 50 : 1) as an eluent affording 5-methoxyspiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthrene] as a pale-yellow solid (310 mg, 0.623 mmol) in 77% yield. m.p. 226.5 - 227.5 °C

$^1$H NMR (400 MHz, Chloroform-d) $\delta$ 9.13 (d, $J = 8.2$ Hz, 1H), 8.94 (d, $J = 8.5$ Hz, 1H), 8.89 (d, $J = 8.3$ Hz, 1H), 8.70 (d, $J = 8.4$ Hz, 1H), 8.56 (d, $J = 7.9$ Hz, 1H), 8.50 (d, $J = 7.9$ Hz, 1H), 8.37 (d, $J = 8.4$ Hz, 1H), 7.89 (t, $J = 7.5$ Hz, 1H), 7.81 (t, $J = 7.8$ Hz, 2H), 7.59 (t, $J = 7.6$ Hz, 1H), 7.51 – 7.40 (m, 3H), 7.15 – 7.06 (m, 2H), 7.01 (t, $J = 7.5$ Hz, 1H), 6.93 (d, $J = 8.2$ Hz, 1H), 6.78 – 6.67 (m, 2H), 6.13 (s, 1H), 3.58 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-d) $\delta$ 156.32, 150.51, 148.76, 148.63, 142.97, 142.33, 141.65, 136.90, 131.86, 130.71, 130.57, 129.00, 128.94, 128.42, 127.90, 127.56, 127.47, 127.19, 127.10, 126.95, 126.54, 126.26, 126.19, 125.97, 125.04, 124.90, 124.75, 123.76, 123.73, 123.49, 123.31, 123.22, 123.13, 122.90, 122.38, 99.89, 77.37, 77.26, 77.06, 76.74, 67.22, 55.61.

HRMS (ESI) calcd. for C_{52}H_{34}O_{3} [M+Na]$^+$ 757.2713; found 757.2718.

Synthesis of spiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthren]-5-ol (7)

5-methoxyspiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthrene] (6) (260 mg, 0.52 mmol) and boron tribromide (653 mg, 2.16 mmol) were combined in a 50 mL round-bottom flask and dissolved in dry dichloroethane (20 mL) under an argon atmosphere. The reaction was allowed to proceed for 5 hours at room temperature, followed by the addition of water at 0°C. The organic phase was combined and washed with brine and water, then dried with anhydrous MgSO$_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 50 : 1) as an eluent affording spiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthren]-5-ol (7) as a pale-yellow solid (185 mg, 0.38 mmol) in 73% yield. m.p. 197.5 - 198.6 °C

$^1$H NMR (400 MHz, Chloroform-d) $\delta$ 9.09 (d, $J = 8.2$ Hz, 1H), 8.93 (d, $J = 8.6$ Hz, 1H), 8.86 (d, $J = 8.3$ Hz, 1H), 8.69 (d, $J = 8.4$ Hz, 1H), 8.53 (d, $J = 7.9$ Hz, 1H), 8.49 (d, $J = 7.9$ Hz, 1H), 8.28 (d, $J = 8.4$ Hz, 1H), 7.87 (t, $J = 7.6$ Hz, 1H), 7.83 – 7.75 (m, 2H), 7.58 (t, $J = 7.7$ Hz, 1H), 7.54 – 7.40 (m, 3H), 7.15 – 6.99 (m, 3H), 6.89 (d, $J = 8.2$ Hz, 1H), 6.75 (d, $J = 7.5$ Hz, 1H), 6.70 (d, $J = 7.6$ Hz, 1H), 6.11 (s, 1H).
**13C NMR (101 MHz, Chloroform-d)** \(\delta\) 156.32, 150.51, 148.76, 148.63, 142.97, 142.33, 141.65, 136.90, 131.86, 130.71, 130.57, 129.00, 128.94, 128.42, 127.90, 127.56, 127.47, 127.19, 127.10, 126.95, 126.54, 126.26, 126.19, 125.97, 125.04, 124.90, 124.75, 123.76, 123.73, 123.49, 123.31, 123.22, 123.13, 122.90, 122.38, 99.89, 77.37, 77.26, 77.06, 76.74, 67.22, 55.61.

**HRMS (ESI)** calcd. for C\(_{37}\)H\(_{22}\)O [M+H]+ 483.1743; found 483.1705.

**Compound NP-b**

This compound was prepared according to the same procedure as that of **NP-b**, except that the eluent for column chromatography is petroleum ether/ethyl acetate (v/v = 50 : 1) as an eluent. The product **NP-b** is a pale-yellow solid in 46% yield. m.p. 179.5 - 180.6 °C.

**1H NMR (400 MHz, Chloroform-d)** \(\delta\) 9.44 (d, \(J = 8.0\) Hz, 1H), 9.06 (d, \(J = 8.2\) Hz, 1H), 8.91 (d, \(J = 8.6\) Hz, 1H), 8.84 (d, \(J = 8.3\) Hz, 1H), 8.66 (d, \(J = 8.3\) Hz, 1H), 8.52 – 8.45 (m, 2H), 8.27 (d, \(J = 8.4\) Hz, 1H), 7.87 – 7.81 (m, 1H), 7.81 – 7.74 (m, 2H), 7.56 (t, \(J = 7.8\) Hz, 1H), 7.49 – 7.44 (m, 2H), 7.42 – 7.38 (m, 2H), 7.28 (d, \(J = 8.5\) Hz, 1H), 7.20 (s, 1H), 7.09 – 7.04 (m, 2H), 7.02 – 6.98 (m, 1H), 6.93 (d, \(J = 8.3\) Hz, 2H), 6.89 – 6.85 (m, 3H), 6.72 (d, \(J = 7.8\) Hz, 1H), 6.67 (d, \(J = 7.6\) Hz, 1H), 6.46 (d, \(J = 8.0\) Hz, 1H), 6.09 (s, 1H), 3.85 (s, 3H), 3.81 (s, 3H).

**13C NMR (101 MHz, Chloroform-d)** \(\delta\) 193.78, 162.24, 161.70, 160.79, 152.27, 150.38, 148.62, 148.50, 142.96, 142.28, 141.46, 136.81, 132.49, 132.44, 131.79, 130.79, 130.68, 130.60, 129.31, 129.20, 128.90, 128.38, 128.29, 128.11, 127.98, 127.62, 127.55, 127.19, 127.14, 126.93, 126.57, 126.29, 126.09, 125.43, 124.99, 124.96, 124.85, 124.82, 124.68, 123.85, 123.75, 123.48, 123.34, 123.22, 123.11, 122.94, 122.39, 77.38, 77.06, 76.75, 66.86, 55.45, 55.43.

**HRMS (ESI)** Calcd. for C\(_{54}\)H\(_{36}\)O\(_3\) [M+H]+ 733.2738; found 733.2719.
2. NMR Spectra

Fig. S1 $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of 5-methoxy-benzofluoren-7(H)-one.

Fig. S2 $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of 5-methoxy-benzofluoren-7(H)-one.
**Fig. S3** $^1$H NMR spectrum (400 MHz, DMSO-$d_6$, 298 K) of 5-methoxy-7-(1,2,2-triphenylvinyl)-7$H$-benzo[c]fluoren-7-ol

**Fig. S4** $^{13}$C NMR spectrum (101 MHz, DMSO-$d_6$, 298 K) of 5-methoxy-7-(1,2,2-triphenylvinyl)-7$H$-benzo[c]fluoren-7-ol
Fig. S5 $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-indene]

Fig. S6 $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-indene]
Fig. S7 $^1$H NMR spectrum (400 MHz, CDCl₃, 298 K) of 2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden]-5-ol

Fig. S8 $^{13}$C NMR spectrum (101 MHz, CDCl₃, 298 K) of 2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden]-5-ol
**Fig. S9** $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of 5-methoxyspiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthrene]

**Fig. S10** $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of 5-methoxyspiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthrene]
Fig. S11 $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of spiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthren]-5-ol

Fig. S12 $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of spiro[benzo[c]fluorene-7,13'-indeno[1,2-l]phenanthren]-5-ol
**Fig. S13** $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of NP

**Fig. S14** $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of NP
Fig. S15 $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of NP-a

Fig. S16 $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of NP-a
Fig. S17 $^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of NP-b

Fig. S18 $^{13}$C NMR spectrum (101 MHz, CDCl$_3$, 298 K) of NP-b
3. MS Spectra

**Fig. S19** HR-ESI-TOF-MS of 5-methoxy-7-{1,2,2-triphenylvinyl}-7H-benzo[c]fluoren-7-ol

**Fig. S20** HR-ESI-TOF-MS of 5-methoxy-2',3'-diphenylspiro[benzo[c]fluorene-7,1'-indene]
Fig. S21 HR-ESI-TOF-MS of 2',3'-diphenylspiro[benzo[c]fluorene-7,1'-inden]-5-ol

Fig. S22 HR-ESI-TOF-MS of 5-methoxyspiro[benzo[c]fluorene-7,13'-indenopheno[1,2-l]phenanthrene]
Fig. S23 HR-ESI-TOF-MS of spiro[benzo[c]fluorene-7,13’-indeno[1,2-l]phenanthren]-5-ol

Fig. S24 HR-ESI-TOF-MS of NP-a
4. Optical Properties of NPs in the solution

Fig. S26 UV-Vis absorption spectra of **NP-a** in chloroform with various concentrations upon irradiation with UV light (365 nm, 200 mW) for 50 seconds
**Fig. S27** Color change of NP-a and NP-b in chloroform (8.0 x 10^-5 M) upon UV irradiation (365nm, 260mW/cm²) to PSS

**Fig. S28** Photochromic curves over time at $\lambda_{max}$ of NP-b and NP in chloroform (8 x 10^-5 mol/L) upon UV irradiation (365nm, 260mW/cm²); (b) Thermal fading curves of NP-a, NP-b and NP in chloroform (8 x 10^-5 mol/L) at 298 K

**Fig. S29** Thermal fading curves with kinetics parameters of (a) NP-a, (b) NP-b and (c) NP in chloroform (8 x 10^-5 mol/L) at 298 K
Table S1 Photophysical data of NP-a in various solvents (5 × 10^{-5} mol/L) upon irradiation with UV light (365 nm, 200 mW) for 50 s

<table>
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<th>Solvent</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>( A_{\text{max}} )</th>
<th>( \varepsilon/\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1} )</th>
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5. Optical Properties of PMMA Film Doped with NP-b

Fig. S30 (a) UV-Vis absorption spectra of the PMMA doped with NP-b without UV irradiation; (b) UV-Vis absorption spectra of the PMMA doped with NP-b upon UV irradiation (365nm, 260mW/cm^2) to PSS; (c) Photochromic curve over time at \( \lambda_{\text{max}} \) of the PMMA doped with NP-b; (d) Thermal fading curve of the PMMA doped with NP-b at 298 K.
Fig. S31 Absorbance values at $\lambda_{\text{max}}$ of the process of color generation and decoloration of the PMMA film doped with NP-b at room temperature.

6. X-ray Crystallographic Analysis.

Single crystals of NP-a were grown by slowly diffusing $n$-hexane into the chloroform solution.

Table S2 X-ray crystal structure refinement data for NP-a.

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<th>Identification code</th>
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<tr>
<td>a/Å</td>
<td>11.6774(3)</td>
</tr>
<tr>
<td>b/Å</td>
<td>12.0992(3)</td>
</tr>
<tr>
<td>c/Å</td>
<td>14.8445(4)</td>
</tr>
<tr>
<td>$\alpha$/°</td>
<td>88.277(2)</td>
</tr>
<tr>
<td>$\beta$/°</td>
<td>72.382(2)</td>
</tr>
<tr>
<td>$\gamma$/°</td>
<td>71.540(2)</td>
</tr>
<tr>
<td>Volume/Å³</td>
<td>1891.08(9)</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>$\rho_{\text{calc}}$ g/cm$^3$</td>
<td>1.291</td>
</tr>
<tr>
<td>$\mu$/mm$^{-1}$</td>
<td>0.613</td>
</tr>
<tr>
<td>F(000)</td>
<td>772.0</td>
</tr>
<tr>
<td>Radiation</td>
<td>CuK$_{\alpha}$ ($\lambda = 1.54184$)</td>
</tr>
<tr>
<td>2$\theta$ range for data collection/°</td>
<td>7.724 to 153.356</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-14 $\leq$ h $\leq$ 14, -15 $\leq$ k $\leq$ 15, -18 $\leq$ l $\leq$ 15</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>24115</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>7655 [R$<em>{\text{int}}$ = 0.0264, R$</em>{\text{sigma}}$ = 0.0253]</td>
</tr>
<tr>
<td>Data/restraints/parameters</td>
<td>7655/0/517</td>
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<tr>
<td>Goodness-of-fit on F2</td>
<td>1.059</td>
</tr>
<tr>
<td>Final R indexes [$I &gt; 2\sigma (I)$]</td>
<td>R$_1$ = 0.0383, wR$_2$ = 0.1023</td>
</tr>
<tr>
<td>Final R indexes [all data]</td>
<td>R$_1$ = 0.0416, wR$_2$ = 0.1049</td>
</tr>
<tr>
<td>Largest diff. peak/hole / e Å$^3$</td>
<td>0.43/-0.28</td>
</tr>
</tbody>
</table>
7. References