Supporting Information for

Novel Photochromic Infinite Coordination Polymer Particles Derived from Diarylethene Photoswitch

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1. Methods and Materials

All reagents and spectrograde solvents were purchased from Sigma-Aldrich, TCI and SAMCHUN and used as received. The $^1$HNMR and $^{13}$C NMR spectra were obtained using a JEOL JNM-AL300 spectrometer at 300 in CDCl$_3$, DMSO-d6, with tetramethylsilane as the internal reference. High resolution mass spectrometry (HRMS) spectra were obtained with JEOL JMS-700 spectrometer. Fourier transform infrared (FT-IR) spectroscopy measurements were performed using a JASCO FTIR-4200 instrument. TGA was performed using a TGA Q5000 IR / SDT Q600 (TA) Thermal Analyzer. FE-TEM was performed using a JEM-2100F (JEOL) Field Emission Transmission Electron Microscopy. FE-SEM was performed using a LEO SUPRA 55, GENESIS 2000 (Carl Zeiss, EDAX) Field Emission Scanning Electron Microscope. BET was performed using a BELSORP-max (MP) BET Surface area and Pore size Analyzer. Flash column chromatography was performed with Merck silica gel 60 (70-230 mesh). UV and visible irradiations were performed with standard lamps used for visualizing TLC plates (VL6L; 312 nm, 8 mW/cm$^2$) and a 400 W tungsten lamp and the samples were placed in a glass chamber maintained at room temperature. UV absorption spectra were recorded on a Shimadzu UV-3100 spectrophotometer in spectroscopy grade DMF. Photochromic changes were monitored using a 500 W xenon lamp (Newport-74000) equipped with a monochromator (Newport- 66921).
2. Experimental Procedures

**Compound 3**

To a 100mL two-neck flask was loaded 1\(^1\) (920 mg, 1.28 mmol), 2\(^2\) (491mg, 3.07 mol), CuI (28 mg, 0.15 mmol) and Pd(PPh\(_3\))\(_2\)Cl\(_2\) (50 mg, 0.07 mmol). Then degased triethyl -amine (40 mL) was added. The reaction mixture was heated to reflux overnight. The resulting mixture was cooled to room temperature, solvent was evaporated under a reduced pressure. Then the residue was purified by column chromatography (SiO\(_2\), EA:Hexane = 10:1) to afford brown yellow solid ( 552 mg, 0.71 mmol) of 3 in a 54.95% yield.

\(^1\)HNMR (300 MHz, CDCl\(_3\)): \(\delta\) (ppm): 2.23 (s, 3.6H), 2.49 (s, 2.4H), 3.92 (s, 6H), 7.34-8.03 (m, 14H). \(^{13}\)CNMR (300 MHz, CDCl\(_3\)): \(\delta\) (ppm): 166.4, 147.7, 138.2, 138.1, 132.4, 131.5, 131.4, 129.5, 128.1, 128.0, 127.7, 125.5, 125.3, 121.9, 121.7, 119.1, 118.9, 92.0, 89.3, 52.3, 52.2, 15.3. HRMS (FAB\(^+\)): \(m/z\) calcd. for C\(_{43}\)H\(_{26}\)F\(_6\)O\(_4\)S\(_2\) 784.1177, found [M+H] 785.1265

\(\text{H}_2\text{BDC}^3\)

To a stirred solution (30 mL, EtOH/H\(_2\)O/CH\(_2\)Cl\(_2\) = 9:1:5, V/V) of 3 (671 mg, 0.86 mmol) was added KOH (480 mg, 8.6 mmol) at room temperature. Then the reaction
mixture was heated to 35°C for 12h, monitored by TLC plate. The resulting mixture was cooled to room temperature, then the mixture was filtered over a Buchber funnel and the collected solid was washed with CH$_2$Cl$_2$ and deionized water. The solid product was then dried at 60°C for 12 h. Finally, got light yellow solid (645 mg, 0.85 mmol) of H$_2$BDC in a 99.11% yield.

$^1$HNMR (300 MHz, DMSO-d6): δ (ppm): 2.32 (s, 3.0H), 2.53 (s, 23.0H), 7.40-8.22 (m, 14H), 13.17 (s, 2H). $^{13}$CNMR (300 MHz, DMSO-d6): δ (ppm): 166.7, 145.8, 137.8, 137.7, 131.5, 131.4, 130.7, 130.6, 129.6, 129.5, 128.3, 128.0, 126.4, 126.0, 125.7, 121.8, 118.0, 117.9, 91.7, 91.6, 89.2, 15.0. HRMS (FAB+): m/z calcd. for C$_{41}$H$_{22}$F$_6$O$_4$S$_2$: 756.0864, found [M] 756.0872.

DAE-ICP$^{4-7}$

H$_2$BDC (56.6 mg, 0.075 mmol) and Zn(NO$_3$)$_2$·6H$_2$O (65.0 mg, 0.219 mmol) was dissolved in 7.4 mL of DMF in a 20mL screw top vial, the solution was dispensed evenly into 10 vials(5mL size), then the vials were kept standing at 100°C in an oven for 24h. The samples were cooled to room temperature slowly, collected with a nylon membrane filters (0.45µm, diameter 47 mm) and washed with fresh DMF, then CHCl$_3$. The solid product was then dried in oven at 200°C for 12 h to release DMF. Finally, yellow solid (17.5mg) of DAE-ICP was afforded.
3. NMR spectra

$^1$HNMR of compound 3

$^{13}$CNMR of compound 3
\(^1\)HNMR of H\(_2\)BDC

\(^{13}\)CNMR of H\(_2\)BDC
4. EDX spectra of DAE-ICP

Fig. S1 EDX spectra of DAE-ICP.
5. Photo-graphic images of solid state $\text{H}_2\text{BDC}$

Fig. S2 (A) The conformational change of ligand $\text{H}_2\text{BDC}$ upon irradiation with UV and visible light; (B) Photo-graphic images of solid state $\text{H}_2\text{BDC}$ upon alternative irradiation with UV and Visible light.
6. FT-IR spectra

Fig. S3 FT-IR spectra of H$_2$BDC and DAE-ICP.
7. Nitrogen adsorption isotherm of DAE-ICP

![Nitrogen adsorption isotherm of DAE-ICP measured at 77 K: (black square- open form; red circle- close form).](image)

**Fig. S4** Nitrogen adsorption isotherm of DAE-ICP measured at 77 K: (black square- open form; red circle- close form).

![Brunauer–Emmett–Teller (BET) of DAE-ICP measured in N$_2$ at 77 K.](image)

**Fig. S5** Brunauer–Emmett–Teller (BET) of DAE-ICP measured in N$_2$ at 77 K.
9. TGA diagram of activated DAE-ICP

Fig. S6 TGA diagram of DAE-ICP.
10. Reference