Electronic Supplementary Information

A Triphenylene-based Conjugated Microporous Polymer: Construction, Gas Adsorption, and Fluorescent Detection Properties

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1. General

Solid-state NMR experiment was carried on a Varian Infinityplus-400 wide-bore (89 mm) NMR spectrometer at a proton frequency of 399.7 MHz using a 5 mm double-resonance HX CP/MAS NMR probe. IR spectra were measured using a Bio-Rad FTS-6000 spectrometer with KBr pellets. The powder X-ray diffraction spectra were recorded on a Bruker D8 FOCUS diffractometer at 40 kV/40 mA. Thermogravimetric analysis was carried out on a NETZSCH TG 209 analyzer with a heating rate of 10 °C min^{-1} from ambient temperature to 800 °C under a nitrogen atmosphere. The scanning electron microscopy experiments were carried out on a JEOL JSM-6701F microscope operated at 5 kV. The solid state photoluminescent spectra were measured on a Hitachi F-4500 fluorescence spectrophotometer. The fluorescence of the suspension of TP-CMP was measured by dispersing 3 mg of grounded sample in 2 mL DMF and subsequently placed in a quartz cell of 1 cm width. All titrations were carried out by gradually adding nitrobenzene in an incremental fashion. Their corresponding fluorescence emission spectra were recorded with λ_{ex} = 300 nm at 298 K. Low-pressure gas adsorption measurements were performed using an ASAP 2020 M gas adsorption analyzer. UHP-grade gases were used in the measurements. The N_2 isotherm measurements were carried out at 77 K in a liquid nitrogen bath and 273 K in an ice water mixture bath. The H_2 sorption isotherms were collected at 77 K in a liquid nitrogen bath and 87 K in a liquid argon bath. The CO_2 and CH_4 sorption isotherms were collected at 273 K in an ice water mixture bath and 298 K in an electric heating jacket. The dry samples were loaded into sample tubes and activated under high vacuum (less than 10^{-5} Torr) at 180 °C. The apparent surface areas were calculated from nitrogen adsorption data by multipoint BET analysis. The apparent micropore distributions were calculated from nitrogen adsorption data by the NLDFT method using a cylindrical pore size model for pillared clay.

2. Synthesis of TP-CMP

TP-CMP was synthesized in a similar procedures to literature.[1] A mixture of 2,3,6,7,10,11-hexabromotriphenylene[2] (150 mg, 0.21 mmol) and 1,4-benzene diboronic acid (106 mg, 0.63 mmol) in dimethylformamide (DMF, 15 mL) was degassed for 15 min. To the mixture was added an aqueous solution of K_2CO_3 (2.0 M, 1.6 mL) and tetrakis(triphenylphosphine) palladium(0) (24.7 mg). The mixture was stirred at 150 °C for 24 h under N_2, and then was cooled to room temperature and poured into water. The resultant precipitate was collected by filtration and further washed by Soxhlet extractions for 24 h sequentially with water, dichloromethane, and methanol, respectively. The solids were dried under vacuum at 60 °C for 8 h to give TP-CMP (94 mg) as a gray solid in quantitative yield.

References:

[1] L. Chen, Y. Honsho, S. Seki, D. Jiang, *J. Am. Chem. Soc.* **2010**, *132*, 6742-6748.

[2] R. Breslow, B. Jaus, R. Q. Kluttz, C.-Z. Xia, *Tetrahedron*, **1982**, *38*, 863-867.

3. IR spectrum of TP-CMP

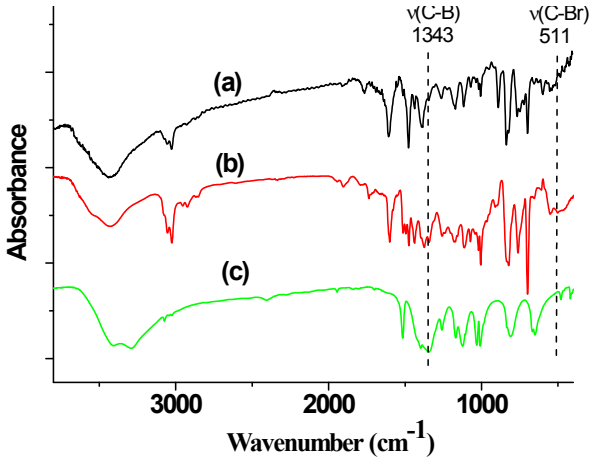

Figure S1. FTIR spectra of (a) **TP-CMP**, **(b)** 2,3,6,7,10,11-hexabromotriphenylene **and (c)** 1,4-benzene diboronic acid

4. TGA trace and DSC profile of TP-CMP

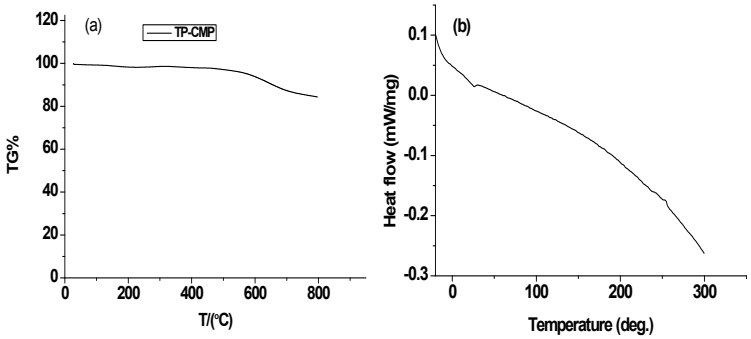

Figure S2. TGA trace (a) and DSC profile (b) of **TP-CMP**

5. Powder X-ray diffraction of TP-CMP

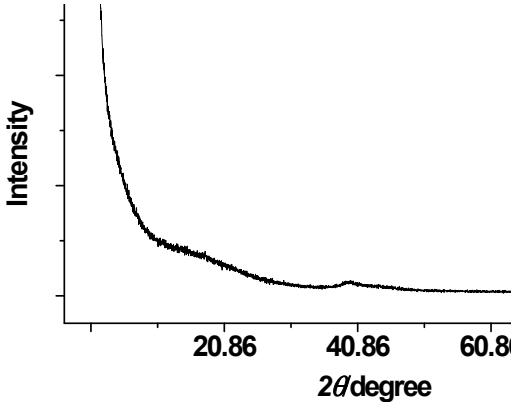

Figure S3. Powder X-ray diffraction of **TP-CMP**

6. Isosteric heat of H_2 and CO_2 adsorption

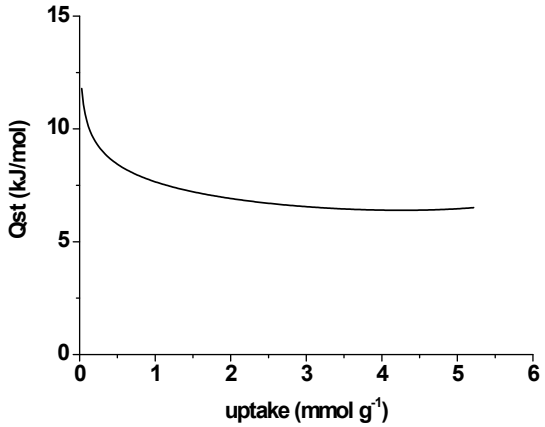

Figure S4. Plot of the isosteric heat of adsorption of H_2 versus the uptake amount of H_2.

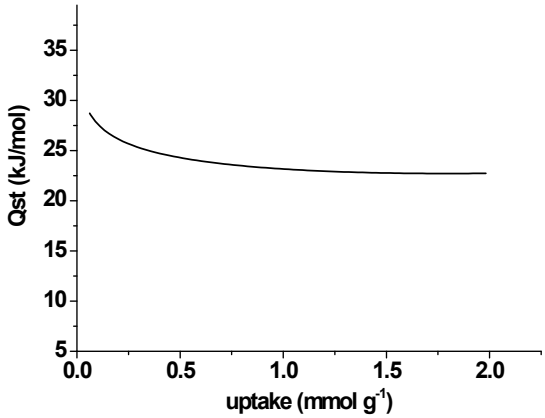

Figure S5. Plot of the isosteric heat of adsorption of CO_2 versus the uptake amount of CO_2

7. Adsorption selectivity of CO_2 over N_2

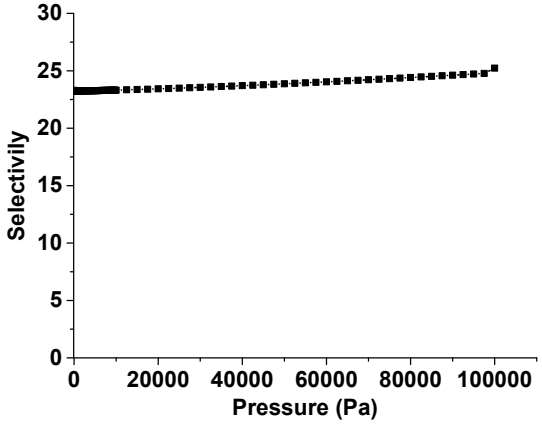

Figure S6. Plot of the adsorption selectivity of CO_2/N_2 at a composition of 15% CO_2 and 85% N_2 at 273 K

8. Fluorescence response of TP-CMP dispersed in DMF upon the addition of different solvents

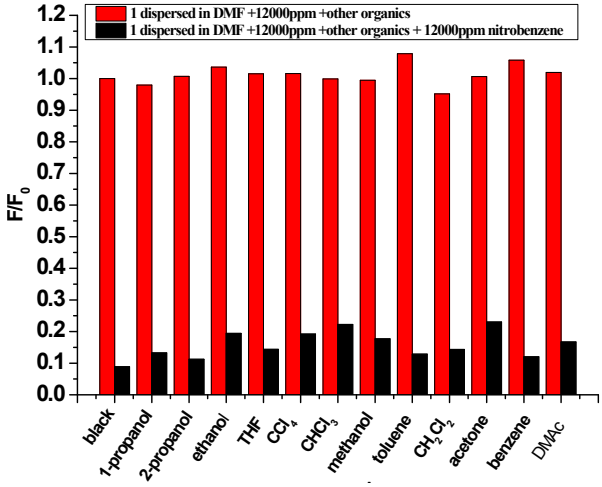

Figure S7 Fluorescence intensity ratio histograms of **TP-CMP** dispersed in DMF on the addition of different solvents with (black) and without (red) nitrobenzene. Emission intensities at 475 nm were selected.