# Electronic Supplementary Information

## Ultrahigh volatile iodine uptake by hollow microspheres formed from a heteropore covalent organic framework

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## Section 1. Instruments and Methods

### Fourier transform infrared spectroscopy (FTIR)

Fourier transform infrared spectroscopy (FTIR) was carried out with a Nicolet 380 FTIR spectrometer. The samples for IR study were prepared as KBr pellets.

### Thermal gravimetric analysis (TGA)

Thermal gravimetric analyses were carried out on a Waters TGA Q500 by heating the samples from 25 to 950 or 1000 ℃ under nitrogen atmosphere at a heating rate of 10 ℃ /min.

### UV-vis absorption spectra (UV-vis)

UV-vis experiments were performed on a Unico 4802 UV-vis double beam spectrophotometer.

### Transmission electron microscopy (TEM) and Energy dispersive X-ray spectroscopy (EDX)

Transmission electron microscopy and Energy dispersive X-ray spectroscopy (EDX) were performed on a Tecnai G2 F20 S-TWIN or a GEOL JEM-2100 instrument.

### Powder X-ray diffraction (PXRD)

Powder X-ray diffraction measurement was carried out with an X'Pert PROX system using monochromated Cu/K α (λ = 0.1542 nm). The sample was spread on the square recess of XRD sample holder as a thin layer.

### Nitrogen adsorption-desorption isotherm measurements

The measurements were carried out using a Quadrasorb SI MP. Before gas adsorption measurements, the as-prepared sample (~50 mg) was activated by being immersed in anhydrous 1,4-dioxane for 12 h. The solvent was decanted and the sample was dried under dynamic vacuum at 160 ℃ for 4 h. The resulting sample was then used for gas adsorption measurements from 0 to 1 atm at 77 K. The Brunauer-Emmett-Teller (BET) method was utilized to calculate the specific surface area. By using the non-local density functional theory model, the pore size distribution curve was derived from the sorption data.

**Structural simulations and powder X-ray diffraction analysis**

The Pawley refinement of the experimental PXRD was conducted by the Reflux module in the Materials Studio 7.0. Before the simulations, the structure was firstly optimized in Gaussian 09 package by semiempirical calculations at PM3 level. The simulation of the two possible structures was carried out in Accelrys Materials Studio 7.0 software package. The stimulated PXRD patterns were determined by the Reflex module. P1 space group was used for the simulations.

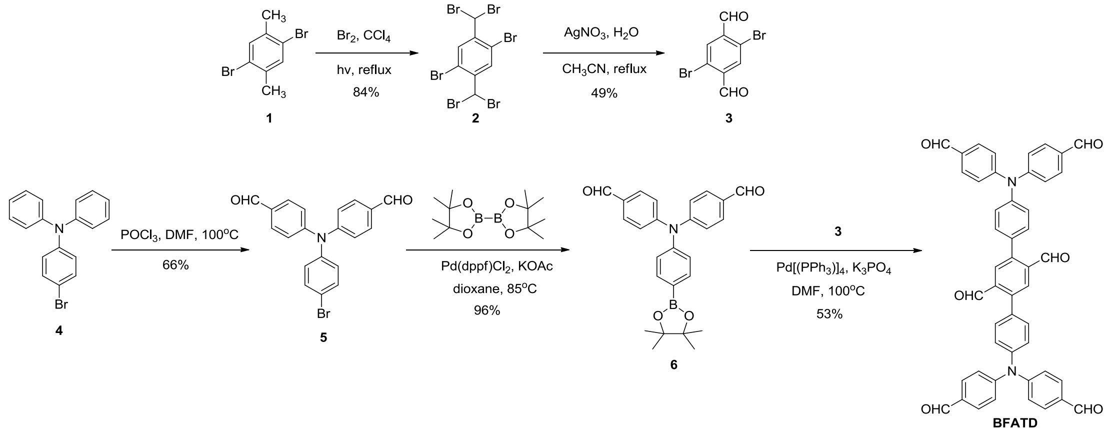
**Experiment procedure for the uptake of iodine vapor**

The iodine capture experiment was performed in the following procedure. Activated **SIOC-COF-7** (43.6 mg) in a small beaker and excess iodine were placed in a sealed glass container, heated at 75 ℃ under ambient pressure. Some contact time later, the COF sample was cooled down to room temperature and weighed. The iodine uptake of **SIOC-COF-7** was calculated by weight gain: $\alpha = [(m_2 - m_1)/m_1] \times 100$ wt %, where $\alpha$ is the iodine uptake, $m_1$ and $m_2$ are the mass of **SIOC-COF-7** sample before and after being exposed to iodine vapor, respectively. The iodine capture experiments were conducted three times and a good repeatability was observed.

**Experiment procedure for the uptake of iodine in solution phase**

The iodine capture experiment in solution phase was performed in the following procedure. Iodine (40.0 mg) was dissolved in n-hexane (3.0 mL) and then activated **SIOC-COF-7** (30.0 mg) was added. Four days later, UV-vis absorption of the solution was recoded. The amount of iodine remained in solution was determined by using the working curve established (Figure S10). Then the amount of iodine captured by the COF can be calculated through subtracting the amount of iodine remained in solution from the initial amount of iodine.

**Section 2. Synthesis and Characterizations**




**1,4-dibromo-2,5-bis(dibromomethyl)benzene (2)** was synthesized following a reported procedure[1] with minor modifications as detailed below. To a refluxing solution of 1,4-dibromo-2,5-dimethylbenzene (1.3 g, 5.0 mmol) in carbon tetrachloride (100 mL), which was irradiated with a 500 W incandescent lamp, a solution of bromine (1.3 mL, 25.3 mmol) in carbon tetrachloride (5 mL) was added dropwise. The reaction mixture was stirred under reflux with concomitant irradiation by the same lamp for 12 h. After being cooled to room temperature, the reaction mixture was washed successively with an aqueous solution of $Na_2SO_3$ and water, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. Recrystallization of the crude product from ethyl acetate yielded compound **2** as white crystals (2.4 g, 84%). $^1$H NMR (400 MHz, $CDCl_3$): δ 8.13 (s, 2 H), 6.93 (s, 2H).

**2,5-dibromoterephthalaldehyde (3)** was synthesized following a reported procedure[1] with minor modifications as detailed below. A solution of $AgNO_3$ (1.3 g, 7.7 mmol) in water (3.5 mL) was added to a suspension of 1,4-dibromo-2,5-bis(dibromomethyl)benzene (1.0 g, 1.7 mmol) in acetonitrile (24 mL) and the resulting mixture was stirred and heated to reflux under an argon atmosphere for about 8 h. The reaction mixture was filtered while hot, and the solid was washed with hot acetonitrile. The filtrate was cooled to room temperature to allow crystallization of the product. The resulting need-like crystals were collected by filtration, and the filtrate was concentrated to allow crystallization again. The combined crystals were dissolved in dichloromethane and the insoluble fraction was filtered off. The solvent was evaporated to yield compound **3** (0.25 g, 49%). $^1$H NMR (400 MHz, $CDCl_3$): δ 10.35 (s, 2H), 8.16 (s, 2H).

**4,4'-((4-bromophenyl)azanediyl)dibenzaldehyde (5)** was synthesized following a reported procedure[2] with minor modifications as detailed below. 4-bromo-N,N-diphenylaniline (6.0 g, 18.5 mmol) was dissolved in DMF (23 mL, 296 mmol) in a 250 mL flask. Under cooling with ice phosphorus oxychloride was added (18.5 mL, 198 mmol) dropwise. The solution was heated for 36 h at 100 ℃. Upon being cooled to room temperature, the reaction was quenched by pouring it into ice-cold water. The reaction solution was neutralized with 2N NaOH solution, whereby a brown solid precipitated out. The solid was filtered, washed with water and ethanol. The crude product was purified by flash column chromatograph (dichloromethane/hexane 3:1) to give compound **5** as a yellow solid (4.64 g, 66%). $^1$H NMR (400 MHz, $CDCl_3$): δ 9.91 (s, 2H), 7.79 (d, $J$ = 8.6 Hz, 4H), 7.50 (d, $J$ = 8.7 Hz, 2H), 7.18 (d, $J$ = 8.6 Hz, 4H), 7.05 (d, $J$ = 8.7 Hz, 2H).

**4,4'-((4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)azanediyl)dibenzaldehyde (6).** Compound **5** (5.0 g, 13.1 mmol), bis(pinacolato)diborane (4.0 g, 15.8 mmol), potassium acetate (3.9 g, 39.7 mmol), $Pd(dppf)_2Cl_2$ (0.3 g, 0.4 mmol), and dried 1,4-dioxane (90 mL) were added in a 250 mL flask. The mixture was degassed through three freeze–pump–thaw cycles under an argon atmosphere and then stirred at at 100 ℃ for 24 h. After being cooled to room temperature, the reaction mixture was extracted with ethyl acetate and died over $MgSO_4$. After removed of solvent under reduced pressure, the crude product was purified by flash column chromatograph (petroleum ether/ethyl acetate 10:1) to give compound **6** as a light yellow solid (5.4 g, 96%). $^{1}H$ NMR (400 MHz, $CDCl_3$): δ 9.90 (s, 2H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 8.7 Hz, 4H), 7.19 (d, *J* = 8.6 Hz, 4H), 7.15 (d, *J* = 8.4 Hz, 2H), 1.46-1.27 (m, 12H). $^{13}C$ NMR (125 MHz, $CDCl_3$): δ 190.50, 151.81, 148.18, 136.56, 131.59, 131.30, 125.55, 123.27, 84.01, 24.88. MS (ESI): *m/z* 428.4 $[M+H]^+$ . HRMS (ESI): Calcd for $C_{26}H_{27}BNO_4$ $[M+H]^+$: 427.2064. Found: 427.2064.

**4,4''-bis(bis(4-formylphenyl)amino)-[1,1':4',1''-terphenyl]-2',5'-dicarbaldehyde (BFTDA).** A mixture of compound **3** (200 mg, 0.69 mmol), compound **6** (586 mg, 1.37 mmol), $K_3PO_4$ (182 mg, 0.86 mmol) and $Pd[P(Ph_3)]_4$ (81 mg, 0.07 mmol) was dissolved in DMF (10 mL) in a 25 mL flask. The mixture was degassed through three freeze–pump–thaw cycles under an argon atmosphere and then stirred at 100 ℃ for 24 hours. After being cooled to room temperature, the reaction mixture was extracted with dichloromethane. The organic layer was washed with water, dried over $MgSO_4$, filtered and evaporated. The crude product was purified by flash column chromatograph (dichloromethane/ethyl acetate 50:1) to give **BFTDA** as a bright yellow solid (532 mg, 53%). $^{1}H$ NMR (500 MHz, DMSO-$d_6$): δ 10.11 (s, 2H), 9.91 (s, 4H), 8.02 (s, 2H), 7.89 (d, *J* = 8.6 Hz, 8H), 7.62 (d, *J* = 8.4 Hz, 4H), 7.35 (d, *J* = 8.4 Hz, 4H), 7.29 (d, *J* = 8.6 Hz, 8H). $^{13}C$ NMR (125 MHz, $CDCl_3$): δ 191.28, 190.47, 151.66, 146.34, 143.56, 136.49, 133.43, 131.94, 131.64, 131.48, 130.49, 126.27, 123.52. MS (MALDI-TOF): *m/z* 732.2. HRMS (MALDI-TOF): Calcd for $C_{48}H_{32}N_2O_6$: 732.2251. Found: 732.2255.

**Preparation of SIOC-COF-7.** A mixture of BFATD (30 mg, 0.04 mmol), 1,4-diminobenzene (13.3 mg, 0.12 mmol), 1,4-dioxane (0.5 mL), 1,3,5-trimethylbenzene (0.5 mL) and acetic acid (6 M (aq.), 0.1 mL) was placed in a glass ampoule. The mixture was sonicated for 3 minutes and then degassed through three freeze–pump–thaw cycles. After that the tube was sealed under vacuum and then warmed to room temperature. The mixture was heated to 120 ℃ for 3 days without disturbance. After being cooled to room temperature, the solvent was evaporated, the yellow residue was washed with large amount of 1,4-dioxane and dichloromethane, and dried under vacuum to yield the COF (31.4 mg, 80.8%). Anal. Calcd. For $C_{66}H_{44}N_8$: C, 83.52; H, 4.67; N, 11.81. Found: C, 80.00; H, 4.78; N, 10.99.

**References for the synthesis**

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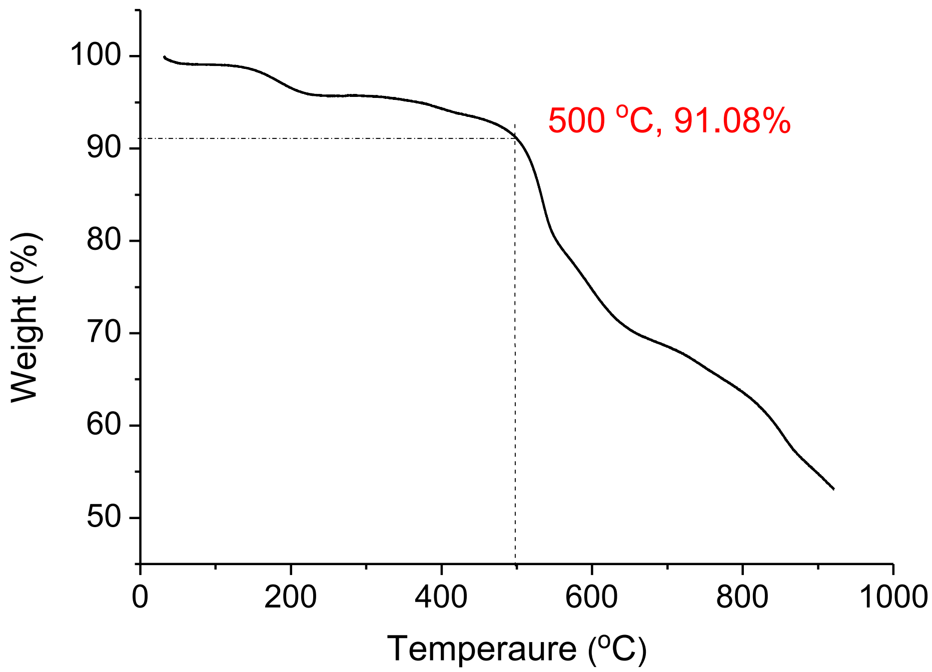


**Fig. S1** TGA profile of **SIOC-COF-7**.

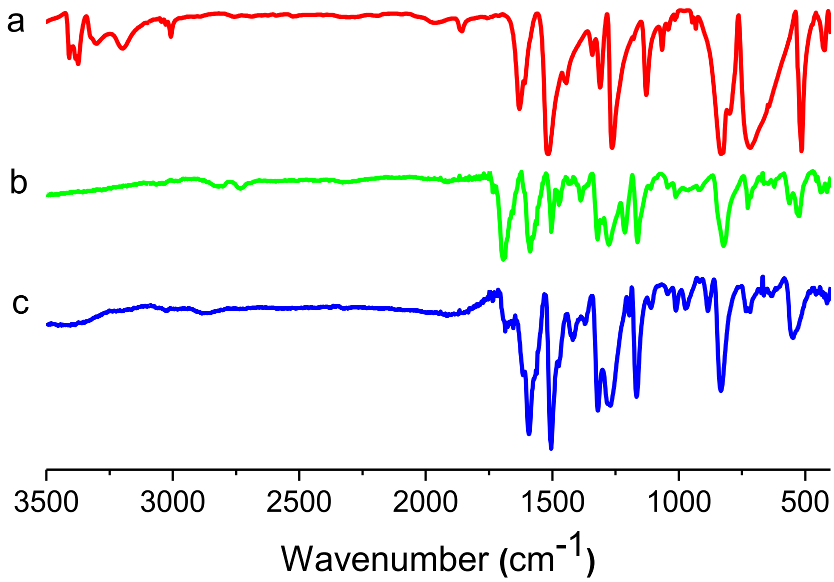


**Fig. S2** FTIR spectra of (a) 1,4-diaminobenzene, (b) BFATD, and (c) **SIOC-COF-7**.

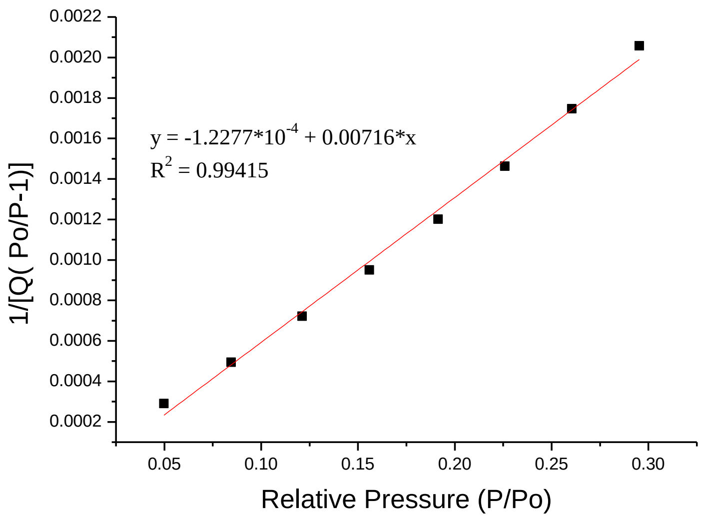


**Fig. S3** BET surface area plot for **SIOC-COF-7** calculated from the isotherm.

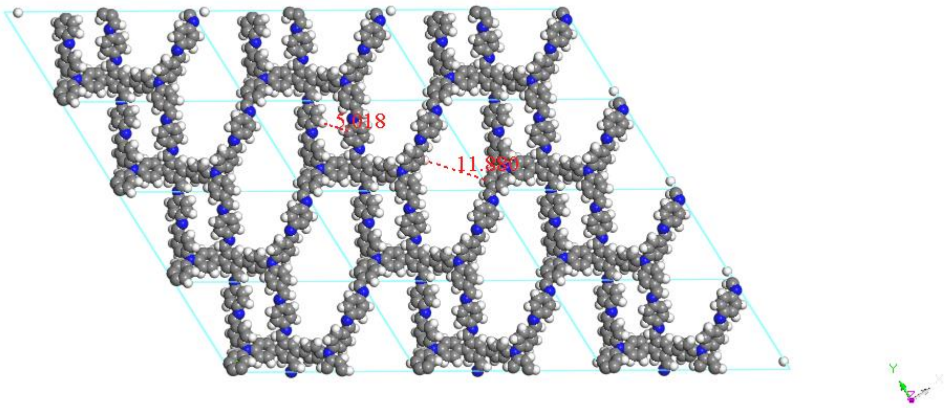

**Fig. S4** Illustration for pore size distribution of **SIOC-COF-7** with eclipsed AA stacking.

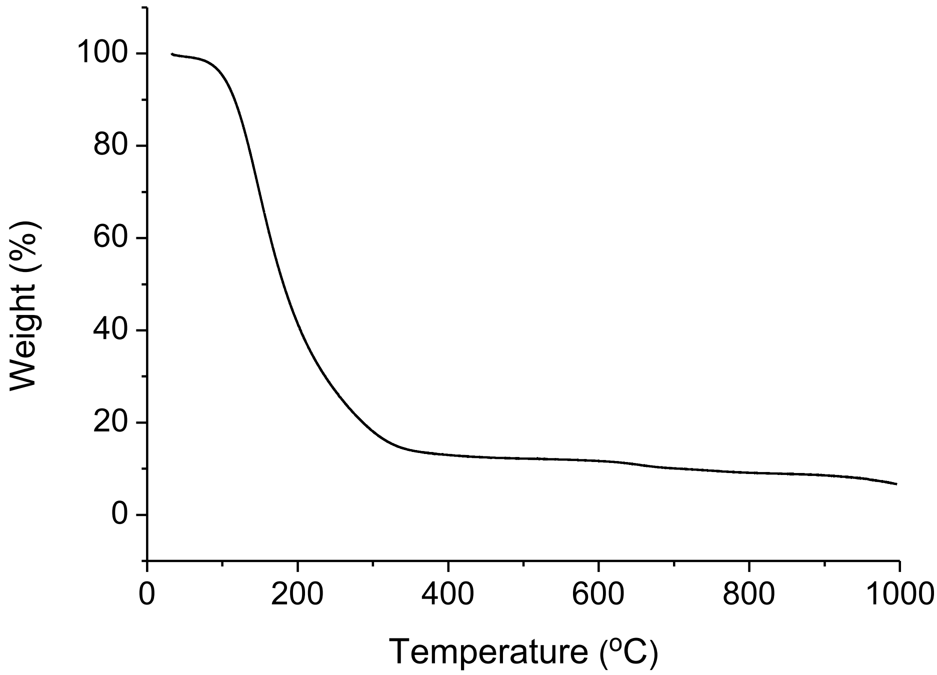


**Fig. S5** TGA profile of iodine-loaded **SIOC-COF-7**.

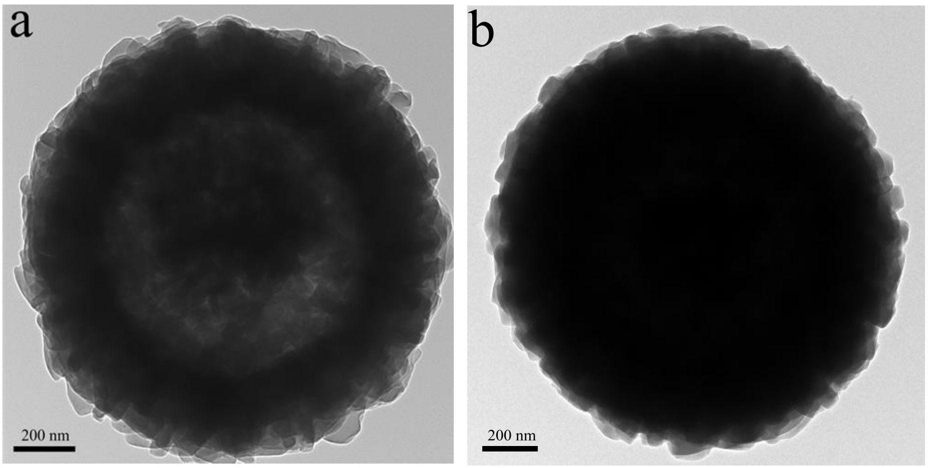


**Fig. S6** TEM images of (a) **SIOC-COF-7** and (b) iodine-loaded **SIOC-COF-7**.

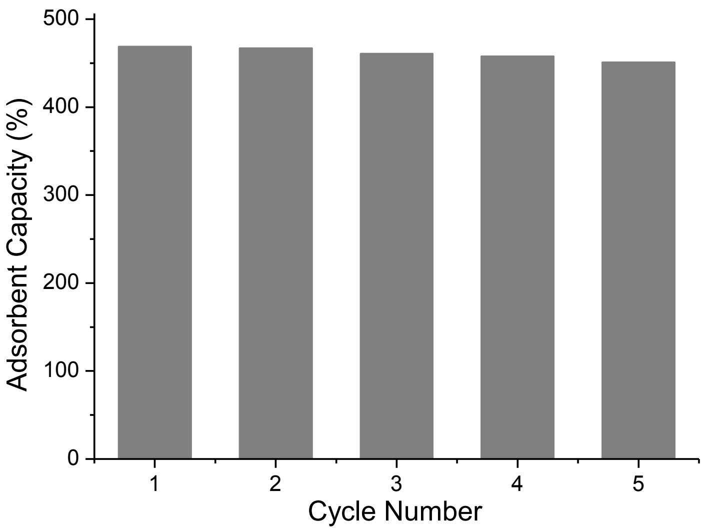


**Fig. S7** Reusability of **SIOC-COF-7** for iodine capture. A sample with initial iodine uptake of 469 wt % was used for the recycle test.

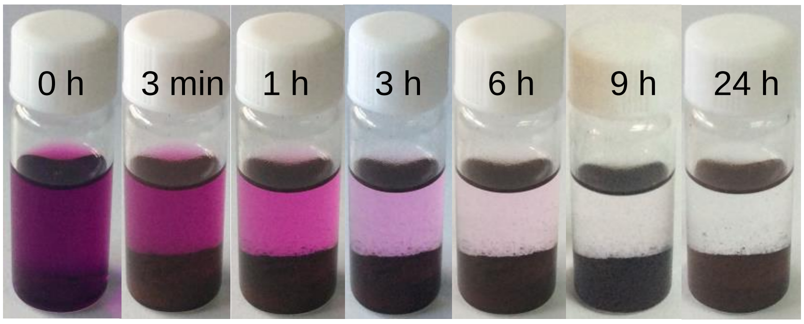


**Fig. S8** Photographs showing progress of iodine capture after **SIOC-COf-7** (30 mg) was immersed in a hexane solution of iodine (10.0 mmol $L^{-1}$, 3 mL).

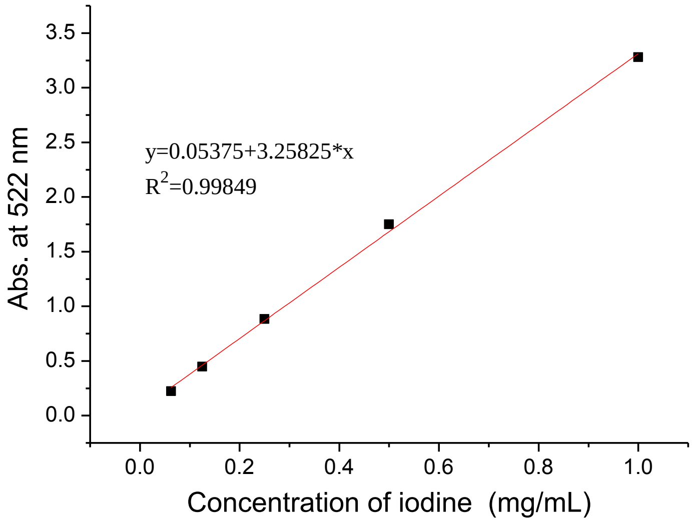


**Fig. S9** Working curve for the estimation of iodine uptake in solution.

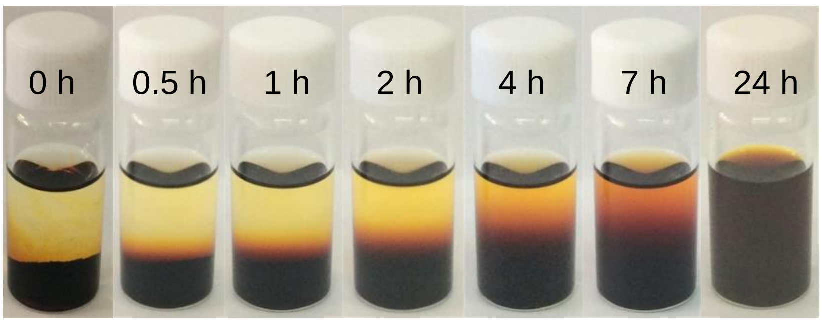


**Fig. S10** Photographs showing progress of iodine release from the iodine-loaded **SIOC-COF-7** after it was immersed in ethanol.

**Table S1.** Summary of iodine uptake properties of porous materials.

| Adsorbent | | Temperature (℃) | pressure | $S_{BET}$ ($m^2g^{-1}$) | Iodine capacity (mg $I_2$/g) | References |
|---|---|---|---|---|---|---|
| 1 | **SIOC-COF-7** | 75 | 1 bar | 618 | 4810 | This work |
| 2 | HCMP-3(reduced) | 85 | 1 bar | 82 | 3360 | S1 |
| 3 | AzoPPN | 77 | 1 bar | 400 | 2900 | S2 |
| 4 | PAF-24 | 75 | 1 bar | 136 | 2760 | S3 |
| 5 | PAF-23 | 75 | 1 bar | 82 | 2710 | S3 |
| 6 | PAF-25 | 75 | 1 bar | 262 | 2600 | S3 |
| 7 | Azo-Trip | 77 | 1 bar | 510 | 2380 | S4 |
| 8 | NiMoS chalcogels | 60 | 1 bar | 490 | 2250 | S5 |
| 9 | CMPN-3 | 70 | 1 bar | 1368 | 2080 | S6 |
| 10 | NiP-CMP | 77 | 1 bar | 2630 | 2020 | S7 |
| 11 | PAF-1 | 25 | 40 Pa | 5600 | 1860 | S8 |
| 12 | NTP | 75 | 1 bar | 1067 | 1800 | S9 |
| 13 | JUC-Z2 | 25 | 40 Pa | 2081 | 1440 | S8 |
| 14 | Cu-BTC | 75 | 1 bar | – | 1750 | S10 |
| 15 | ZIF-8 | 75 | 1 bar | 1875 | 1200 | S11 |
| 16 | Activated carbon | 75 | 1 bar | – | 300 | S9 |
| 17 | Ag@Zeolite Mordenites | 95 | 1 bar | – | 275 | S12 |
| 18 | Ag@Mon-POF | 70 | 1 bar | 690 | 250 | S13 |
| 19 | CC3 | 20 | 1 bar | – | 364 | S14 |

**References for Table S1**

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**Table S2.** Fractional atomic coordinates for the unit cell of **SIOC-COF-7** with AA stacking.

**SIOC-COF-7**: Space group symmetry P1

a = 32.35 Å, b=18.36 Å, c= 3.82 Å

α = β = 90°, γ = 122.04 °

| Element | Number | u ( Å ) | v ( Å ) | w ( Å ) |
|---|---|---|---|---|
| H | 1 | 0.17119 | 0.097278 | 0.780994 |
| H | 2 | 0.24511 | 0.099715 | 0.810212 |
| H | 3 | 0.32448 | 0.363944 | 0.447521 |
| H | 4 | 0.25274 | 0.367589 | 0.495969 |
| H | 5 | 0.22994 | 0.386286 | 1.047022 |
| H | 6 | 0.24724 | 0.529947 | 0.966128 |
| H | 7 | 0.12371 | 0.431881 | 0.265095 |
| H | 8 | 0.11126 | 0.290255 | 0.307042 |
| H | 9 | 0.0675 | 0.208816 | 0.641 |

| | | | | |
|---|---|---|---|---|
| H | 10 | -0.00696 | 0.088439 | 0.830777 |
| H | 11 | 0.07014 | -0.0101 | 1.37599 |
| H | 12 | 0.14633 | 0.115814 | 1.213048 |
| H | 13 | 0.17178 | 0.589678 | 0.400403 |
| H | 14 | 0.30262 | 0.104146 | 0.568392 |
| H | 15 | 0.45774 | 0.358131 | 0.943725 |
| H | 16 | 0.44829 | 0.114795 | 0.608323 |
| H | 17 | 0.51711 | 0.108517 | 0.799198 |
| H | 18 | 0.56455 | 0.32992 | 1.460329 |
| H | 19 | 0.49552 | 0.334168 | 1.295446 |
| H | 20 | 0.49688 | 0.048895 | 1.292669 |
| H | 21 | 0.48271 | -0.09047 | 1.340272 |
| H | 22 | 0.63687 | 0.014657 | 1.477846 |
| H | 23 | 0.65265 | 0.157157 | 1.423467 |
| H | 24 | 0.66275 | 0.222938 | 0.91423 |
| H | 25 | 0.74657 | 0.343971 | 0.923267 |
| H | 26 | 0.70472 | 0.478774 | 1.625515 |
| H | 27 | 0.62368 | 0.354086 | 1.658741 |
| H | 28 | 0.35863 | 0.399998 | 0.927898 |
| H | 29 | 0.80913 | 0.487296 | 1.097979 |
| H | 30 | 0.52702 | 0.583997 | 0.991052 |
| H | 31 | 0.5594 | 0.731537 | 1.178889 |
| H | 32 | 0.41209 | 0.672667 | 1.344499 |
| H | 33 | 0.37971 | 0.525137 | 1.155497 |
| H | 34 | 0.32747 | 0.759251 | 0.888907 |
| H | 35 | 0.36716 | 0.914953 | 0.862919 |
| H | 36 | 0.23866 | 0.885718 | 0.365394 |
| H | 37 | 0.19891 | 0.729755 | 0.390576 |

| | | | | |
|---|---|---|---|---|
| H | 38 | 0.88354 | 0.590902 | 1.222915 |
| H | 39 | 0.96023 | 0.728963 | 1.185457 |
| H | 40 | 0.88833 | 0.857102 | 1.556047 |
| H | 41 | 0.8113 | 0.71872 | 1.594009 |
| H | 42 | 0.38632 | 1.047457 | 0.940945 |
| H | 43 | 0.58097 | 0.854945 | 1.442391 |
| H | 44 | 0.94466 | 0.953289 | 1.130606 |
| C | 1 | 0.16817 | -2.67548 | -0.30509 |
| C | 2 | 0.11578 | -2.82853 | -0.12442 |
| C | 3 | 0.20467 | -2.7644 | -0.31129 |
| C | 4 | 0.20489 | -2.84021 | -0.26139 |
| C | 5 | 0.2474 | -2.84074 | -0.26959 |
| C | 6 | 0.29353 | -2.76591 | -0.3503 |
| C | 7 | 0.29133 | -2.6945 | -0.46042 |
| C | 8 | 0.24936 | -2.69294 | -0.42841 |
| C | 9 | 0.20629 | -2.60437 | -0.12825 |
| C | 10 | 0.21593 | -2.52208 | -0.17636 |
| C | 11 | 0.18676 | -2.50553 | -0.39135 |
| C | 12 | 0.1473 | -2.57682 | -0.55524 |
| C | 13 | 0.13891 | -2.65911 | -0.52214 |
| C | 14 | 0.07063 | -2.83747 | -0.19963 |
| C | 15 | 0.02663 | -2.90801 | -0.08751 |
| C | 16 | 0.02411 | -2.97478 | 0.106545 |
| C | 17 | 0.06893 | -2.96296 | 0.2061 |
| C | 18 | 0.11307 | -2.89152 | 0.101413 |
| C | 19 | 0.19772 | -2.41914 | -0.44783 |
| C | 20 | 0.33848 | -2.76281 | -0.30213 |
| C | 21 | 0.33725 | -2.84032 | -0.33962 |

| | | | | |
|---|---|---|---|---|
| C | 22 | 0.37401 | -2.85207 | -0.23745 |
| C | 23 | 0.41982 | -2.7771 | -0.14135 |
| C | 24 | 0.42233 | -2.69809 | -0.13083 |
| C | 25 | 0.38351 | -2.6884 | -0.18469 |
| C | 26 | 0.46283 | -2.77778 | -0.0531 |
| C | 27 | 0.47233 | -2.83914 | -0.19159 |
| C | 28 | 0.51222 | -2.84187 | -0.08812 |
| C | 29 | 0.54686 | -2.78415 | 0.153764 |
| C | 30 | 0.54032 | -2.71805 | 0.268025 |
| C | 31 | 0.49981 | -2.71562 | 0.172995 |
| C | 32 | 0.635 | -2.72189 | 0.275503 |
| C | 33 | 0.57703 | -2.88089 | 0.319111 |
| C | 34 | 0.52957 | -2.9549 | 0.314947 |
| C | 35 | 0.52088 | -3.03682 | 0.354303 |
| C | 36 | 0.5586 | -3.05182 | 0.402702 |
| C | 37 | 0.60556 | -2.97864 | 0.429773 |
| C | 38 | 0.61462 | -2.896 | 0.39221 |
| C | 39 | 0.67198 | -2.7214 | 0.07981 |
| C | 40 | 0.71976 | -2.65173 | 0.083941 |
| C | 41 | 0.73345 | -2.57662 | 0.270856 |
| C | 42 | 0.69648 | -2.57691 | 0.463777 |
| C | 43 | 0.64893 | -2.64756 | 0.471642 |
| C | 44 | 0.39072 | -2.60479 | -0.10806 |
| C | 45 | 0.78349 | -2.50476 | 0.258028 |
| C | 46 | 0.26009 | -2.26782 | -0.35583 |
| C | 47 | 0.45102 | -2.45683 | 0.055118 |
| C | 48 | 0.84079 | -2.35633 | 0.406967 |
| C | 49 | 0.5014 | -2.39694 | 0.070346 |

| | | | | |
|---|---|---|---|---|
| C | 50 | 0.51972 | -2.31346 | 0.179581 |
| C | 51 | 0.48819 | -2.28634 | 0.280337 |
| C | 52 | 0.43777 | -2.34657 | 0.269456 |
| C | 53 | 0.41943 | -2.43012 | 0.160049 |
| C | 54 | 0.30762 | -2.21336 | -0.22851 |
| C | 55 | 0.33011 | -2.12502 | -0.24328 |
| C | 56 | 0.30571 | -2.08745 | -0.3864 |
| C | 57 | 0.25851 | -2.1419 | -0.51919 |
| C | 58 | 0.23601 | -2.23026 | -0.50428 |
| C | 59 | 0.88388 | -2.35111 | 0.299017 |
| C | 60 | 0.92759 | -2.27277 | 0.279148 |
| C | 61 | 0.93038 | -2.19589 | 0.363211 |
| C | 62 | 0.8877 | -2.20132 | 0.482317 |
| C | 63 | 0.84407 | -2.27972 | 0.504608 |
| C | 64 | 0.36375 | -1.93923 | -0.22995 |
| C | 65 | 0.54935 | -2.13792 | 0.423961 |
| C | 66 | 0.97704 | -2.04902 | 0.197673 |
| N | 1 | 0.16189 | -2.75852 | -0.25912 |
| N | 2 | 0.58594 | -2.79524 | 0.265505 |
| N | 3 | 0.23881 | -2.35659 | -0.3285 |
| N | 4 | 0.43469 | -2.54003 | -0.06088 |
| N | 5 | 0.79528 | -2.43388 | 0.416463 |
| N | 6 | 0.32607 | -1.99876 | -0.39715 |
| N | 7 | 0.50504 | -2.20138 | 0.373858 |
| N | 8 | 0.97454 | -2.11716 | 0.3189 |

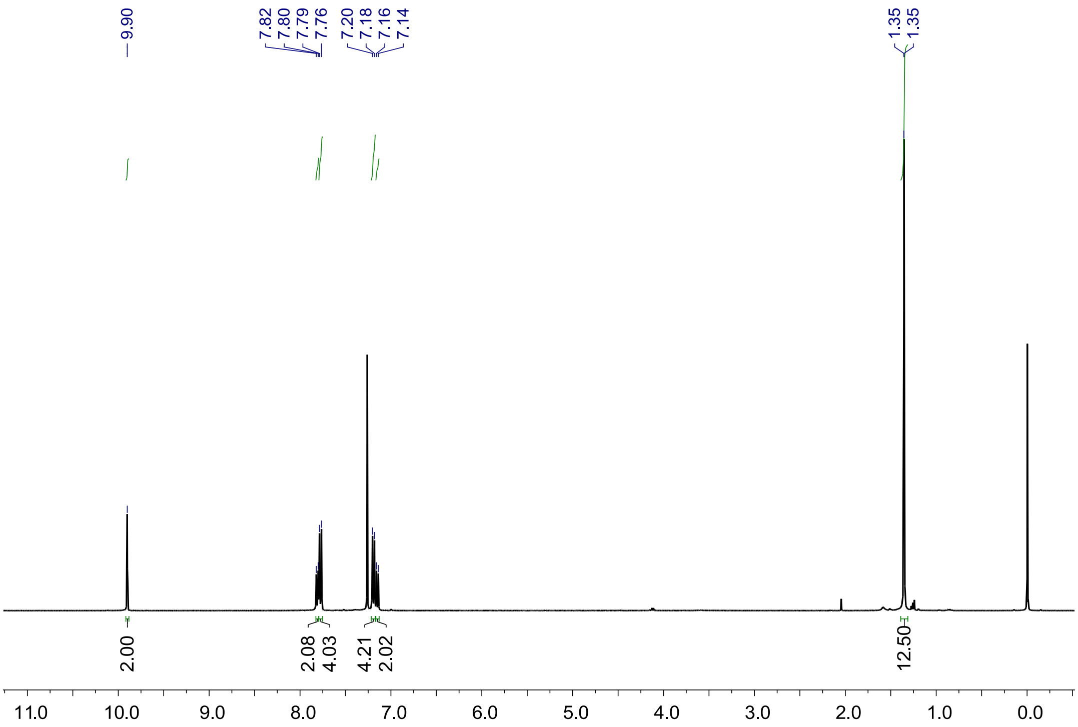


**Fig. S9** $^{1}$H NMR (400 MHz, $CDCl_3$) spectrum of compound **6**.

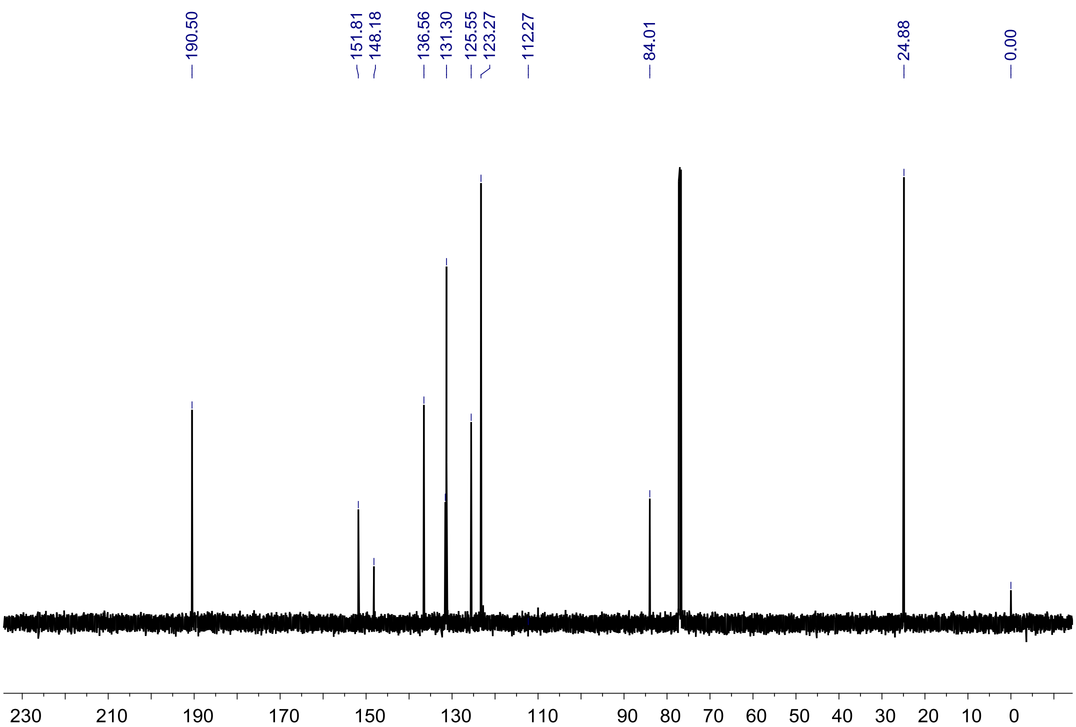


**Fig. S10** $^{13}$C NMR (125 MHz, $CDCl_3$) spectrum of compound **6**.

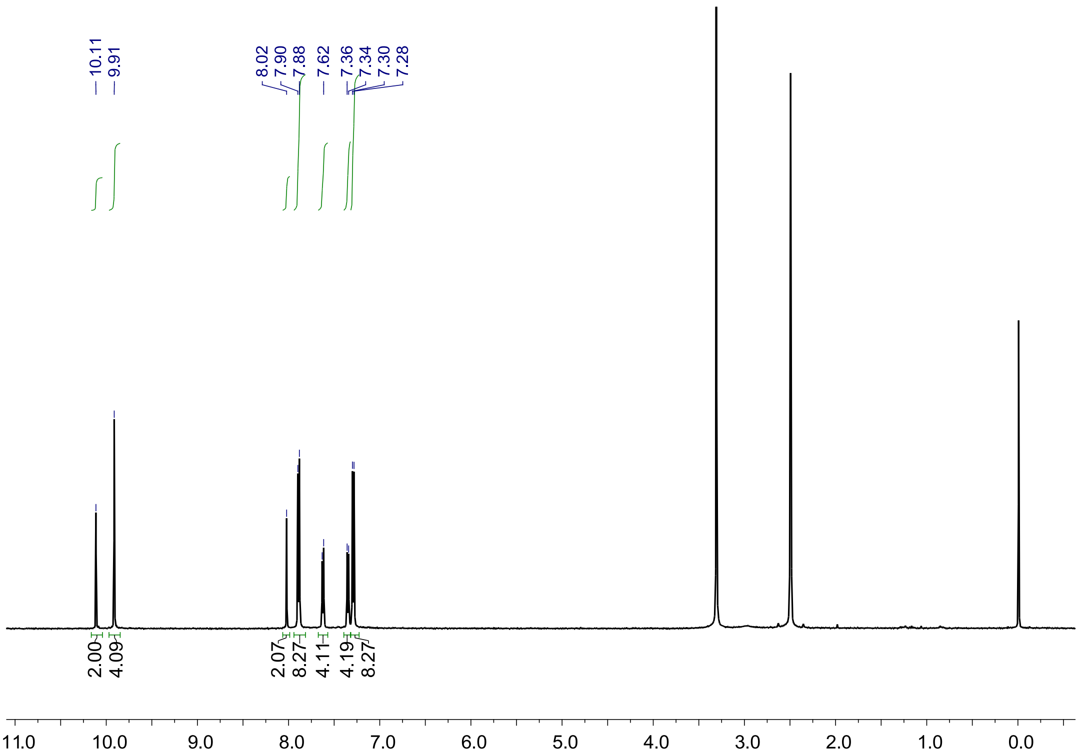


**Fig. S11** $^{1}H$ NMR (500 MHz, DMSO-$d_6$) spectrum of **BFATD**.

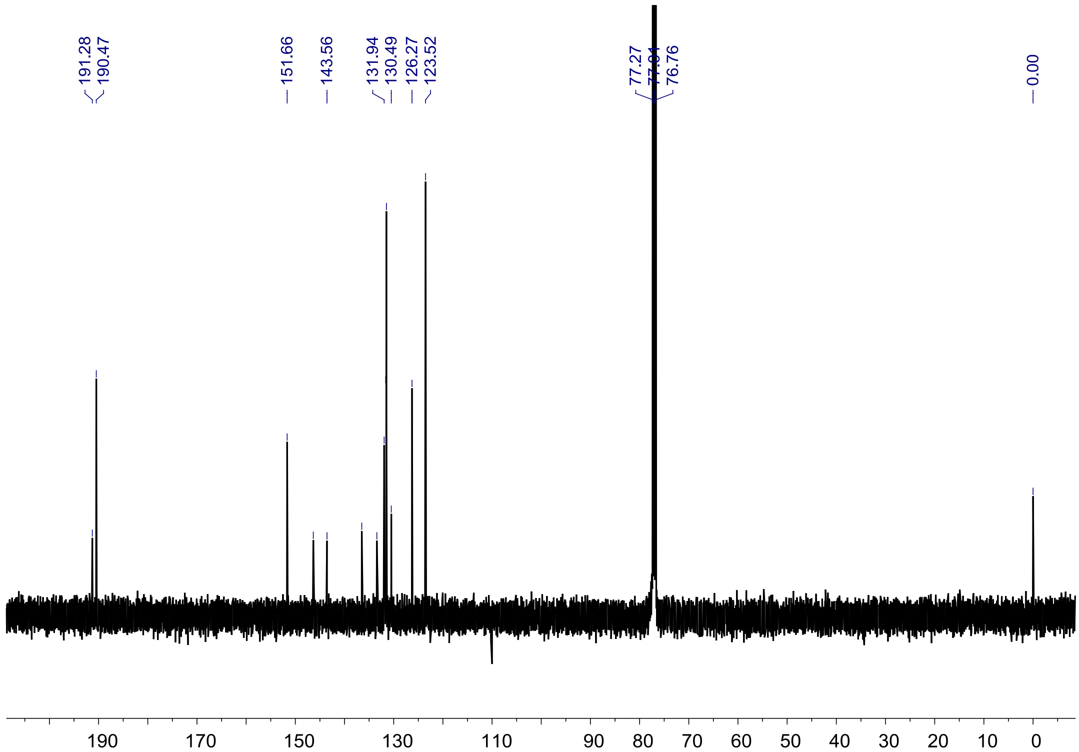


**Fig. S12** $^{13}C$ NMR (125 MHz, $CDCl_3$) spectrum of compound **BFATD**.