

## **Electronic Supplementary Information**

**Constructing a magnetic ionic covalent organic polymer through post-synthesis  
functionalization approach for efficient iodine/iodide adsorption**

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## 1. Characterization

Fourier Transform Infrared Spectroscopy (FT-IR) was used to determine the structure and surface functional groups (model: PE Frontier NIR, America). The images from the scanning electron microscope (SEM) were captured using a Thermo Scientific microscope (model: Apreo 2, America). The images transmission electron microscopy (TEM) were captured using a Thermo Scientific microscope (model: JEM-2100F, Jeol Ltd., Japan) after the specimens were dispersed in ethanol and placed on holey copper grids. The thermal stability of the samples was measured using a thermogravimetric (TGA) analyzer (model: Discovery SDT650, America) by scanning from ambient temperature to 800°C at a heating rate of 10°C min<sup>-1</sup> under nitrogen atmosphere. The X-ray photoelectron spectroscopy (XPS) was recorded using a Thermo Fisher Scientific (model: Shimadzu/Krayos AXIS Ultra DLD, Japan) to study the form of adsorbed molecule iodine. Ultraviolet-visible (UV-Vis) spectroscopic analyses were performed on a Persee UV-Vis spectrophotometer (model: T-9, Beijing). Raman spectra were acquired using a HORIBA JobinYvon Aramis equipped with a 532 nm diode laser (model: Lab RAM HR Evolution, France). The magnetic properties of the sample were tested at ambient temperature using a vibrating sample magnetometer (VSM) (model: LakeShore7404, America). The specific surface areas were evaluated by Micromeritics instrument (model: ASAP 2020, America). The CPMA S <sup>1</sup>H and <sup>13</sup>C NMR measurements were carried out with spectrometer operating at 400 and 101 MHz, respectively (model: Bruker AVANCE NEO500M, Germany).

## 2. Uptake of iodine

### 2.1. Iodine vapor adsorption capacity

$$Q_t = \frac{(m_t - m_1) - (m_{r,t} - m_{r,0})}{m_1 - m_0} \quad (\text{S1})$$

Where  $Q_t$  ( $\text{g g}^{-1}$ ) is the static  $\text{I}_2$  uptake capacity at time  $t$ ,  $m_t$  ( $\text{g}$ ) is the weight of the third vial at time  $t$ ,  $m_1$  is the weight of the third vial before the adsorption experiment,  $m_0$  is the weight of first vial without IMF-COP-Fe,  $m_{r,t}$  is the weight of the second vial at time  $t$ ,  $m_{r,0}$  is the weight of second vial before the adsorption experiment.

### 2.2. Equations of adsorption capacity

$$Q_t = \frac{(C_0 - C_t)V}{m} \quad (\text{S2})$$

Where  $Q_t$  ( $\text{mg g}^{-1}$ ) is the equilibrium capacity of IMF-COP-Fe for iodine/iodide;  $C_0$  ( $\text{mg L}^{-1}$ ) is the initial concentration of the iodine-cyclohexane solution (iodide solution);  $C_t$  ( $\text{mg L}^{-1}$ ) is the concentration of iodine-cyclohexane solution (iodide solution) when the adsorption time is  $t$ ;  $m$  ( $\text{g}$ ) is the mass of IMF-COP-Fe;  $V$  ( $\text{L}$ ) indicates the iodine-cyclohexane solution (iodide solution) volume.

### 2.3. Adsorption kinetics and the internal diffusion models

$$\ln(Q_e - Q_t) = \ln Q_e - k_1 t \quad (\text{S3})$$

$$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + \frac{t}{Q_e} \quad (\text{S4})$$

$$Q_t = K p t^{0.5} + C \quad (\text{S5})$$

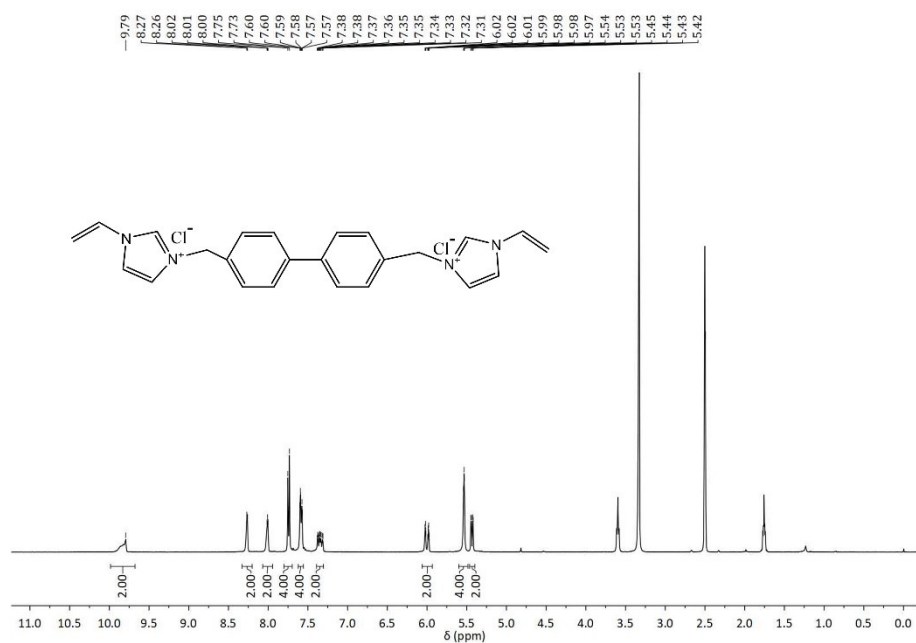
Where  $k_1$  ( $\text{min}^{-1}$ ) and  $k_2$  ( $\text{g mg}^{-1} \text{min}^{-1}$ ) are the kinetic constants of the pseudo-first-order and pseudo-second-order kinetic model, the adsorbed amount of iodine is  $Q_e$  ( $\text{mg g}^{-1}$ ) at equilibrium and  $Q_t$  ( $\text{mg g}^{-1}$ ) at  $t$  ( $\text{min}$ ).

## 2.4. Langmuir and Freundlich models

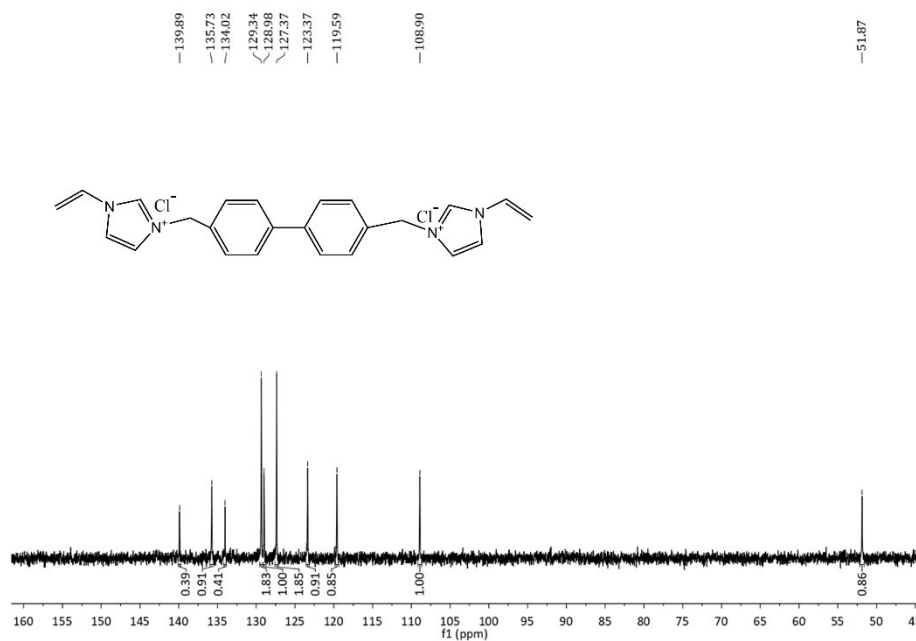
$$\frac{C_e}{Q_e} = \frac{C_e}{Q_0} + \frac{1}{Q_0 K_c} \quad (\text{S6})$$

$$\ln Q_e = \ln K_F + \frac{1}{n} \ln C_e \quad (\text{S7})$$

The equilibrium adsorption capacity of IMF-COP-Fe is denoted by  $Q_e$  ( $\text{mg g}^{-1}$ ).  $C_e$  ( $\text{mg L}^{-1}$ ) is the concentration of iodide in the solution at equilibrium for IMF-COP-Fe.  $Q_0$  ( $\text{mg g}^{-1}$ ) is the theoretical maximum adsorption capacity based on the Langmuir model. The adsorption intensity coefficient is denoted by  $n$ , while  $K_c$  and  $K_F$  represent the adsorption equilibrium coefficients for the Langmuir and Freundlich models, respectively.



**Fig. S1** <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 9.79 (s, 2H), 8.26 (d, J = 3.1 Hz, 2H), 8.07 – 7.94 (m, 2H), 7.74 (d, J = 8.1 Hz, 4H), 7.62 – 7.56 (m, 4H), 7.39 – 7.30 (m, 2H), 6.06 – 5.93 (m, 2H), 5.60 – 5.48 (m, 4H), 5.43 (dd, J = 8.8, 2.4 Hz, 2H).



**Fig. S2** <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ 139.89, 135.73, 134.02, 129.34, 128.98, 127.37, 123.37, 119.59, 108.90, 51.87.

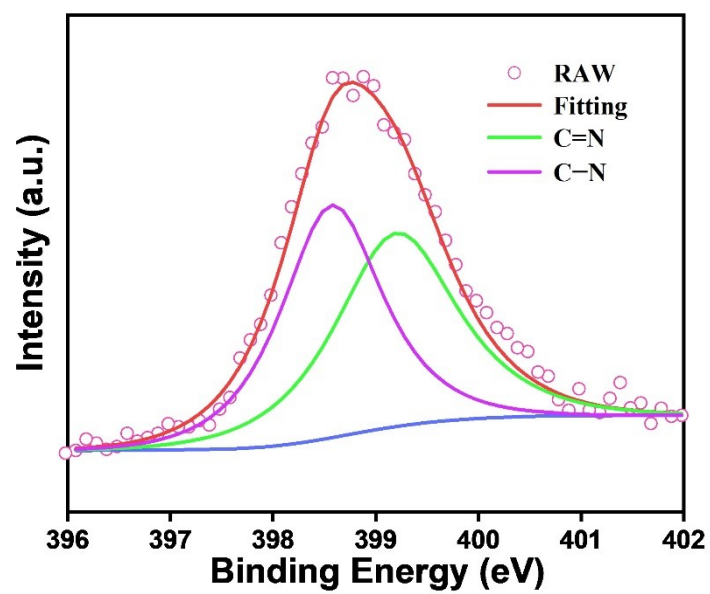


Fig. S3 N 1s XPS spectra of COP.

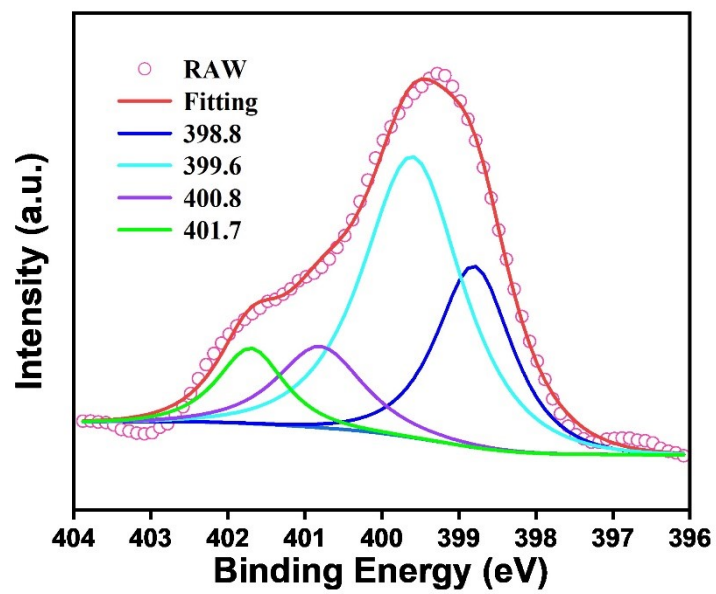


Fig. S4 N 1s XPS spectra of IMF-COP-Fe.

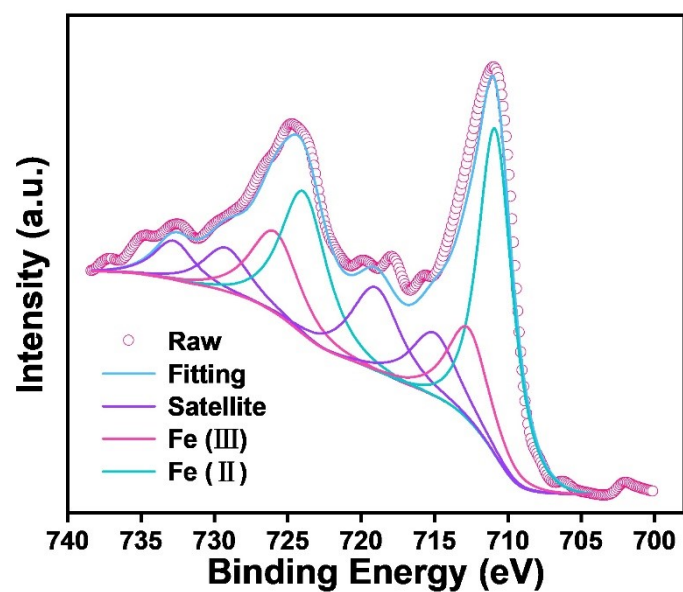


Fig.S5 Fe 2p XPS spectra of IMF-COP-Fe.

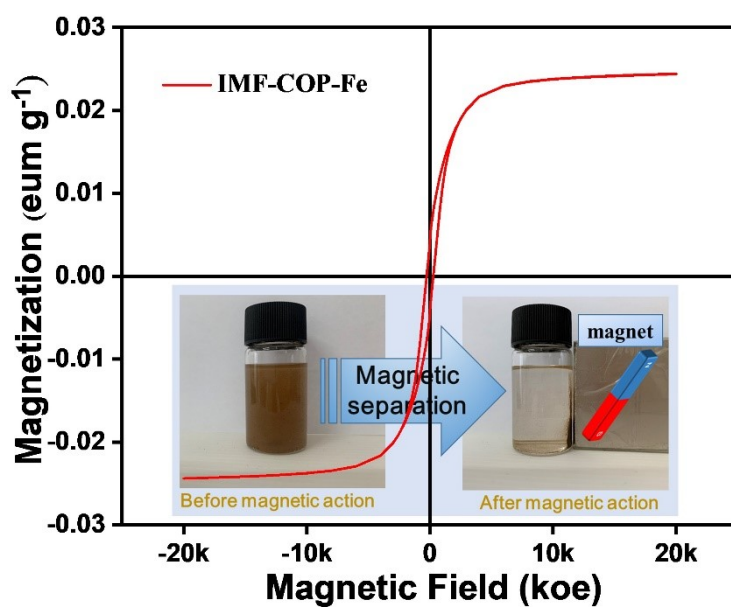
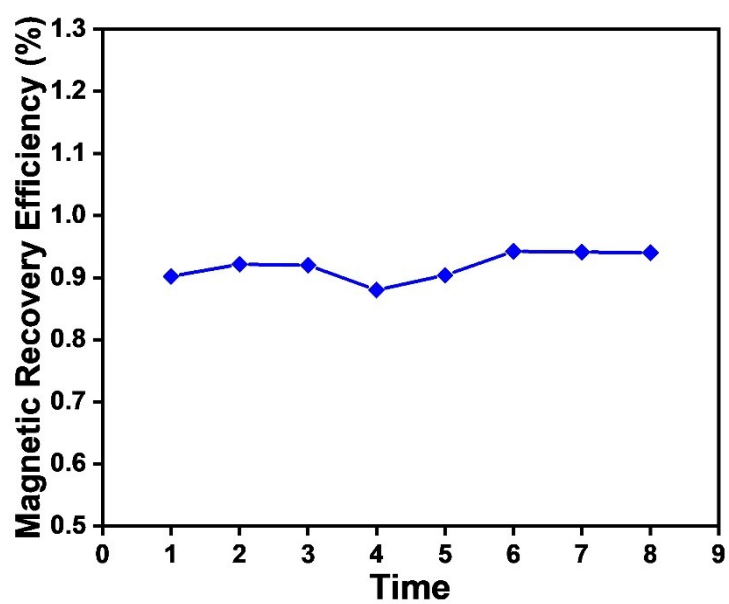
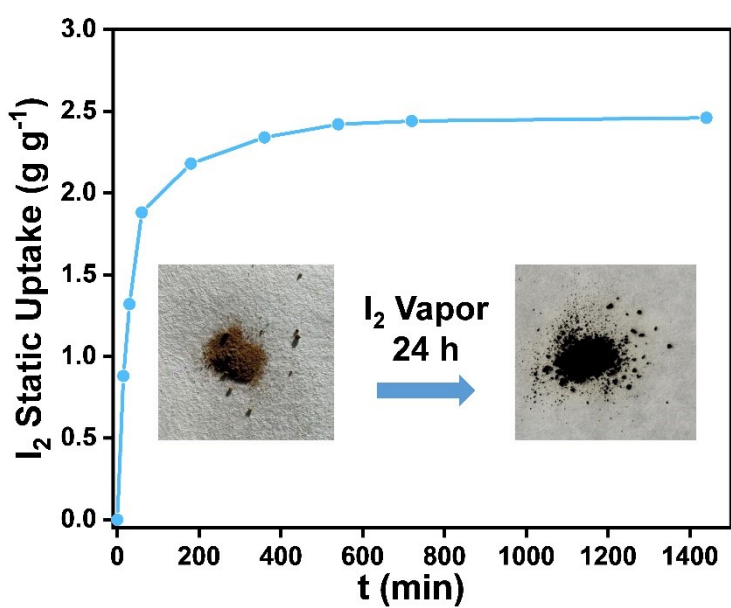


Fig. S6 VSM from the IMF-COP-Fe (inset: magnetic separation of IMF-COP-Fe from cyclohexane solution under an external magnet).



**Fig. S7** The magnetic recovery efficiency of IMF-COP-Fe.



**Fig. S8** Static I<sub>2</sub> vapor adsorption kinetics on IMF-COP-Fe upon exposure to I<sub>2</sub> vapor at 75°C.



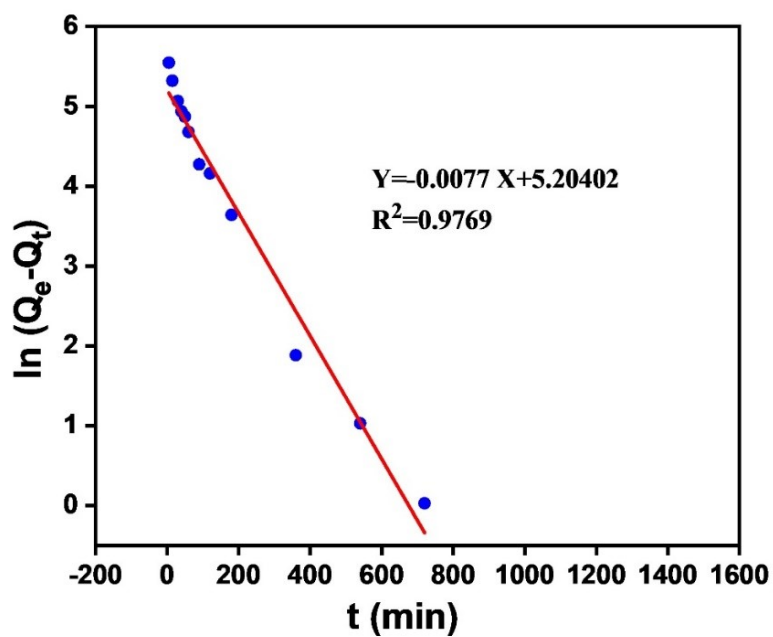


Fig. S9 Pseudo-first-order kinetic model of iodine uptake on IMF-COP-Fe.

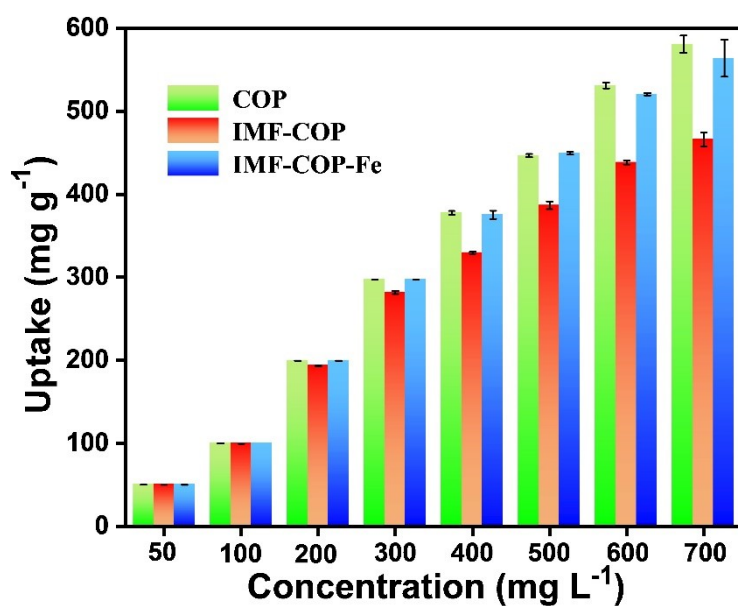


Fig. S10 The maximum adsorption capacity of COP, IMF-COP and IMF-COP-Fe at different concentrations of iodine-cyclohexane solution.

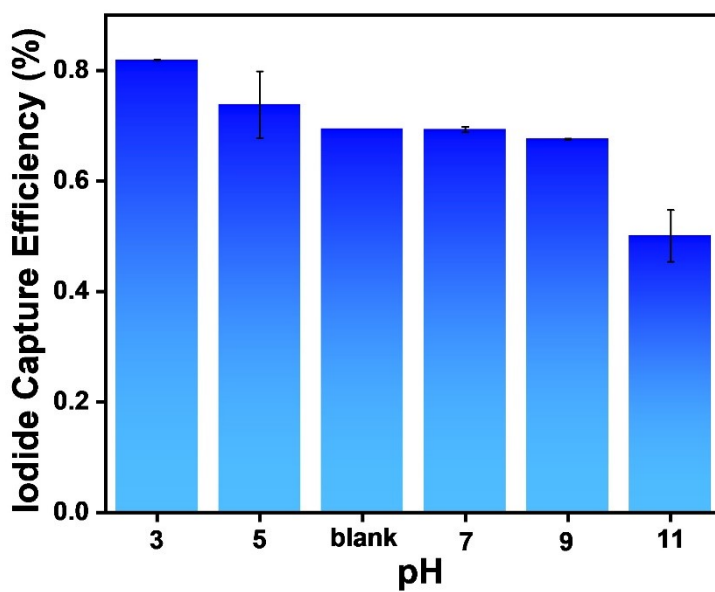


Fig. S11 Effect of pH on iodide removal efficiency of IMF-COP-Fe.

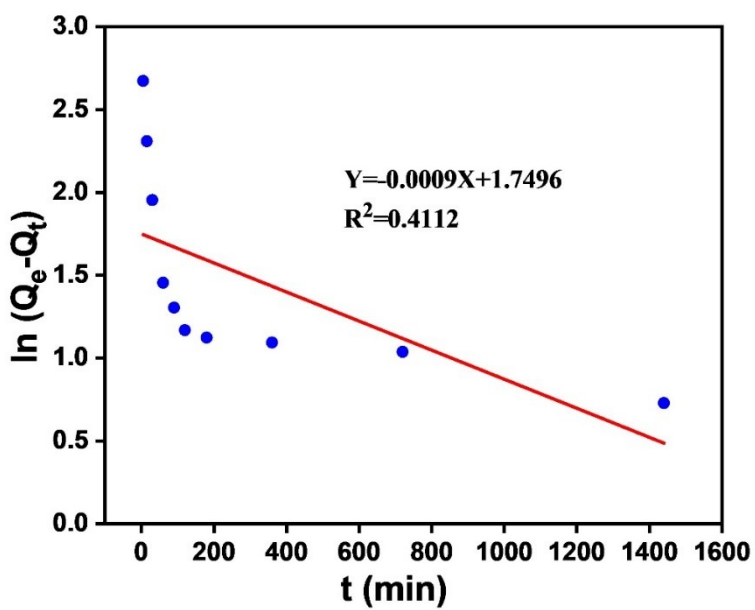


Fig. S12 Pseudo-first-order kinetic model of iodide uptake on IMF-COP-Fe.

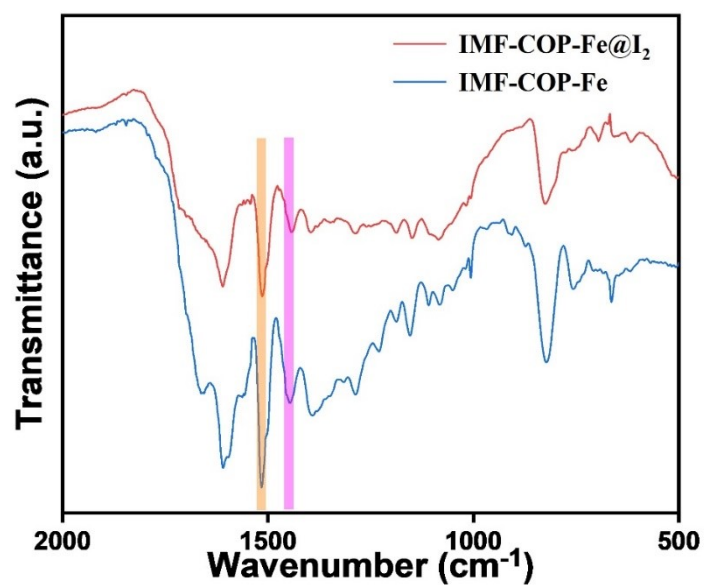


Fig. S13 The FT-IR analysis of IMF-COP-Fe and IMF-COP-Fe@I<sub>2</sub>.

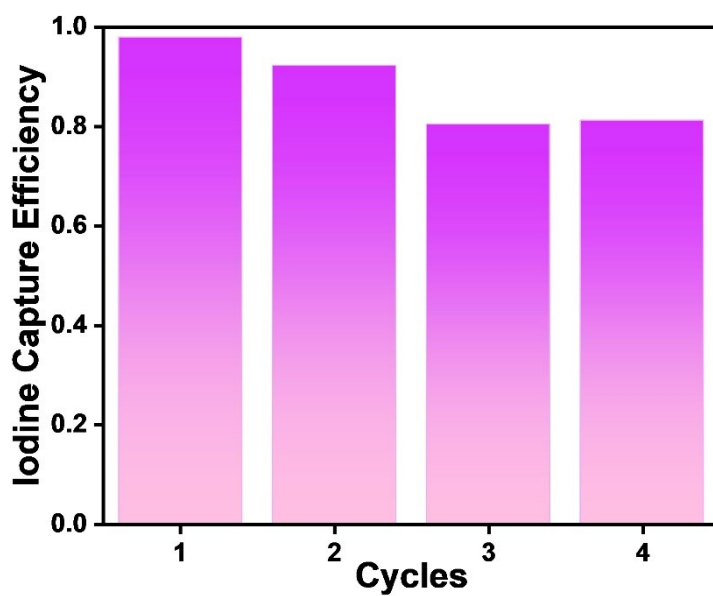


Fig. S14 Recycling test for IMF-COP-Fe adsorption on iodine.

**Table S1** Pseudo-first-order and pseudo-second-order model parameters of adsorption iodine for IMF-COP-Fe.

Adsorbent	Pseudo-first-order model			Pseudo-second-order model		
	$Q_e$	$k_1$	$R^2$	$Q_e$	$k_2$	$R^2$
	( $\text{mg g}^{-1}$ )	( $\text{min}^{-1}$ )		( $\text{mg g}^{-1}$ )	( $\text{g mg}^{-1} \text{min}^{-1}$ )	
IMF-COP-Fe	182.00	0.0077	0.9769	414.94	0.0001167	0.9999

**Table S2** Pseudo-first-order and pseudo-second-order model parameters of adsorption iodide for IMF-COP-Fe.

Adsorbent	Pseudo-first-order model			Pseudo-second-order model		
	$Q_e$	$k_1$	$R^2$	$Q_e$	$k_2$	$R^2$
	( $\text{mg g}^{-1}$ )	( $\text{min}^{-1}$ )		( $\text{mg g}^{-1}$ )	( $\text{g mg}^{-1} \text{min}^{-1}$ )	
IMF-COP-Fe	5.75	0.0009	0.4112	77.58	0.02163	0.9999

**Table S3** Textural properties of different samples.

sample	$S_{\text{BET}}^{\text{a}}$ ( $\text{m}^2 \cdot \text{g}^{-1}$ )	$V_{\text{p}}^{\text{b}}$ ( $\text{cm}^3 \cdot \text{g}^{-1}$ )	$D_{\text{av}}^{\text{c}}$ (nm)
COP	37.10	0.074	7.97
IMF-COP	18.86	0.042	8.99
IMF-COP-Fe	22.10	0.059	10.76

<sup>a</sup> Surface area calculated from  $\text{N}_2$  adsorption isotherms using the BET equation.

<sup>b</sup> Pore volume calculated from nitrogen uptake at  $p/p_0 = 0.99$ .

<sup>c</sup> Average pore size.

**Table S4** The comparison of iodine uptake capacities with other reported adsorbent materials.

Adsorbent	Category	Guest molecules	Adsorption capacity(mg g <sup>-1</sup> )	Ref.
T_COP-1	COPs	I <sub>2</sub>	1045	1
T_COP-2	COPs	I <sub>2</sub>	970	1
T_COP-3	COPs	I <sub>2</sub>	950	1
SIOC-COF-7	COFs	I <sub>2</sub>	1270	2
mICOP-1@agar	COPs	I <sub>2</sub>	1152.5	3
ICOP-1	COPs	I <sub>2</sub>	695.5	3
P-COFs	COFs	I <sub>2</sub>	1300	4
PIPCOP	COPs	I <sub>2</sub>	1950	5
PT-POP	POPs	I <sub>2</sub>	340	6
DaTd-COF	COFs	I <sub>2</sub>	666.79	7
P-TzTz	POPs	I <sub>2</sub>	494.09	8
SCNU-Z4	MOFs	I <sub>2</sub>	332	9
Mxene-PILs	Composites (PILs)	I <sub>2</sub>	170	10
Th-MOF	MOFs	I <sub>2</sub>	1046	11
PHCPs	HCPs	I <sub>2</sub>	469	12
AZO-TPA	Composites	I <sub>2</sub>	661.79	13
AZO-TPA-600	Composites	I <sub>2</sub>	775.36	13
UA-DT	Composites	I <sub>2</sub>	334.5	14
Complexes 1	Composites	I <sub>2</sub>	638.5	15
nano Cu <sub>2</sub> O/Cu-C	Composites	I <sup>-</sup>	41.2	16

$\text{Cu}_{0.1}\text{Zn}_{0.9}\text{@NC}$	Composites	$\text{I}^-$	(pH=3) 235.5	17
$\text{Ag}^0\text{-UiO-66-(OH)}_2$	Composites	$\text{I}^-$	531.98	18
$\text{Ag}^+\text{@UiO-66-(COOH)}_2$	MOFs	$\text{I}^-$	235.5	19
MXene-PDA- $\text{Bi}_6\text{O}_7$	Composites	$\text{I}^-$	64.65	20
$\beta\text{-Bi}_2\text{O}_3$	Metal oxides	$\text{I}^-$	239.5	21
$\sigma\text{-Bi}_2\text{O}_4\text{@PES}$	Composites	$\text{I}^-$	95.4	22
Purolite A530E	Resins	$\text{I}^-$	275.16	23
HDPy-bent	Composites	$\text{I}^-$	80	24
Hal/ $\text{Ag}_2\text{O-2}$	Composites	$\text{I}^-$	57.5	25
$\text{Cu/Al}_2\text{O}_3$ aerogels	Aerogels	$\text{I}^-$	407.6	26
Alg-BO	Composites	$\text{I}^-$	111.8	27
SiPyR-N4	Resins	$\text{I}^-$	124	28
CMPs-1	CMPs	$\text{I}^-$	(t=10°C)16.93	29
CAU-17	Composites	$\text{I}^-$	268.9	30
PGM220%- $\text{Ag}^+$	Composites	$\text{I}^-$	100.82	31
IMF-COP-Fe	Composites (ILs)	$\text{I}_2/\text{I}^-$	563.92(700 mg $\text{L}^{-1}$ )/109.90	This work

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