Supporting Information for

Efficient Removal of Bisphenols Pollutants on Imine-Based Covalent Organic Frameworks: Adsorption Behavior and Mechanism

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TABLE OF CONTENTS

TEXT

TABLES

FIGURES

Text S1. Instrumental analysis

The calibration curve of bisphenol S and bisphenol A were drawn in the concentration range of 0-80 $mg \cdot L^{-1}$, and the concentration were determined by high-performance liquid chromatography (HPLC, Shimadu, Japan) equipped with an UV detector using a SB-C18 column (150 mm×4.6 mm). All samples were filtered through 0.45μm Millipore filters before instrument analysis. The mobile phase was used under the following conditions at the flow rate of 1 $mL \cdot min^{-1}$: acetonitrile, deionized water with 2% acetic acid (50:50, v/v) for BPS; methanol, deionized water with 2% acetic acid (75:25, v/v) for BPA. The determination wavelengths 260 nm, 275 nm for BPS and BPA, respectively [1].

Text S2. Sorption experiments

Batch adsorption experimental conditions and detailed measurement for adsorption kinetics, adsorption isotherm, thermodynamic**,** pH effects, ionic strengthen and reusability experiments were conducted.

Text S3. Adsorption kinetics

For the adsorption kinetics, 8 mg of adsorbent were dispersed in 40 ml of BPS/BPA solution (30 $mg \cdot L^{-1}$) and shaken at 220 rpm and 303 K in a water bath constant temperature oscillator. During adsorption period, the remaining concentration in series of independent sample were measured from 2 min-180 min. Afterward, 1ml of solution was collected periodically and each sample was filtered through a 0.45 μm

membrane filter. The initial and equilibrium concentration of the solutions were analyzed by HPLC. (mobile phase: acetonitrile, deionized water with 2% acetic acid (50:50, v/v) for BPS; methanol, deionized water with 2% acetic acid (75:25, v/v) for BPA. The determination wavelengths 260 nm, 275 nm for BPS and BPA, respectively) [1].Two different kinetics models such as pseudo-first-order kinetics and pseudo-second order kinetics were used to analyze the equilibrium data. The kinetics models equations can be expressed as follows [2, 3]:

Pseudo - first order model: $$\log(q_e - q_t) = \log q_e - k_1 \frac{t}{2.303} \quad (1)$$

Pseudo - second order model: $$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \quad (2)$$

Where, q_e and q_t are the adsorption capacities ($mg \cdot g^{-1}$) at equilibrium and at different time t (min), respectively. k_1 (min^{-1}) and k_2 [$g/(mg \cdot min^{-1})^{-1}$] are the rate constant of the pseudo-first order model and pseudo-second order model, respectively.

Text S4. Adsorption isotherms

For the adsorption isotherm, 8 mg of the COFs adsorbent were added into 40 ml of 10-80 $mg \cdot L^{-1}$ of BPS/BPA solution and shaken at 220 rpm and 303 K for 24 h. Then, 1 mL of the solution was filtered with 0.45 μm membrane, and the residual were measured by above mentioned method.

Two isotherms models such as Langmuir and Freundlich were applied to fit the adsorption data. The equations in linear forms as follows [4, 5]:

Langmuir equations: $$\frac{c_e}{q_e} = \frac{1}{q_{max} k_L} + \frac{c_e}{q_{max}} \quad (3)$$

Freundlich equations: $$ln(q_e) = ln(k_F) + \frac{1}{n} ln(c_e) \quad (4)$$

where, q_e and q_{max} are the adsorption capacity and maximum adsorption capacity ($mg \cdot g^{-1}$), c_e is the concentration at equilibrium ($mg \cdot L^{-1}$), k_L is the Langmuir constant ($L \cdot mg^{-1}$), *1/n* is the intensity of the sorption process, k_F is the Freundlich model constant, *R* is the universal gas constant, *T* is the temperature (K).

Text S5. Adsorption thermodynamic

The adsorption thermodynamics were studied at different temperatures (303, 313 and 323 K) by adding 8 mg of the COFs into 40 ml of 10-80 $mg \cdot L^{-1}$ of BPS/BPA solution and shaken at 220 rpm for 24 h. Then, 1 mL of the solution was filtered with 0.45 μm membrane, and the residual were measured by above mentioned method. The thermodynamic parameters were obtained by the following thermodynamic equations [6, 7]:

$$\Delta G = -RT \ln k_d \tag{5}$$

$$\ln k_d = \frac{\Delta S}{R} - \frac{\Delta H}{RT} \tag{6}$$

$$k_d = \frac{q_e}{c_e} \tag{7}$$

where, R (8.314 J/mol K) and T (k) are universal gas constant and absolute temperature. c_e ($mg \cdot L^{-1}$) and q_e ($mg \cdot g^{-1}$) are equilibrium concentration of adsorbate and equilibrium adsorption amount of adsorbate, respectively. ΔS and ΔH were obtained from intercept and slope of plotting relationship between $\ln k_d$ and *1/T*, respectively.

Text S6. The effect of pH and ionic strength

The pH of BPS/BPA solution was adjusted to 4-10 by adding 0.1 $mol \cdot L^{-1}$ HCl or NaOH solution into desired pH range (4-10). 8 mg of adsorbents were shake with 40

ml of BPS/BPA solutions (30 $mg \cdot L^{-1}$) with varying pH at 303 K for 3 h. The initial and equilibrium concentrations of BPS/BPA were measured by HPLC. The aqueous solution of NaCl was used as control ionic strength and range from 0-1 $mol \cdot L^{-1}$.

Text S7. Regeneration and reuse experiences

Four sorption-regeneration cycles were performed to evaluate the recyclability and reusability of the COFs adsorbent. For sorption, 8 mg adsorbent was added into100 ml centrifuge tube containing 40 ml of 30 $mg \cdot L^{-1}$ BPS/BPA solution. The solution was shaken on a water bath thermostatic oscillator at 220 rpm for 3 h at 303 K. Then, the COFs were separated and collected by an organic filter membrane. For desorption, the collected adsorbent was re-dispersed in 40 ml methanol and the mixture was shaken at 220 rpm for 1 h at 303 K. Then, the regenerated adsorbent was collected by an organic filter membrane from methanol solution and washed several times with deionized water. After drying, the regenerated COFs were used in the next sorption experience.

Table S1. Kinetic model parameters in the adsorption of BPS and BPA on prepared COFs materials

Adsorbate	Adsorbent	$q_{e,exp}$	Pseudo-first-order			Pseudo-second-order		
			$q_{e,cal}$ ($mg \cdot g^{-1}$)	k_1 (min^{-1})	R^2	$q_{e,cal}$ ($mg \cdot g^{-1}$)	k_2 (min^{-1})	R^2
BPS	COF-2	139	43.00	0.021	0.6624	138.89	0.004	0.9991
	COF-1	124	26.94	0.024	0.5995	125.00	0.007	0.9997
BPA	COF-2	115	45.4255	0.020	0.7415	116.28	0.003	0.9984
	COF-1	84	27.8676	0.026	0.5714	84.03	0.004	0.9977

Table S2. Langmuir and Freundlich parameters in the adsorption of BPS and BPA on prepared COFs materials

Adsorbate	Adsorbent	Langmuir model				Freundlich model		
		q_{max} ($mg \cdot g^{-1}$)	K_L ($L \cdot min^{-1}$)	R^2	R_L	K_F ($L \cdot min^{-1}$)$^{1/n}$	n	R^2
BPS	COF-2	200.00	1.01	0.9981	0.03	101.70	4.82	0.7602
	COF-1	158.73	1.13	0.9989	0.03	26.49	2.01	0.8704
BPA	COF-2	149.25	0.61	0.999	0.05	66.83	4.40	0.8794
	COF-1	131.58	0.26	0.9988	0.11	44.58	3.58	0.9577

Table S3. Comparison of adsorption performance of resulting adsorbent toward BPS and BPA with many other adsorbents reported previously

Adsorbate	Adsorbent	Equilibrium time (h)	Q_{max}（L·min^{-1}）	Temperature (℃)	Reference
BPA	PAC-PNIPAM	24	116.3	25	[8]
	MMIPs	12	142.86	25	[9]
	SMZFA	24	114.9	25	[10]
	graphene	6	182	29	[11]
	Conventional AC	5	30.8	25	[12]
	COF-1	3	124.66	30	This work
	COF-2	3	144.58	30	
BPS	NZY	5	25.64	25	[13]
	NZSM-5	2	41	25	[14]
	CA-P-CDP	0.25	48.25	25	[15]
	Fe_3O_4@COF	2	21.78	25	[16]
	Conventional AC	12	123	25	[17]
	COF-1	3	157	30	This work
	COF-2	3	195.24	30	

Table S4. Thermodynamic parameters in the adsorption of BPS and BPA on COF-2 at different temperatures

Adsorbate	Temperature (K)	lnk_d	ΔG ($KJ \cdot mol^{-1}$)	ΔH ($KJ \cdot mol^{-1}$)	ΔS ($J \cdot (mol \cdot K^{-1})^{-1}$)
BPS	303	1.681	-4.236	-37.137	-109.080
	313	1.013	-2.552		
	323	0.773	-1.947		
BPA	303	7.925	-19.965	-82.310	-206.295
	313	6.684	-17.393		
	323	5.906	-15.861		

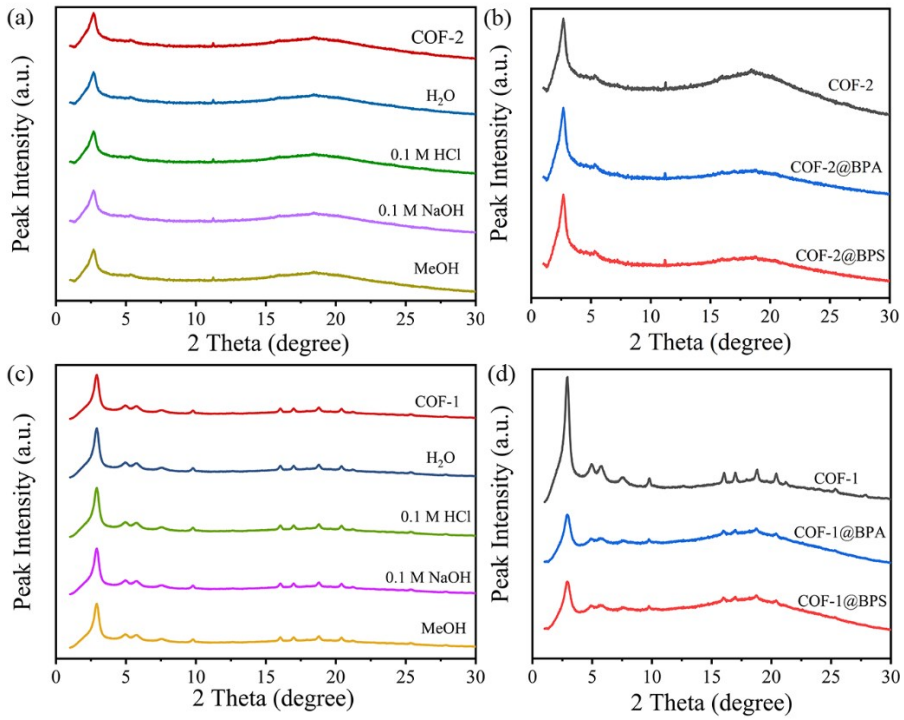

Fig. S1 (a, c) PXRD pattern of COF-1 and COF-2 after treatment with different solvents for 24 h; (b, d) PXRD pattern of before and after adsorption of BPS and BPA onto COF-1 and COF-2

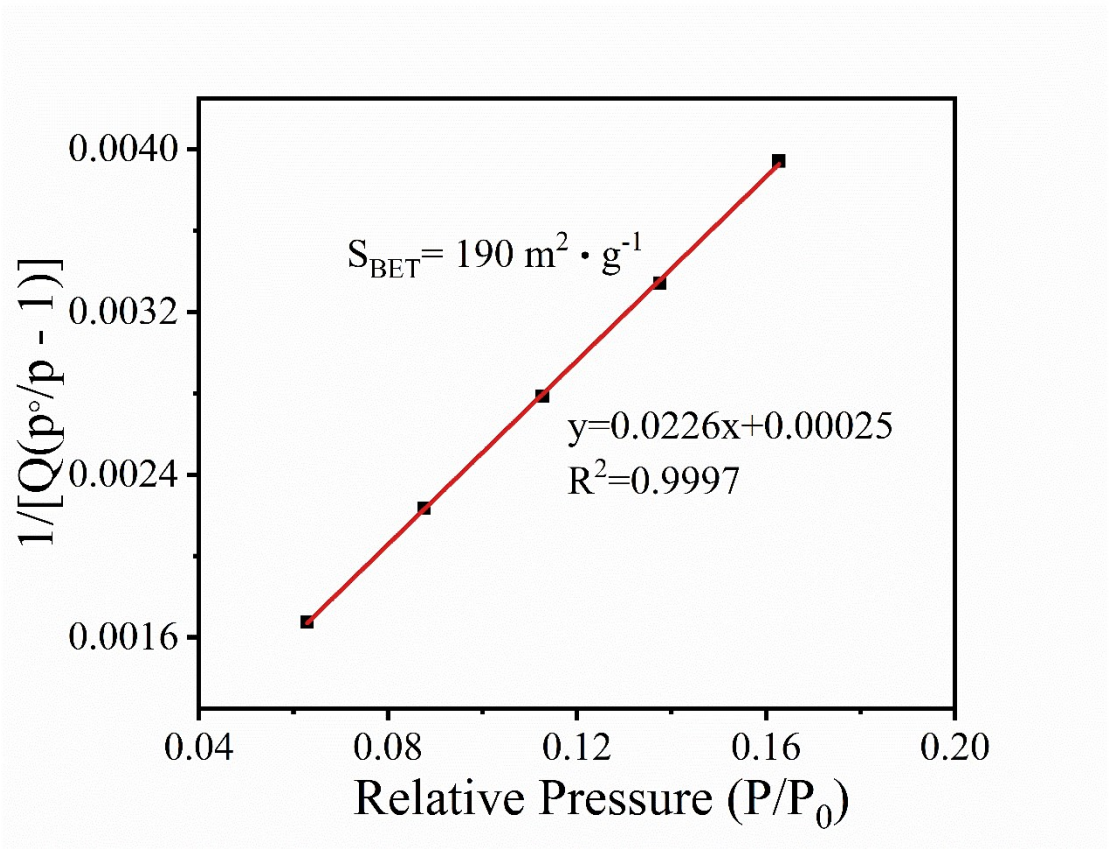

Fig. S2 BET surface area plot for COF-1 calculated from the isotherm

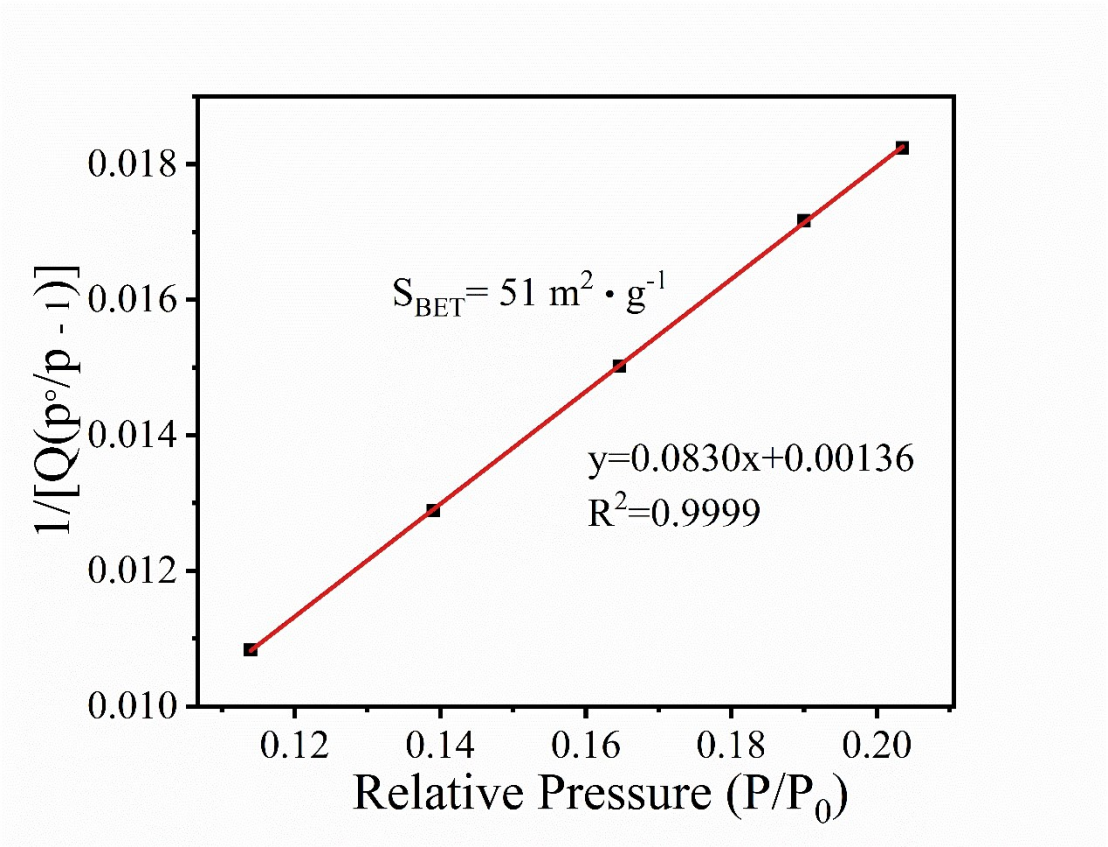

Fig. S3 BET surface area plot for COF-2 calculated from the isotherm

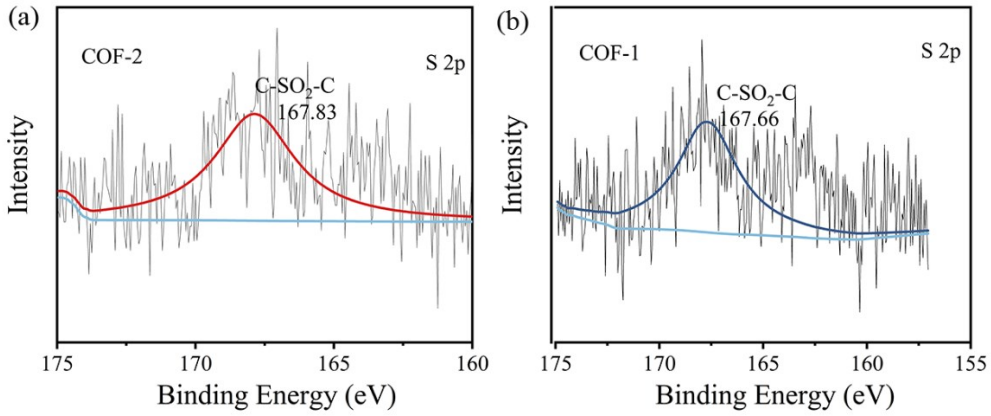

Fig. S4 High deconvolutions of S2p spectra of before and after adsorption of BPS onto COF-1 and COF-2

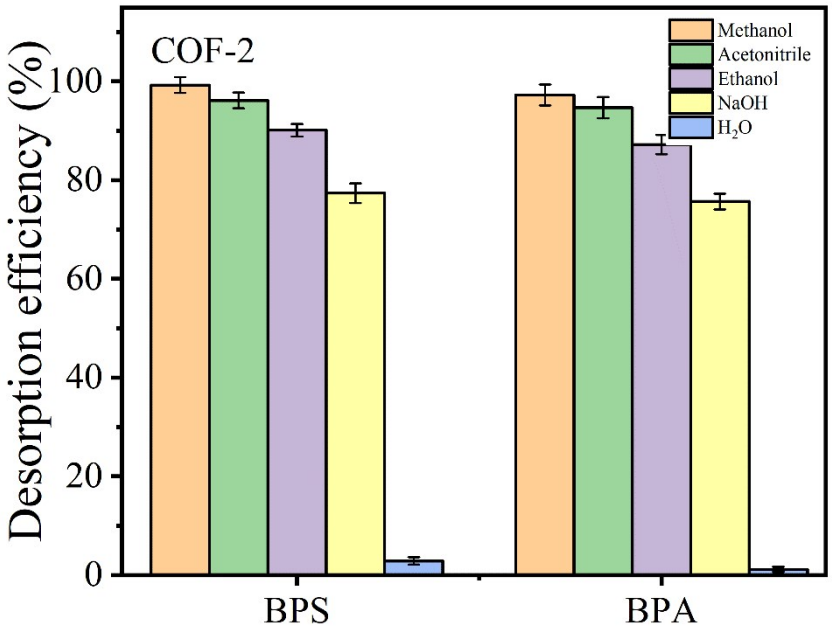

Fig. S5 Desorption percentage of BPS and BPA from COF-2 with di□erent solvents.

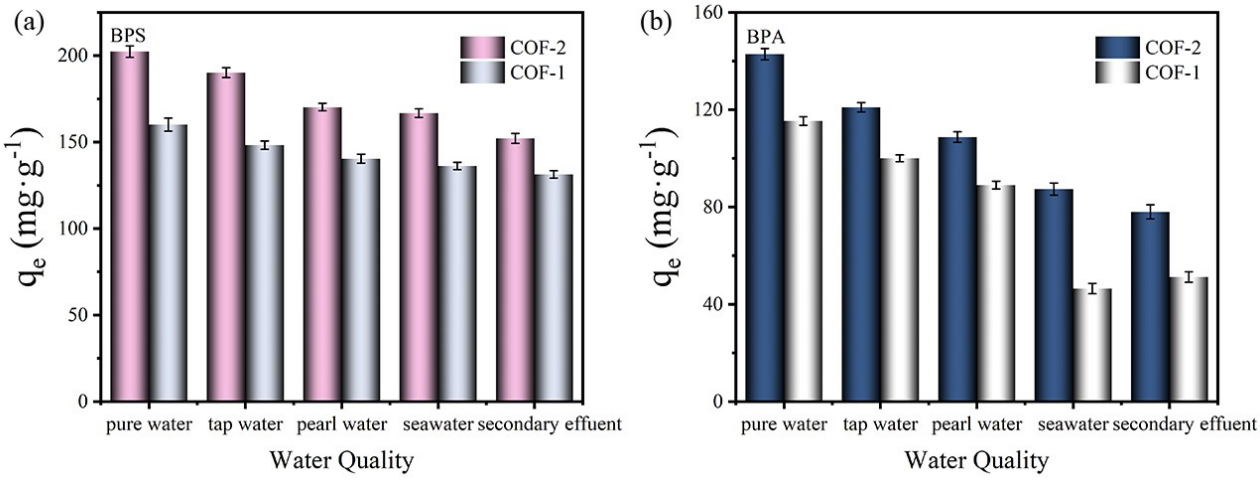

Fig. S6 (a, b) The effect of water quality on adsorption (In each case C_0 = 50 mg·L^{-1}, T = 303 K, t= 24 h, m/V = 0.2 g·L^{-1}).

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