

Electronic Supplementary Information

In-Situ room-temperature fabrication of a covalent organic framework and its bonded fiber for solid-phase microextraction of polychlorinated biphenyls in aquatic products

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Table of Contents

1. Supplementary Figures
2. Supplementary Tables

1. Supplementary Figures

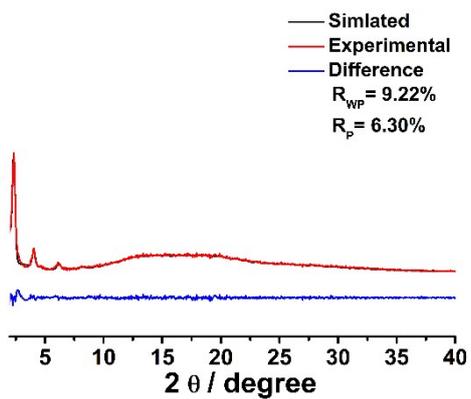


Fig. S1 Pawley refinement of TFPB-BD.

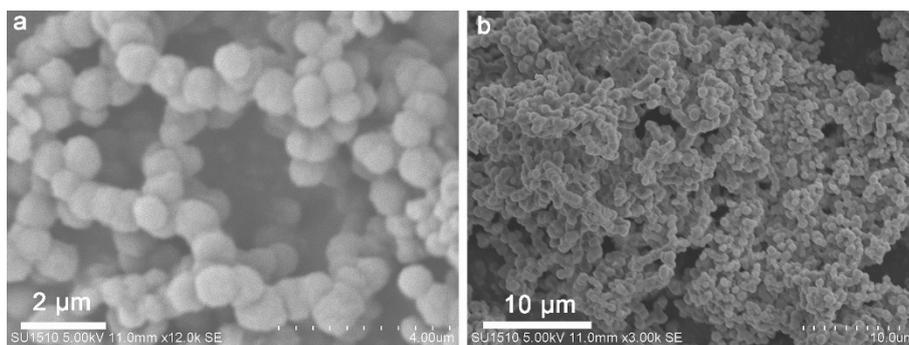


Fig. S2 SEM images of TFPB-BD powder with magnification at (a) 12000 \times ; (b) 3000 \times .

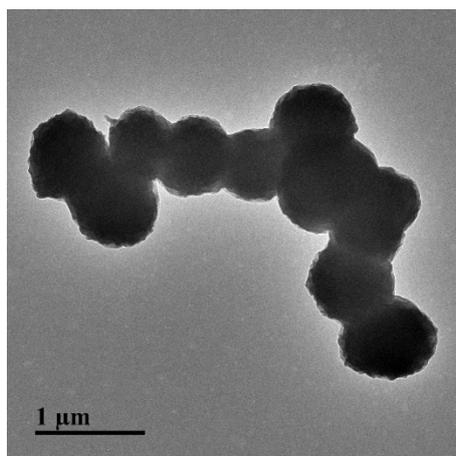


Fig. S3 TEM image of TFPB-BD.

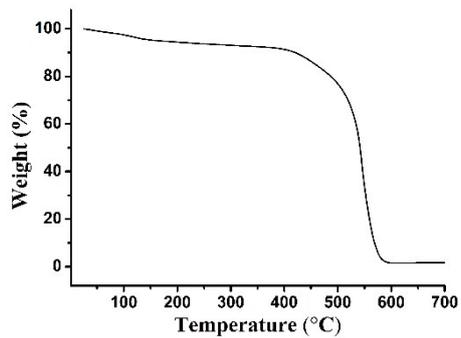


Fig. S4 TGA curves of the TFPB-BD.

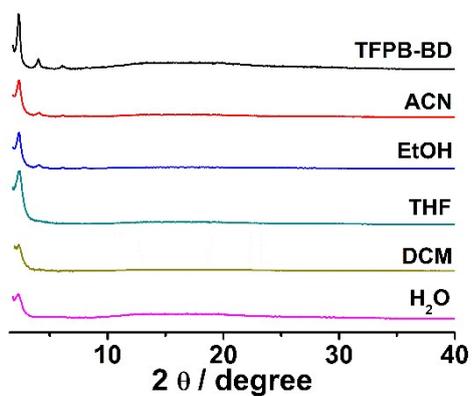


Fig. S5 PXRD patterns of TFPB-BD after treatment with different solvents for 24 h.

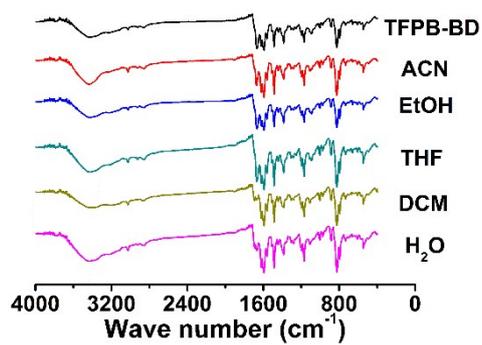


Fig. S6 FT-IR spectra of TFPB-BD after treatment with different solvents for 24 h.

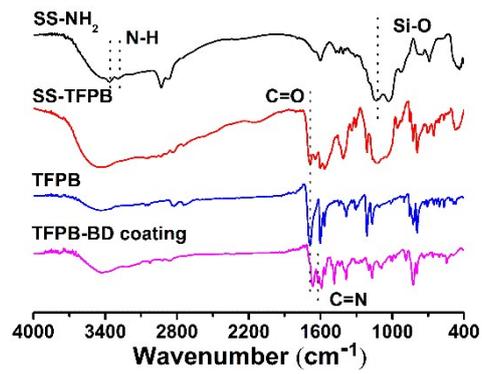


Fig. S7 FT-IR spectra of powders scraped from SS-NH₂ (black), SS-TFPB (red) SS-TFPB-BD (magenta) fibers and monomer TFPB (blue).

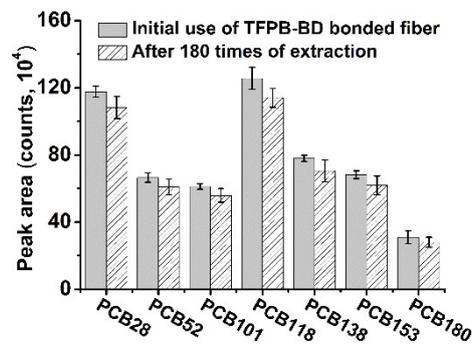


Fig. S8. Comparison of the peak areas of 100 ng L⁻¹ PCBs obtained with the fresh TFPB-BD bonded fiber and the reused TFPB-BD bonded fiber after 180 cycles extraction

2. Supplementary Tables

Table S1 Other Parameters for the Determination of PCBs

Compound	Retention time (min)	MS1→MS2	CE (eV)
PCB28	6.68	255.8→186	30
		257.8→186	32
PCB52	6.91	289.8→220	38
		291.8→220	38
PCB101	7.5	323.7→253.9	34
		325.7→255.9	32
PCB118	7.94	323.7→253.9	30
		325.7→255.8	30
PCB138	8.09	361.7→291.7	34
		359.7→289.7	35
PCB153	8.29	361.7→291.7	28
		359.7→289.8	32
PCB180	8.77	393.7→323.8	38
		395.7→325.7	38

Table S2 Fractional main atomic coordinates for the unit cell of TFPB-BD after Pawley refinement.

TFPB-BD: Space group symmetry P6/m

a= b = 43.7789 Å, c = 4.0603 Å, $\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$

Atom	x	y	z
C1	0.32022	0.68798	0.50000
C2	0.35481	0.70135	0.50000
C3	0.37825	0.73921	0.50000
C4	0.36496	0.76174	0.50000
C5	0.38706	0.79738	0.50000
C6	0.42290	0.81125	0.50000
C7	0.43624	0.78887	0.50000
C8	0.41417	0.75323	0.50000
C9	0.44667	0.84881	0.50000
N10	0.43488	0.87005	0.50000
C11	0.45454	0.90703	0.50000
C12	0.49064	0.92578	0.50000
C13	0.50825	0.96178	0.50000
C14	0.49047	0.98047	0.50000
C15	0.45404	0.96092	0.50000
C16	0.43663	0.92496	0.50000
H17	0.33743	0.75173	0.50000
H18	0.37624	0.81421	0.50000
H19	0.46379	0.79901	0.50000
H20	0.42517	0.73655	0.50000
H21	0.47396	0.85798	0.50000
H22	0.50568	0.91311	0.50000
H23	0.53586	0.97417	0.50000
H24	0.43812	0.97255	0.50000
H25	0.40879	0.91071	0.50000

Table S3 Analytical results ($\mu\text{g kg}^{-1}$, mean \pm s, $n=6$) for the determination of PCBs in aquatic products

Analyte	Snakehead		Bream		Catfish		Crucian		Base shrimp		White shrimp	
	no spiking	spiked with 1.0 $\mu\text{g kg}^{-1}$	no spiking	spiked with 1.0 $\mu\text{g kg}^{-1}$	no spiking	spiked with 1.0 $\mu\text{g kg}^{-1}$	no spiking	spiked with 1.0 $\mu\text{g kg}^{-1}$	no spiking	spiked with 1.0 $\mu\text{g kg}^{-1}$	no spiking	spiked with 1.0 $\mu\text{g kg}^{-1}$
PCB28	0.54 \pm 0.08	1.47 \pm 0.04	0.46 \pm 0.06	1.37 \pm 0.04	<LOD	0.99 \pm 0.09	0.74 \pm 0.06	1.66 \pm 0.04	<LOD	0.98 \pm 0.04	0.57 \pm 0.02	1.55 \pm 0.04
PCB52	0.45 \pm 0.04	1.41 \pm 0.03	0.62 \pm 0.21	1.51 \pm 0.06	<LOQ	0.87 \pm 0.06	1.01 \pm 0.10	1.90 \pm 0.02	<LOD	0.96 \pm 0.01	<LOQ	0.93 \pm 0.05
PCB101	<LOD	0.88 \pm 0.03	0.83 \pm 0.15	1.73 \pm 0.04	<LOQ	0.94 \pm 0.03	0.59 \pm 0.02	1.49 \pm 0.06	<LOD	0.92 \pm 0.08	0.33 \pm 0.05	1.31 \pm 0.07
PCB118	0.83 \pm 0.15	1.78 \pm 0.08	0.97 \pm 0.12	1.95 \pm 0.08	0.61 \pm 0.03	1.49 \pm 0.02	1.34 \pm 0.03	2.24 \pm 0.01	<LOQ	0.95 \pm 0.08	0.39 \pm 0.07	1.32 \pm 0.03
PCB138	0.42 \pm 0.07	1.29 \pm 0.03	1.28 \pm 0.26	2.15 \pm 0.02	0.79 \pm 0.09	1.71 \pm 0.01	1.46 \pm 0.17	2.37 \pm 0.02	<LOD	0.94 \pm 0.01	<LOQ	0.90 \pm 0.01
PCB153	<LOQ	0.98 \pm 0.04	1.48 \pm 0.23	2.43 \pm 0.02	0.84 \pm 0.13	1.72 \pm 0.01	1.04 \pm 0.11	2.01 \pm 0.08	<LOQ	0.89 \pm 0.02	<LOD	0.97 \pm 0.01
PCB180	<LOQ	0.87 \pm 0.06	<LOQ	0.93 \pm 0.03	<LOQ	0.93 \pm 0.09	<LOQ	0.91 \pm 0.01	<LOD	1.00 \pm 0.03	<LOQ	0.95 \pm 0.03