

Supplementary Information

Synthesis of spiro borate-linked covalent organic frameworks (COFs) based on 1,3-diol borates

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1. General Methods

All reagents were commercially available and directly employed without further purification unless stated otherwise. 3,3,9,9 Tetramethyl-2,4,8,10-tetraoxaspiro [5.5] undecane ¹ were prepared according to previously reported procedures, respectively. All spectral data was in agreement with the literature above.

Thin-layer chromatography (TLC) was done on silica gel coated aluminum sheets with F254 indicator and column chromatography separation was performed with silica gel (particle size 0.063-0.200 mm).

Nuclear Magnetic Resonance (NMR) spectra were recorded in CDCl₃ using Bruker DPX 400 MHz NMR spectrometers. Chemical shifts (δ) were expressed in ppm relative to the residual of solvents CDCl₃, (¹H: 7.26 ppm). Coupling constants (*J*) were recorded in Hertz. Abbreviations: s = singlet, d = doublet, t = triplet, m = multiplet.

Fourier-transform infrared spectra (FT-IR) were recorded on a SHIMADZU, IRSpirit-T by pelletizing a sample with KBr.

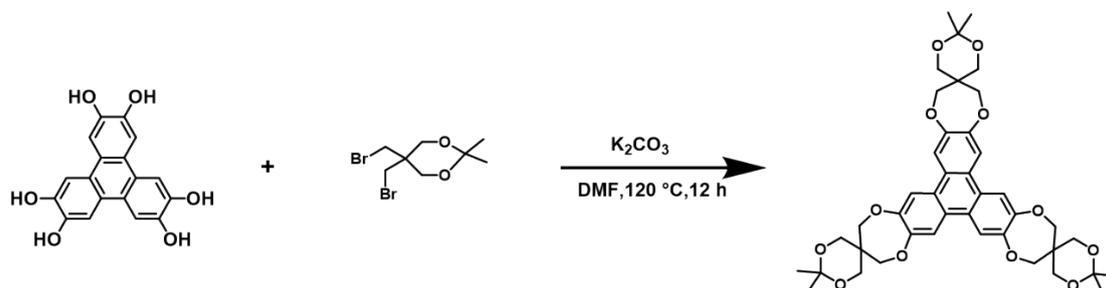
Powder X-ray diffraction data (PXRD) were collected using a Rigaku D/Max 2500 rotating anode X-ray powder diffractometer using Cu K α radiation ($\lambda=1.5406$ Å) operated at 1.6 kW (40 kV, 40 mA) power and equipped with a position sensitive detector with a 10.0 mm divergence height slit. Samples were loaded on zero background sample holders. Data were collected in the range of $2\theta=3$ to 30° with a 0.02° step size and 2° min^{-1} of scan rate. Pawley refinement was performed repeatedly to optimize the lattice parameter until the R_p and R_{wp} values converged.

Field emission scanning electron microscopy (SEM) was carried out on a FEI Nanonova 230, equipped with an energy dispersive spectrometer, with an accelerating voltage of 10 kV and a working distance of 5 mm. All samples were loaded on conductive carbon tape and then prepared by Au sputtering.

High-resolution transmission electron microscopy (HRTEM) was performed with a JEOL JEM-2100F equipped with a field emission gun operated at 200 kV. The sample was suspended in Isopropyl alcohol and drop-cast onto a 200-copper mesh, lacey carbon grid (Ted Pella)

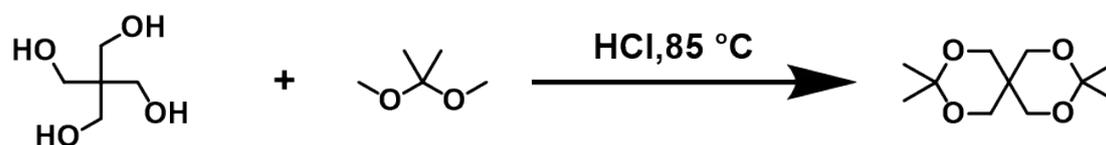
2. Synthetic Details

Synthesis of HHTP-TP



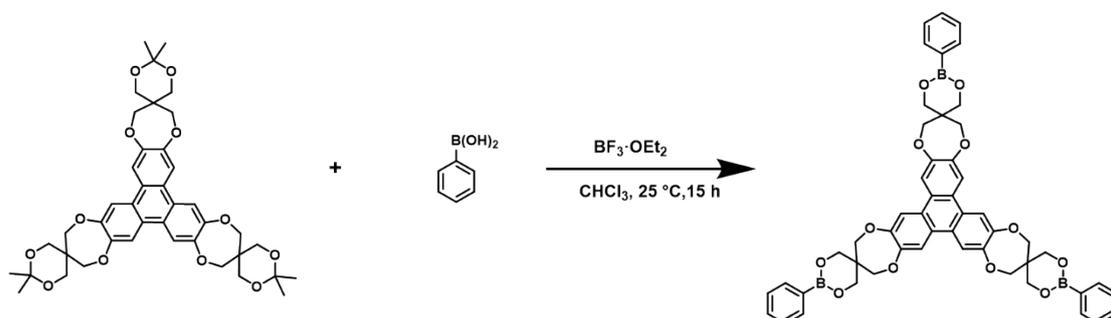
To a solution of 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) (1.0 g, 3.1 mmol) and 5,5-bis(bromomethyl)-2,2-dimethyl-1,3-dioxane (2.81 g, 9.30 mmol) in *N,N*-dimethylformamide (DMF) (100 mL) was added K_2CO_3 (2.98 g, 21.6 mmol). The reaction mixture was heated at 120 °C for 12 h. Then, the resulting mixture was cooled to room temperature and poured into water (100 mL), and added dichloromethane (50 mL). The organic layer was subsequently separated, and was extracted with dichloromethane (3 × 40 mL). The combined organic layers were washed with brine (60 mL) for three times, dried with anhydrous Na_2SO_4 , and concentrated. The residue was purified by silica gel column chromatography to give HHTP-TP as a white solid (0.63 g, 85% yield). 1H NMR (400 MHz, $CDCl_3$): (ppm) 7.85 (s, 6H), 4.24 (s, 12H), 3.89 (s, 12H), 1.50 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.9, 125.2, 123.3, 114.5, 104.4, 98.7, 73.8, 63.4, 60.4, 56.1, 40.3, 32.6. MS (ESI): m/z Calcd. For $C_{42}H_{48}O_{12}$: 744.31, $[M]^+$, found: 744,31. m/z : 744.31.

Synthesis of 3,3,9,9 Tetramethyl-2,4,8,10-tetraoxaspiro [5.5] undecane (PT)



The compound was synthesized as previously reported in literature¹. Sublimation of the solid product formed by the reaction of pentaerythritol with 2,2-dimethoxypropane at 85 °C gave a 70% yield. 1H NMR (500 MHz, $CDCl_3$) δ 3.75 (d, $J = 1.5$ Hz, 8H), 1.42 (d, $J = 1.5$ Hz, 12H).

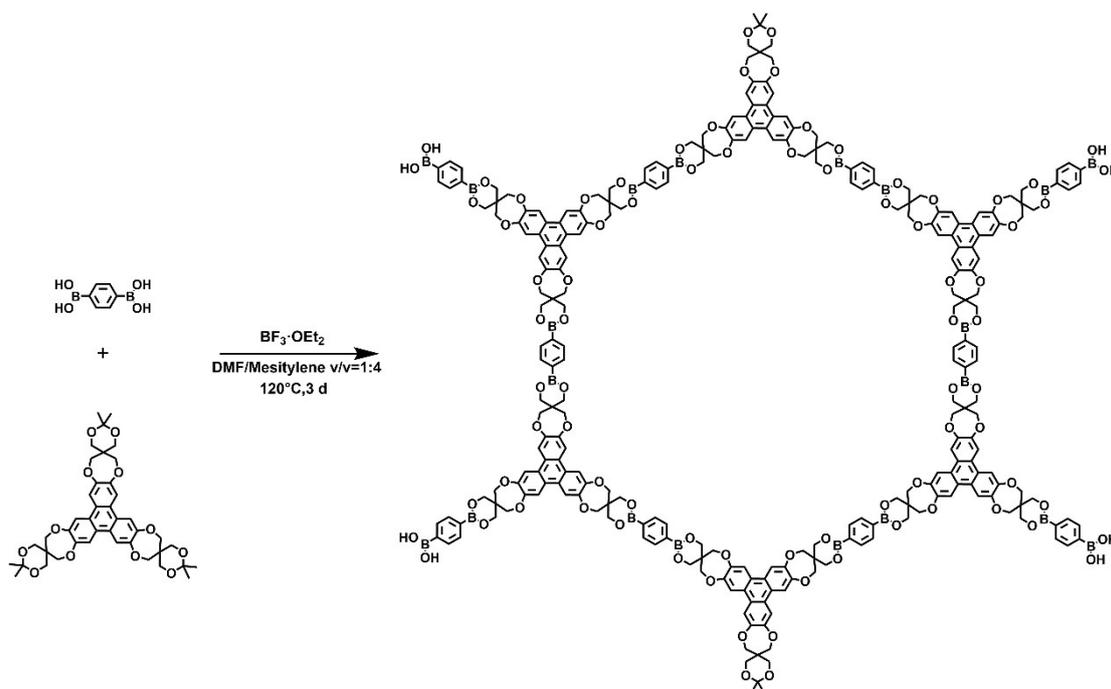
Synthesis of HHTP-PT-R



To a solution of HHTP-TP (10 mg, 0.02 mmol) and phenylboronic acid (5.5 mg, 0.050 mmol) in CHCl_3 (2 mL) was added boron trifluoride etherate (1.9 μL , 0.020 mmol). The reaction mixture was heated at room temperature for 15 h. The white product was obtained in 15.2 mg yield (86%). $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.91~7.85 (m, 14H), 7.48~7.43 (m, 7H), 4.29~4.24 (d, 24H).

3. Synthesis of COFs

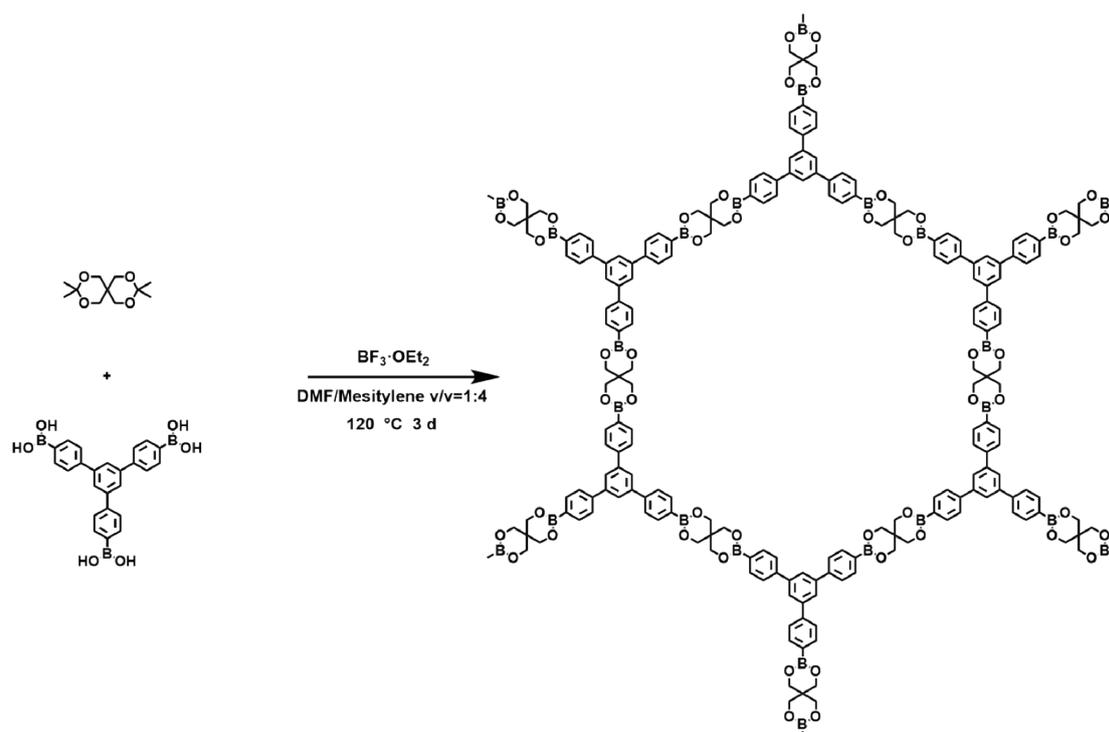
Synthesis of BSCOF-1



A Pyrex tube was charged with HHTP-TP (37.5 mg, 0.0503 mmol), 1,4-benzenediboronic acid (BDDBA) (12.5 mg, 0.075 mmol), boron trifluoride etherate (15 μL) and

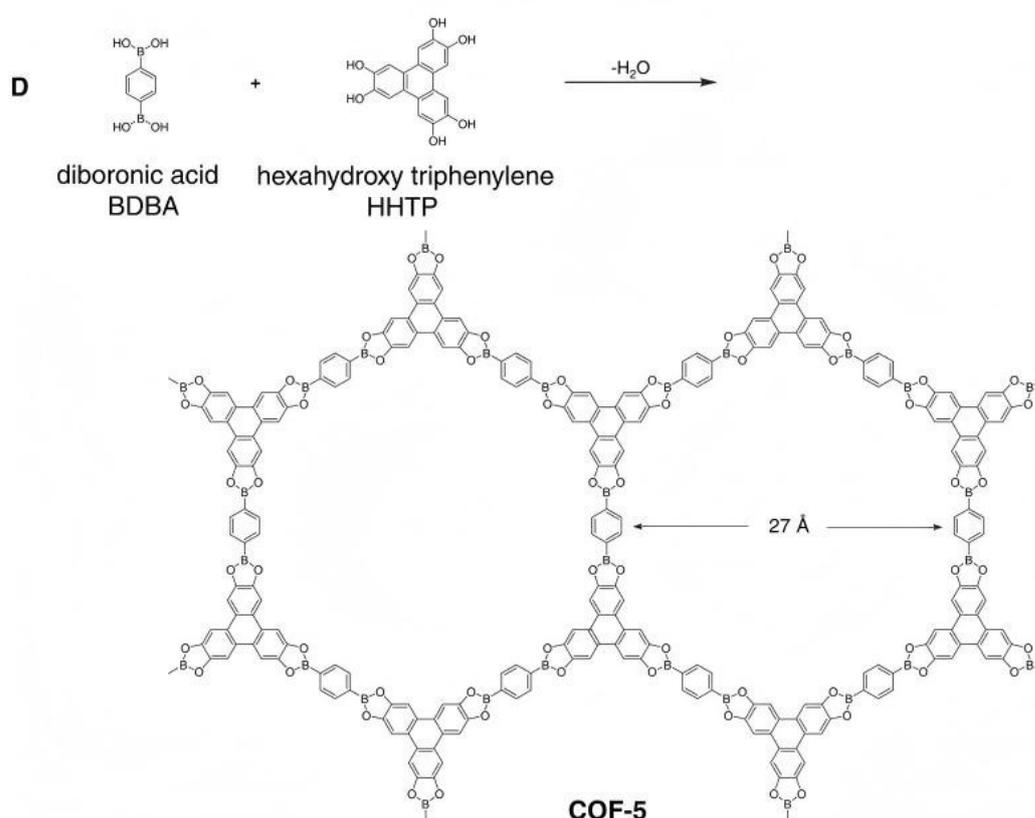
1.5 mL of DMF and 1,3,5-trimethylbenzene (1:4). The tube was flash frozen at 77 K (LN₂ bath) evacuated and flame sealed. Upon sealing the length of the tube was reduced to 15 cm. The reaction mixture was heated at 120 °C for 7 days. Then, reaction mixture was cooled to room temperature and filtered. The filtered solid was soaked in neat THF and acetone (20 mL) for 24 h and then dried under vacuum. Then it was degassed at 80 °C overnight to afford BSCOF-1(33.1 mg, 70.1%).

Synthesis of BSCOF-2



A Pyrex tube was charged with 1,3,5-tris [(4-phenylboronic acid)] benzene (BTPA) (27.6 mg, 0.0600 mmol), PT (12.8 mg, 0.0900 mmol), boron trifluoride etherate (24 μL) and 1.5 mL of DMF:1,3,5-trimethylbenzene (1:4). The tube was flash frozen at 77 K (LN₂ bath), evacuated and flame sealed. Upon sealing the length of the tube was reduced to 15 cm. The reaction mixture was heated at 120 °C for 3 days. Then, reaction mixture was cooled to room temperature, and filtered. The filtered solid was soaked in neat THF and acetone (20 mL) for 24 h and then dried under vacuum. Then it was degassed at 80 °C overnight to afford BSCOF-2 (23.2 mg, 62.7%).

Synthesis of COF-5



The compound was synthesized as previously reported in literature.² A Pyrex tube was charged with BDDBA (25 mg, 0.15 mmol), HHTP (16 mg, 0.050 mmol) and 1 mL of mesitylene and dioxane (1:1). The tube was flash frozen at 77 K (LN₂ bath) and evacuated to an internal pressure of 150 mtorr and flame sealed. Upon sealing the length of the tube was reduced to 18 cm. The reaction mixture was heated at 100 °C for 72 h to yield a free flowing gray-purple powder. Following guest removal COF-5 is obtained as a light gray solid (15 mg, yield 73%).

4.Characterization and Modeling of COFs

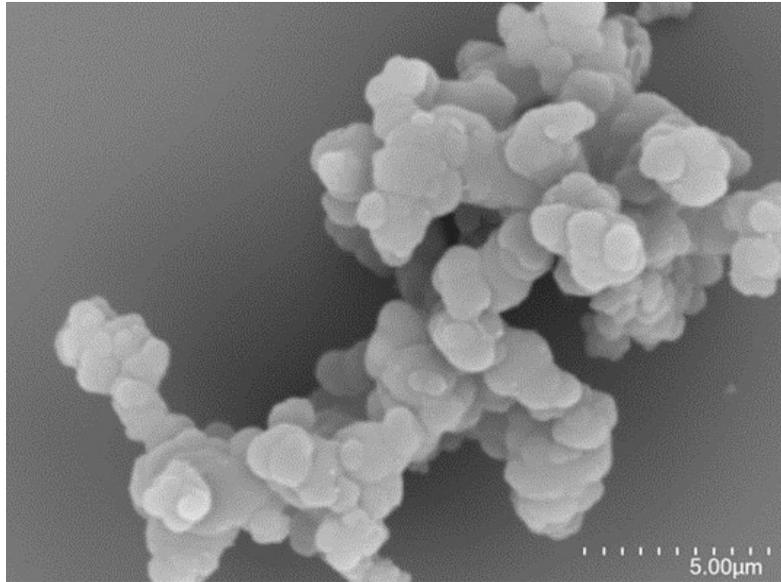


Figure S1. SEM image of BSCOF-1

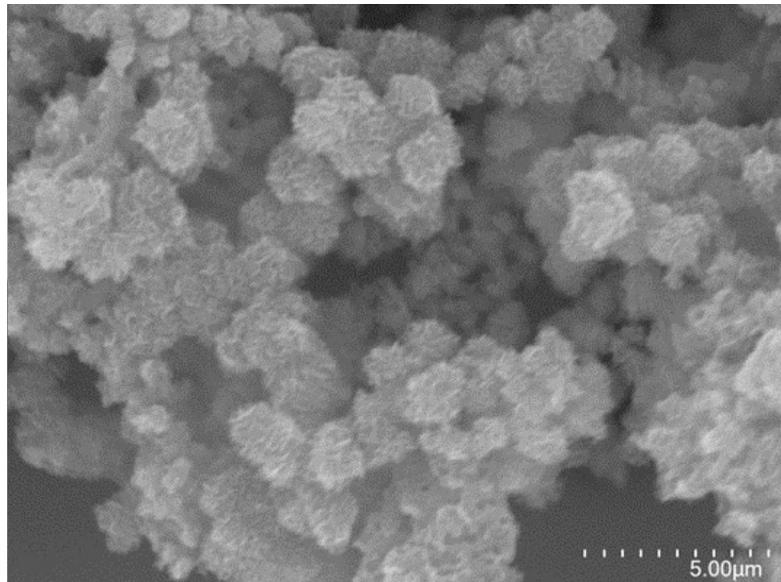


Figure S2. SEM image of BSCOF-2

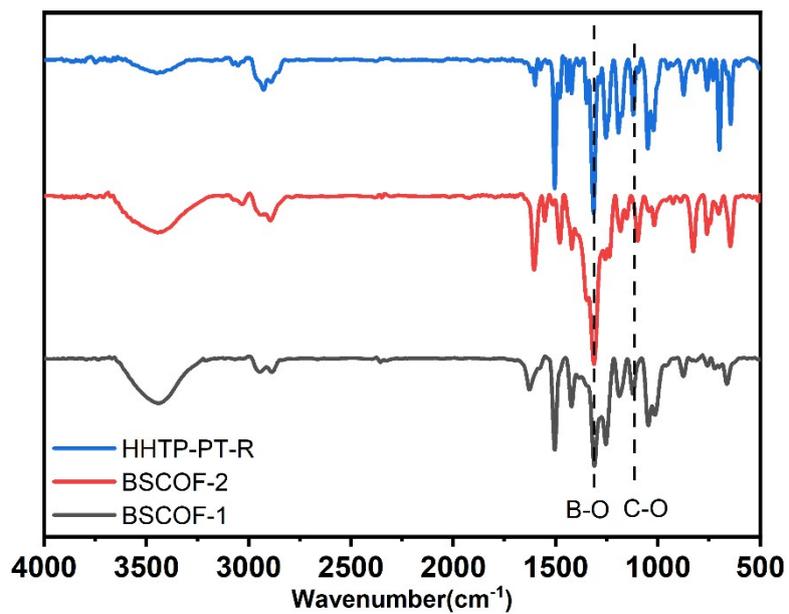


Figure S3. FT-IR spectra of HHTP-PT-R (blue), BSCOF-2 (red), BSCOF-1 (black)

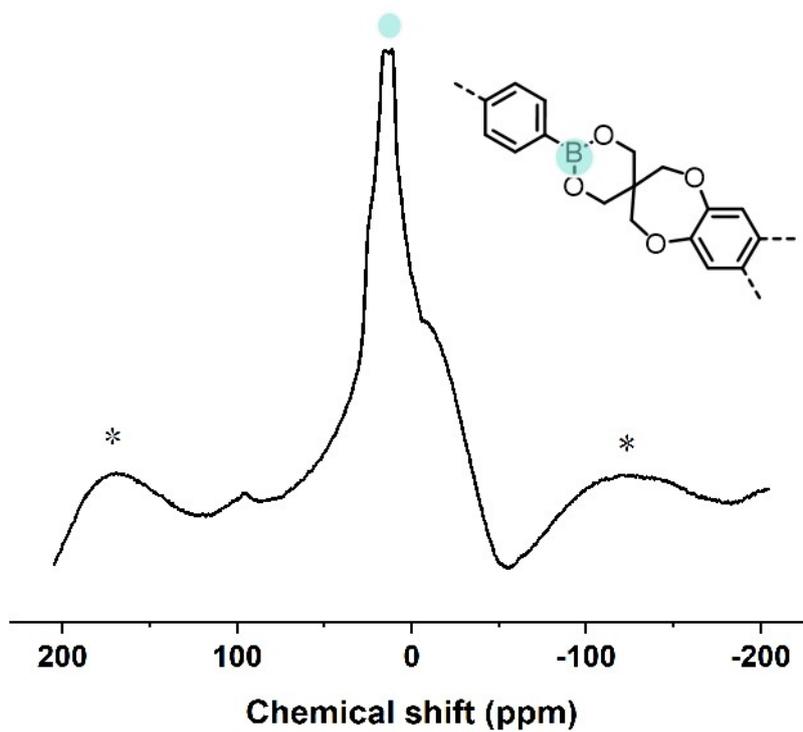


Figure S4. Solid-state ^{11}B NMR (128 MHz) spectrum of BSCOF-1

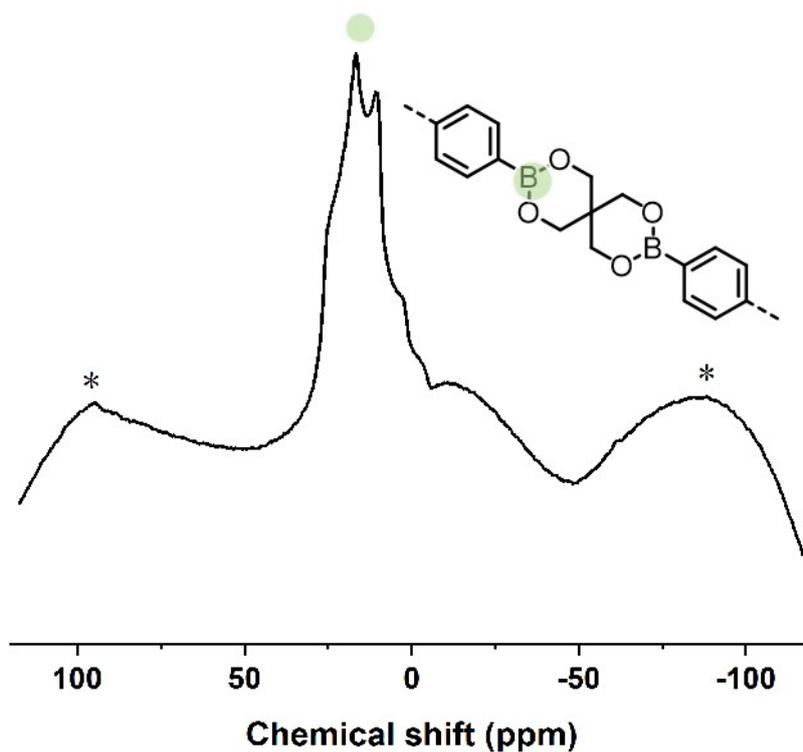


Figure S5. Solid-state ^{11}B NMR (128 MHz) spectrum of BSCOF-2

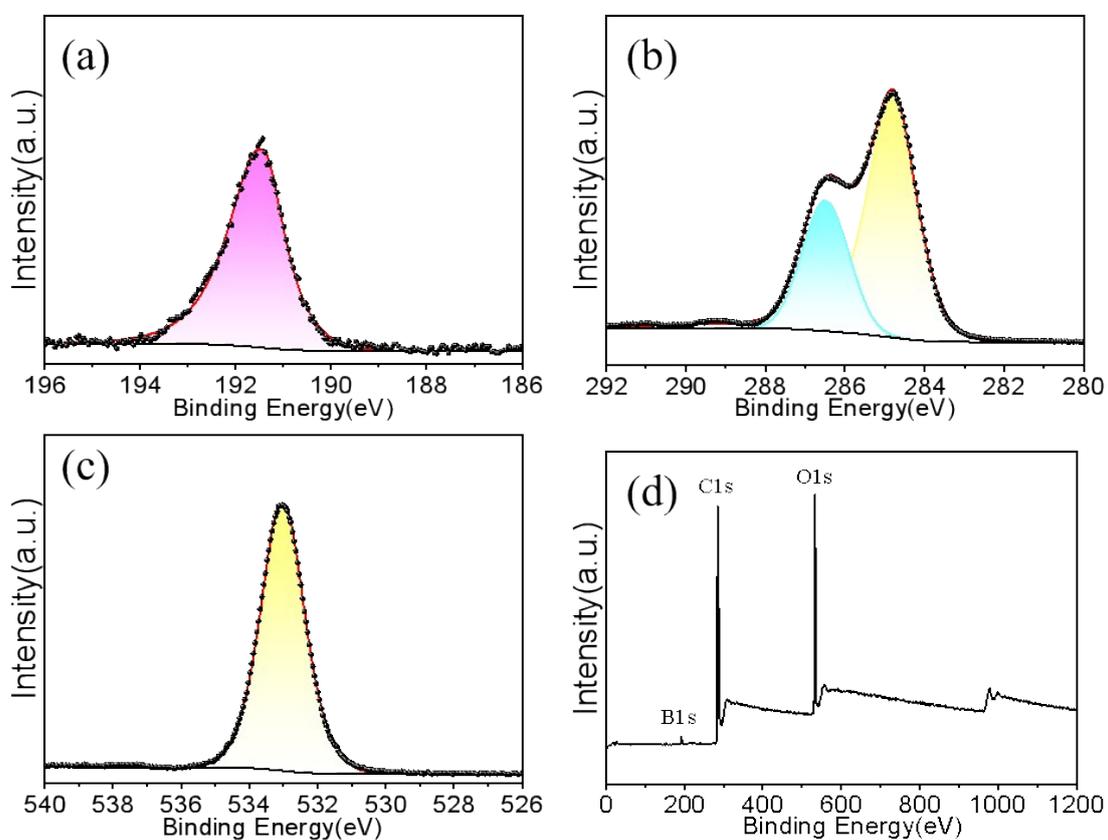


Figure S6. X-ray photoelectron spectroscopy (XPS) characterizations of BSCOF-1. (a) B 1s, (b) C 1s, (c) O 1s, and (d) survey XPS spectra of BSCOD-1

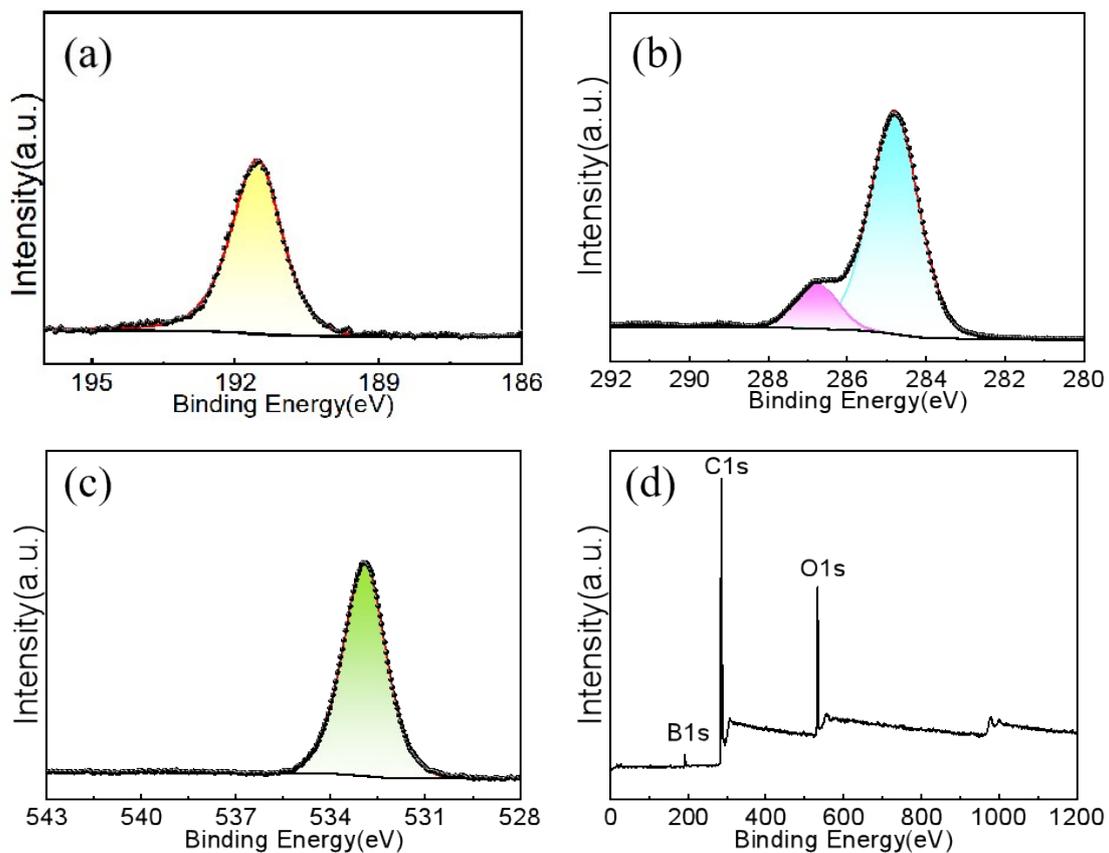


Figure S7. X-ray photoelectron spectroscopy (XPS) characterizations of BSCOF-2; (a) B 1s, (b) C 1s, (c) O 1s, and (d) survey XPS spectra of BSCOD-2

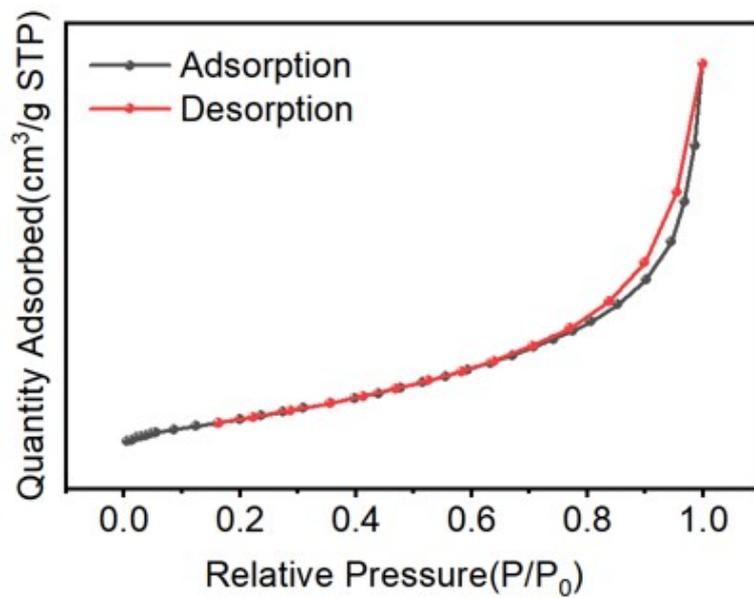


Figure S8. Nitrogen adsorption and desorption isotherms of BSCOF-1

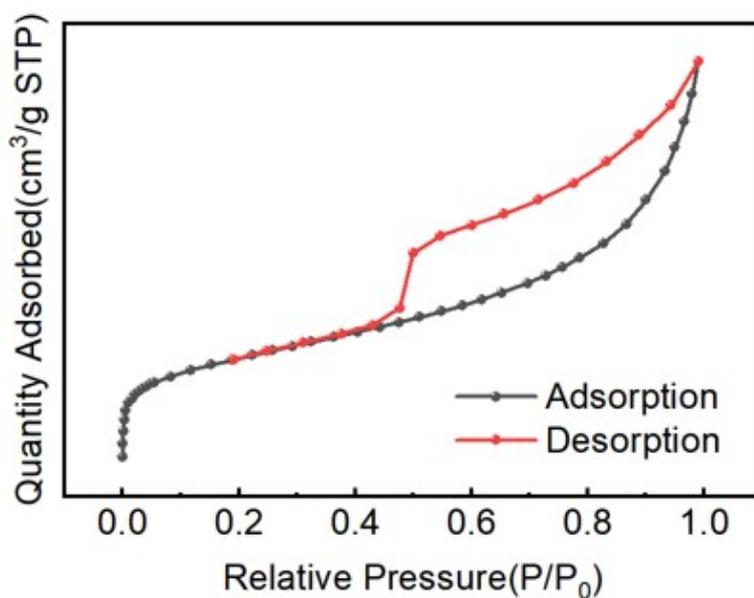


Figure S9. Nitrogen adsorption and desorption isotherms of BSCOF-2

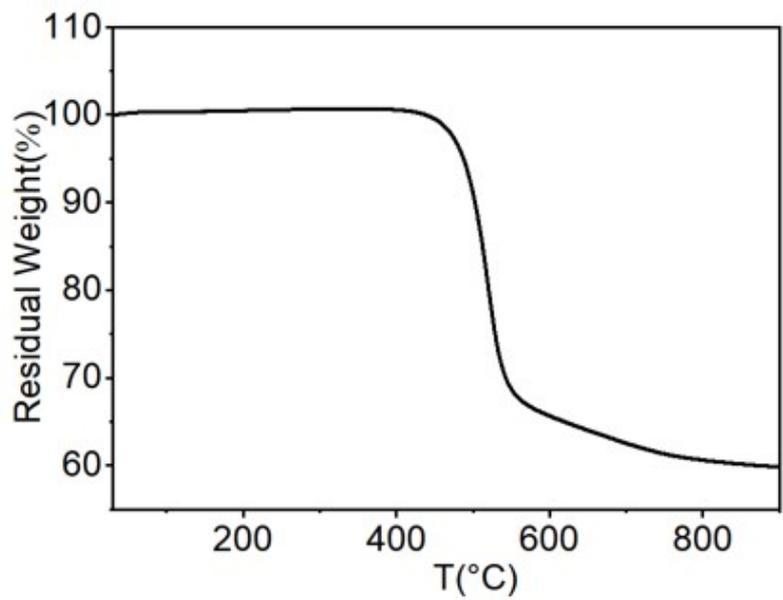


Figure S10. TGA profile of BSCOF-1

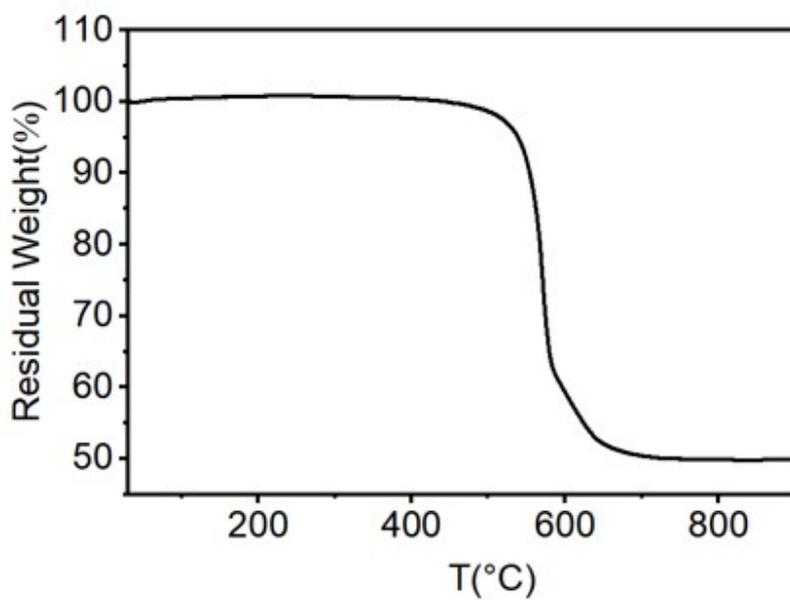


Figure S11. TGA profile of BSCOF-2

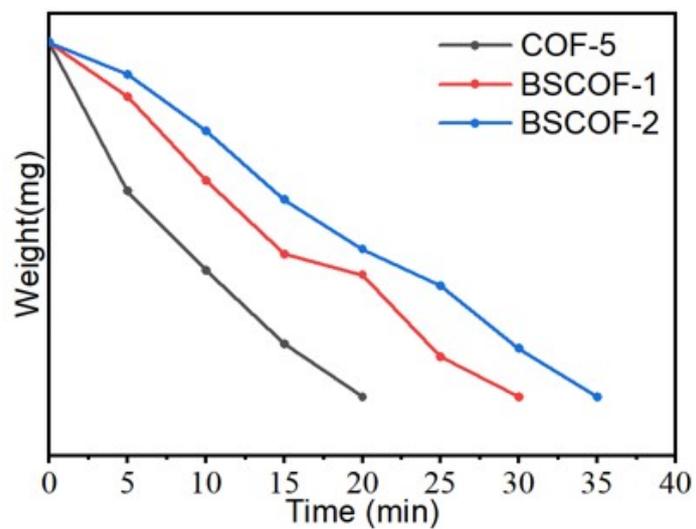


Figure S12. Mass loss of BSCOF-1, BSCOF-2 and COF-5 in water

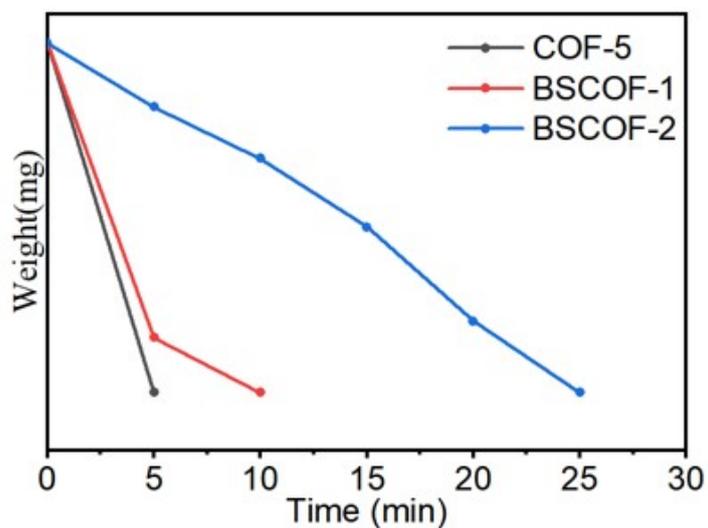


Figure S13. Mass loss of BSCOF-1, BSCOF-2 and COF-5 in HCl (1M)

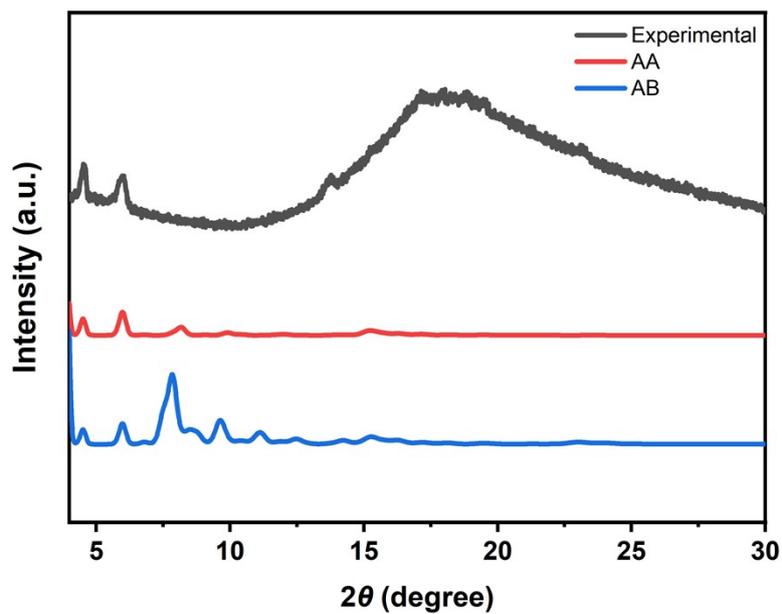


Figure S14. Experimental and simulated PXRD patterns of BSCOF-1

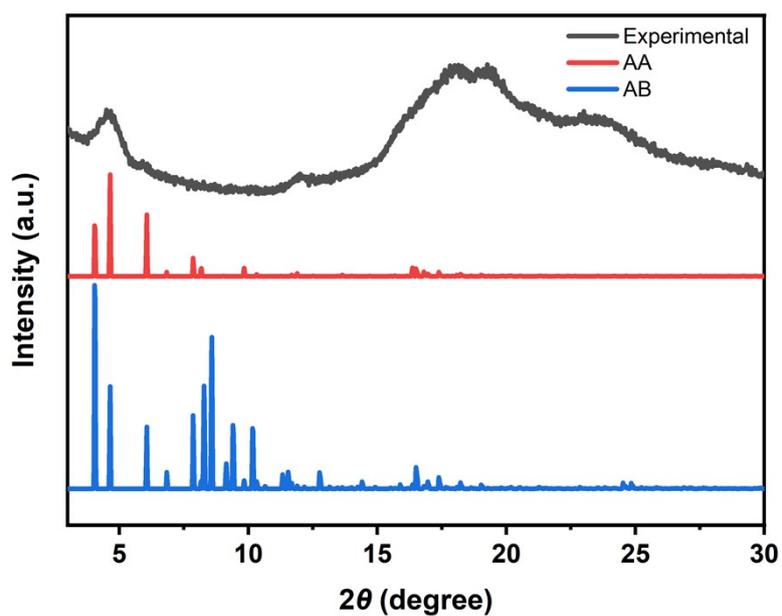


Figure S15. Experimental and simulated PXRD patterns of BSCOF-2

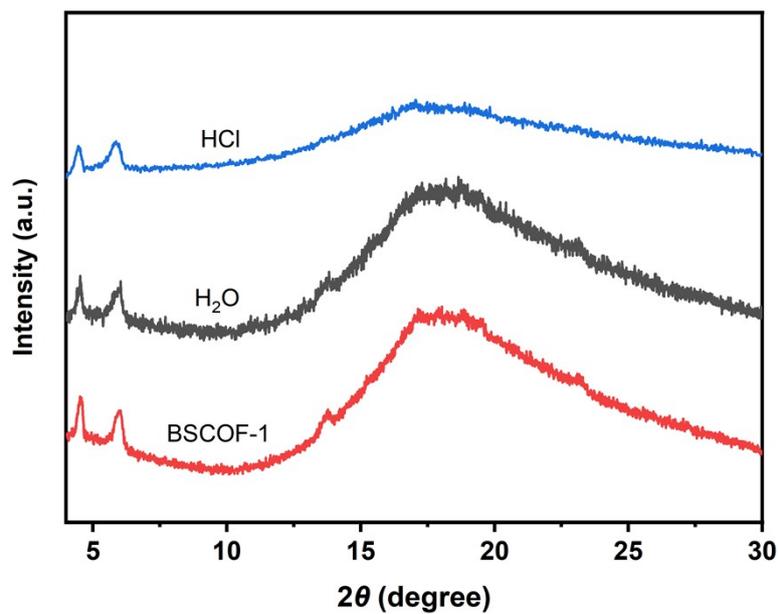


Figure S16. Stability of BSCOF-1 in HCl (1 M) and water.

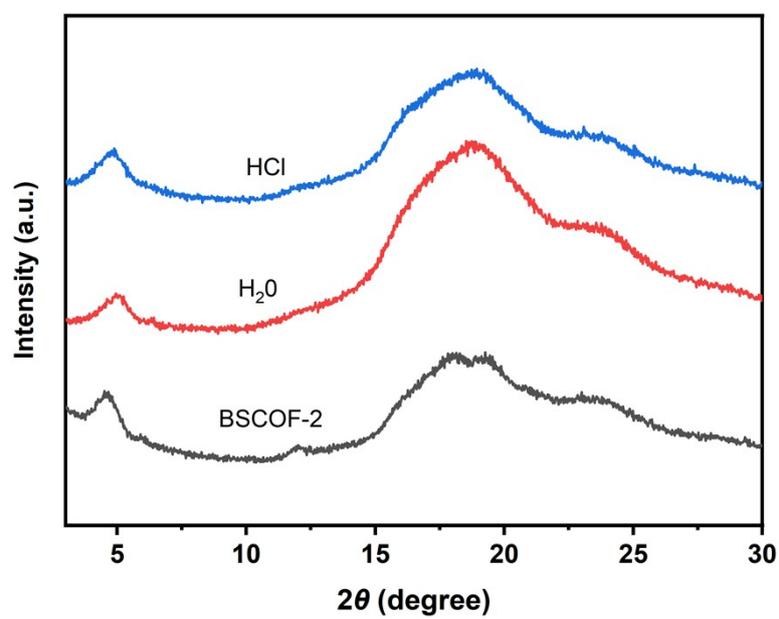


Figure S17. Stability of BSCOF-2 in HCl (1 M) and water.

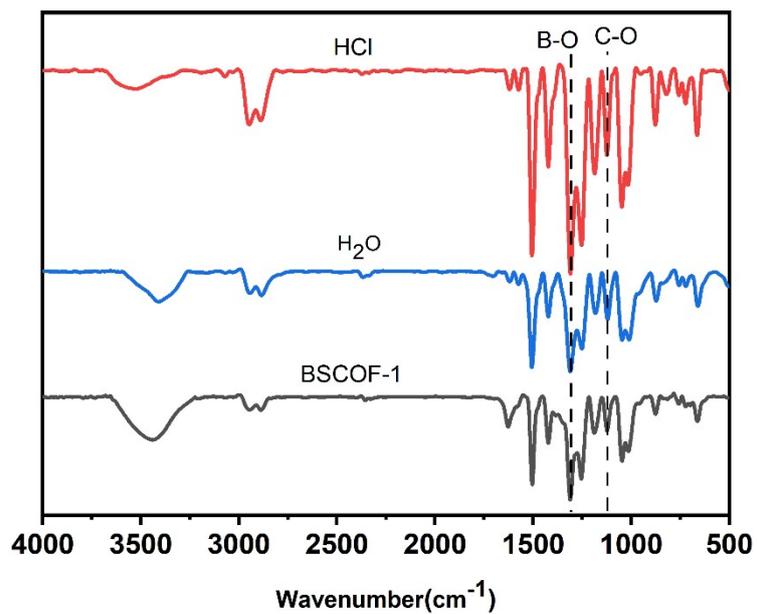


Figure S18. Stability of BSCOF-1 in HCl (1 M) and water.

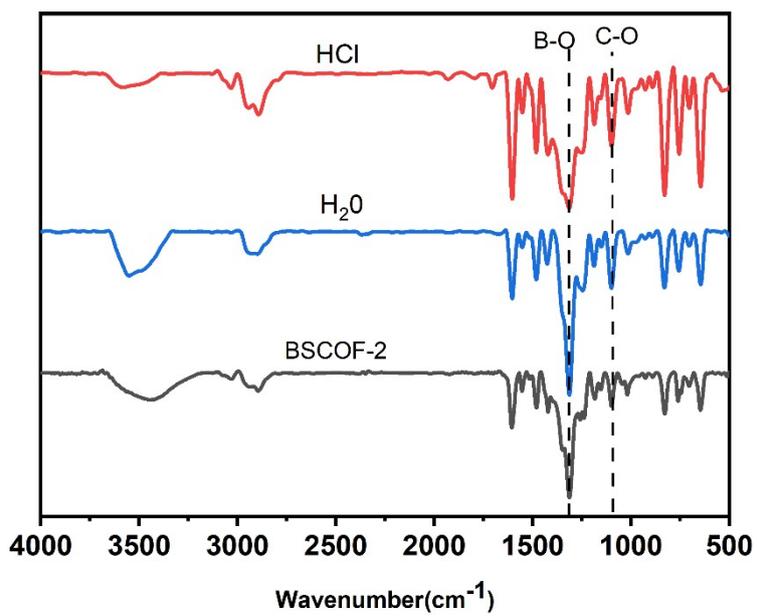


Figure S19. Stability of BSCOF-2 in HCl (1 M) and water.

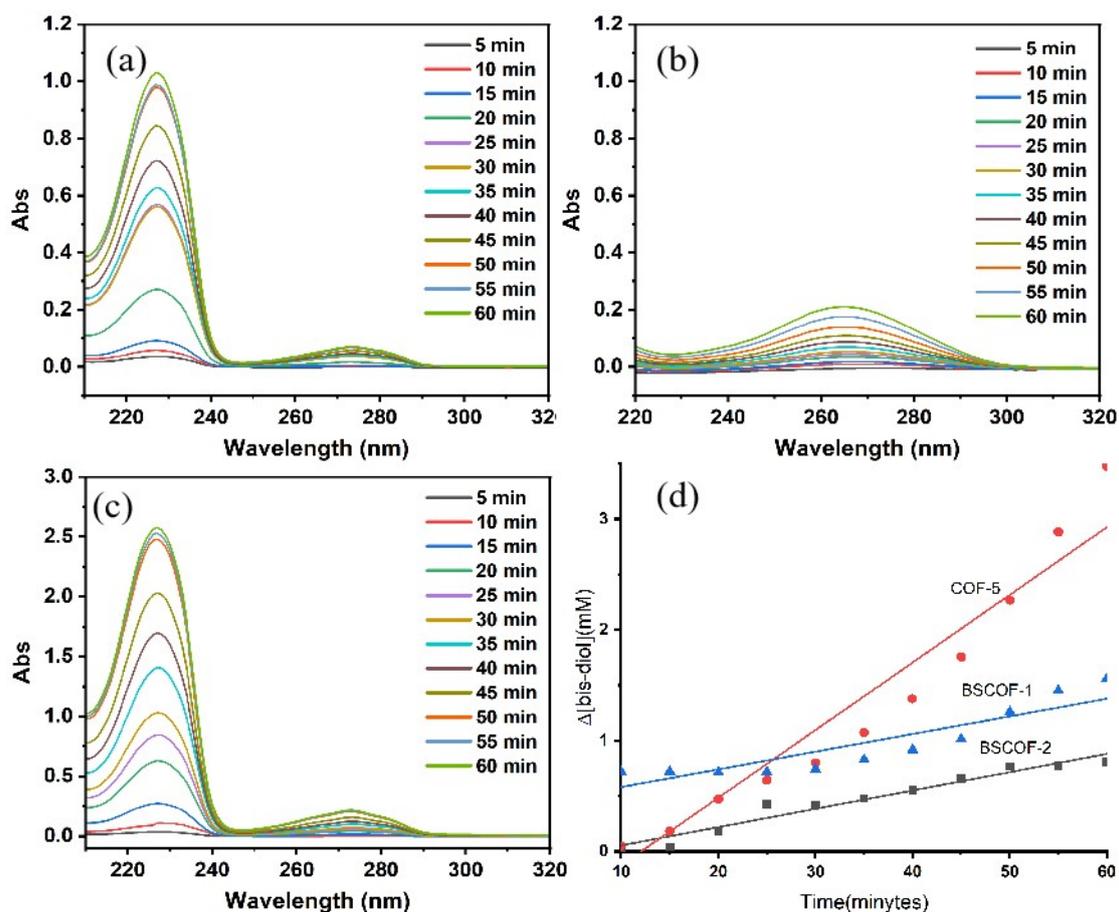


Figure S20. Absorbance spectra showing an increase in the intensity of the peak indicative of the release of bis-diol (230 nm and 270 nm) from the COFs during one hour hydrolysis in water for a) BSCOF-1, b) BSCOF-2, and c) COF-5. d) Comparison of the rate of increase in bis-diol concentration correlating to hydrolysis of BSCOF-1 (blue triangles), BSCOF-2 (gray squares), and COF-5 (red circles) in water.

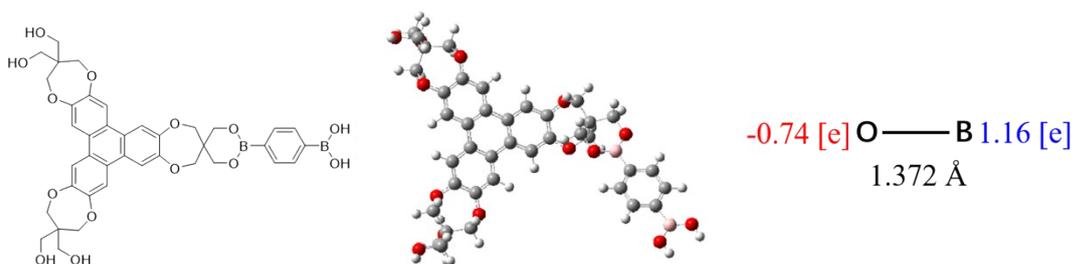


Figure S21. Binding mode between HHTP-PT-1 and water molecules. Bond lengths and NPA charges (blue for positive and red for negative) are included for comparison

5. DFT calculations

Density functional theory (DFT) calculations were performed using the Gaussian 09 software package³. The geometries, were calculated at the B3LYP/6-311G(d,p) level of theory.

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Table S1. Cartesian coordinates of the DFT-optimized monomer and H₂O based on B3LYP/6-311G(d,p).

Symbol	X	Y	Z
C	1.01072958	0.42359495	0.28533718
C	1.32738467	-0.94617282	0.40055155
C	-0.33674758	0.80930625	0.36401797
C	-1.35400547	-0.09882034	0.56814436
C	-1.03412919	-1.46323328	0.71973023
C	0.28380519	-1.85837952	0.62590113
B	-6.85036332	-0.91739036	0.38509199
C	-8.2543502	-0.45459838	-0.12621202
C	-8.93453818	0.6009036	0.49666387
C	-10.19260698	0.99675912	0.06010883
C	-10.81924233	0.34995977	-1.01339438
C	-10.14115904	-0.70770763	-1.63375512
C	-8.88223303	-1.10355868	-1.19796097
B	-12.23444374	0.80064274	-1.51096917
O	-12.79032603	0.1255359	-2.56603383

O	-12.84082526	1.84616767	-0.8650659
O	-1.97303465	-2.43772365	0.93562381
O	-2.63007234	0.39045419	0.63070751
C	-3.04406086	-2.08532763	1.79883421
C	-3.63930438	-0.41915636	0.03941884
C	-4.2062566	-1.43069248	1.04506541
C	-5.11141365	-0.73346149	2.0634487
C	-5.04446144	-2.48368235	0.31680447
O	-6.19079966	-1.90585932	-0.28772338
O	-6.33036418	-0.2923175	1.48904706
C	3.41369018	0.97851731	-0.05540934
C	2.07470881	1.40660333	0.06212243
C	4.40816174	1.94542219	-0.28221557
C	4.11209008	3.28575964	-0.39436719
C	2.78085091	3.718268	-0.26224565
C	1.79516475	2.78050245	-0.03488274
O	2.41443819	5.02056141	-0.43203018
O	5.13078748	4.16066204	-0.68190791
C	2.97382827	5.97814369	0.44981899
C	5.36908333	5.16213167	0.30889414
C	4.43637346	6.37304243	0.1865949
C	4.81724671	7.36370626	1.29698467

C	4.61695806	7.07132107	-1.17980883
O	4.18965169	6.33010705	-2.29244564
O	6.16858458	7.74228618	1.13697898
C	2.7214508	-1.38741994	0.30057297
C	3.74373276	-0.44386915	0.06974457
C	3.07338812	-2.7427315	0.42153355
C	4.38028151	-3.17334156	0.33509675
C	5.40063309	-2.2327046	0.09966682
C	5.06885892	-0.90089117	-0.03250951
O	6.72082211	-2.58028013	0.06899263
O	4.64519895	-4.49739823	0.55033546
C	7.1149258	-3.50445815	-0.94164004
C	5.27877777	-5.19452385	-0.51741216
C	6.79293717	-4.96373738	-0.59312477
C	7.36504794	-5.86912836	-1.68925578
C	7.42887227	-5.33396035	0.7495876
O	8.83637628	-5.22227481	0.63773601
O	6.73963737	-5.54561178	-2.91848023
H	-0.64034171	1.84130336	0.24401461
H	0.47195717	-2.91697034	0.75105848
H	-8.46273412	1.11569852	1.32914517
H	-10.70136476	1.82074955	0.55203741

H	-10.61018323	-1.21985513	-2.46890368
H	-8.36959194	-1.92403827	-1.6924841
H	-13.653908	0.43462788	-2.84508394
H	-13.70297956	2.0954061	-1.20238661
H	-3.37337236	-3.01587749	2.2707512
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H	-4.603502	0.14332847	2.47711999
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H	5.45031071	1.6746673	-0.39417559
H	0.7862585	3.16307868	0.05254005
H	2.33855103	6.86193505	0.33885995
H	2.87548182	5.61353882	1.48458703
H	6.40191661	5.48230736	0.16306387
H	5.28248955	4.70864652	1.30653308
H	4.14769314	8.23663145	1.2398168
H	4.6548637	6.88836619	2.27839621
H	4.02608176	7.99602418	-1.17793876
H	5.67314154	7.36588505	-1.26822545

H	4.55125168	5.44151939	-2.19908787
H	6.38642056	8.38548303	1.81512253
H	2.33002228	-3.50807324	0.60469645
H	5.89245312	-0.21954225	-0.20384951
H	8.19721938	-3.38877655	-1.02444892
H	6.6523625	-3.23659947	-1.89777774
H	5.08004897	-6.25336571	-0.32250232
H	4.81222702	-4.92854823	-1.47206522
H	7.17988501	-6.92035791	-1.41407634
H	8.45182301	-5.72538149	-1.73694726
H	7.02796092	-4.66249149	1.51572278
H	7.13867681	-6.36379574	1.01478124
H	9.19892053	-5.0875521	1.51508216
H	7.17389166	-6.03889578	-3.61752009
O	-7.78830989	-2.76917267	2.3330451
H	-8.37050551	-2.90645374	1.57952919
H	-7.93328868	-1.8458501	2.56315674

Table S2. Cartesian coordinates of the DFT-optimized TS based on B3LYP/6-311G(d,p).

Symbol	X	Y	Z
C	-0.7311697	0.24298582	-0.49722794

C	-1.21001114	-1.08202994	-0.56398789
C	0.64502508	0.46817266	-0.66006252
C	1.53695386	-0.55400549	-0.90979354
C	1.04880716	-1.87101874	-1.030678
C	-0.29644015	-2.11014381	-0.84616702
B	6.96909572	-2.15127427	-0.79690618
C	7.84307089	-1.14844021	0.07011408
C	8.72162303	-0.23410168	-0.5274355
C	9.50174883	0.62351505	0.23847989
C	9.43329758	0.60192334	1.63776187
C	8.55145545	-0.30706098	2.23604624
C	7.77201297	-1.16454133	1.46749964
B	10.30712856	1.56801049	2.50292446
O	10.18725784	1.50164003	3.86741548
O	11.15096291	2.43345843	1.85355978
O	1.84817733	-2.94940464	-1.30568437
O	2.85585396	-0.22127153	-1.04826772
C	2.90162473	-2.72083271	-2.22830885
C	3.79509586	-1.14587102	-0.50708015
C	4.17329031	-2.2202725	-1.53783851
C	5.09544601	-1.63807464	-2.61028411
C	4.90176361	-3.36652747	-0.82952368

O	5.99267326	-2.86444624	-0.09976433
O	6.43573406	-1.47296362	-2.14386351
C	-3.03565127	1.08005478	-0.0611896
C	-1.66287286	1.34660135	-0.24699926
C	-3.90380941	2.16210628	0.16494401
C	-3.45160155	3.46181493	0.21910228
C	-2.08490386	3.73206969	0.03106963
C	-1.22300736	2.68067783	-0.20211767
O	-1.56562383	4.98762628	0.14770567
O	-4.35199964	4.45864882	0.50551758
C	-2.03813526	5.97516522	-0.75121546
C	-4.50601031	5.44991346	-0.51198699
C	-3.43559313	6.54681408	-0.4604316
C	-3.73516716	7.53896654	-1.59425351
C	-3.48887488	7.30677727	0.88371015
O	-3.12700073	6.55499246	2.01230182
O	-5.03292167	8.06787185	-1.41698076
C	-2.63403557	-1.35939746	-0.35791516
C	-3.52980584	-0.29884169	-0.1102494
C	-3.13797999	-2.67106075	-0.38472023
C	-4.47519068	-2.94833559	-0.19667504
C	-5.37100509	-1.89007371	0.04526361

C	-4.8878829	-0.59933227	0.09117542
O	-6.71682618	-2.08758257	0.16784726
O	-4.89483962	-4.24450488	-0.3131024
C	-7.14750074	-2.90493313	1.25313458
C	-5.52554887	-4.80413066	0.83452933
C	-6.99960924	-4.40808615	0.98200536
C	-7.59201698	-5.18113679	2.16522117
C	-7.75412149	-4.78552665	-0.29571667
O	-9.13308877	-4.51934878	-0.11212357
O	-6.86109789	-4.85493395	3.3338191
H	1.07309525	1.45873602	-0.57499744
H	-0.61478924	-3.13955055	-0.94986505
H	8.77950168	-0.17539708	-1.61300021
H	10.17131738	1.32702829	-0.24832054
H	8.47852821	-0.33727077	3.31953138
H	7.09103007	-1.8596716	1.95001819
H	10.73768579	2.11325965	4.35929463
H	11.66411889	3.00970453	2.42250643
H	3.09031577	-3.68278527	-2.71606562
H	2.5758421	-2.01009803	-2.99872969
H	3.38891976	-1.6101132	0.39818263
H	4.66908348	-0.55779345	-0.22131822

H	5.11394098	-2.30227097	-3.48495231
H	4.72558091	-0.65953544	-2.93312463
H	4.22316465	-3.86165514	-0.12793462
H	5.22523688	-4.11656415	-1.56964667
H	-4.96549504	2.01633	0.31795935
H	-0.18055813	2.93953502	-0.33632543
H	-1.30140633	6.78178793	-0.68996232
H	-2.01667684	5.56912884	-1.77500351
H	-5.48904098	5.89354762	-0.34642902
H	-4.50742806	4.95956984	-1.49587465
H	-2.97386685	8.33502799	-1.58041306
H	-3.65034917	7.0193275	-2.56290346
H	-2.78683978	8.14872971	0.83359385
H	-4.49719297	7.73499898	0.98527085
H	-3.58957537	5.71129755	1.95385824
H	-5.19841174	8.70746923	-2.11301413
H	-2.49471004	-3.52316763	-0.56363554
H	-5.61938739	0.17609704	0.27985295
H	-8.20635896	-2.6712866	1.37998829
H	-6.60829383	-2.63232552	2.16686867
H	-5.44950483	-5.88805957	0.70010203
H	-4.97285749	-4.53148416	1.74011002

H	-7.53391449	-6.26023941	1.94755084
H	-8.65328714	-4.92009696	2.26358978
H	-7.33507232	-4.20581421	-1.12448054
H	-7.58755549	-5.85358574	-0.51133501
H	-9.53185298	-4.38569236	-0.9737135
H	-7.29605206	-5.26211048	4.08589148
O	7.86576191	-3.06385485	-1.75121793
H	8.80223382	-2.87706605	-1.62891677
H	7.26595707	-2.29173388	-2.46078959

Table S3. Cartesian coordinates of the DFT-optimized INT based on B3LYP/6-311G(d,p).

Symbol	X	Y	Z
C	1.08039461	0.6472123	-0.45644742
C	1.03780643	-0.75796944	-0.34250718
C	-0.11294323	1.33284257	-0.73171304
C	-1.32299366	0.68590793	-0.87265165
C	-1.37216618	-0.71532268	-0.72204501
C	-0.20247021	-1.40262463	-0.47205379
B	-7.56263315	1.42927518	-1.48167384
C	-8.5098799	0.8272828	-0.38507304
C	-9.59386478	0.02523392	-0.76575075

C	-10.45425613	-0.51633007	0.18048033
C	-10.27447202	-0.26540661	1.54708121
C	-9.20321206	0.55116184	1.9286757
C	-8.33611682	1.08315812	0.98144046
B	-11.24810011	-0.86864433	2.61344083
O	-11.02174814	-0.5737876	3.93310969
O	-12.27653318	-1.66101305	2.17258785
O	-2.52301837	-1.44741803	-0.82635187
O	-2.42053948	1.46068242	-1.12852885
C	-3.68892599	-0.86195502	-0.25884443
C	-3.39340412	0.90760302	-2.00501268
C	-4.41597432	0.0492533	-1.25468209
C	-5.38171987	0.93528463	-0.45628603
C	-5.18225671	-0.78577291	-2.28149893
O	-6.21587488	1.6573017	-1.3403633
C	3.53402544	0.63653477	-0.02702421
C	2.35279759	1.35675574	-0.29979609
C	4.73408723	1.34984848	0.12930058
C	4.79985229	2.72371919	0.01713172
C	3.6184004	3.44051677	-0.25393912
C	2.43059759	2.75598733	-0.39815312
O	3.59933645	4.80044995	-0.42243521

O	6.03004767	3.31338898	0.09595588
C	4.06897903	5.56176433	0.68296735
C	6.22225522	4.31548986	1.08932228
C	5.5946782	5.66686206	0.73134528
C	5.94171296	6.69079643	1.81673478
C	6.13598525	6.14500323	-0.63052029
O	5.43214448	7.26746803	-1.12827766
O	7.34297934	6.70039904	2.00583433
C	2.26677234	-1.50783695	-0.06760652
C	3.48953993	-0.823804	0.09210913
C	2.26330044	-2.90847359	0.0415778
C	3.40511049	-3.63198726	0.31771827
C	4.62465337	-2.94683545	0.48181103
C	4.6470834	-1.57377225	0.35847135
O	5.79256388	-3.58296248	0.80635086
O	3.27609303	-4.97994038	0.50865338
C	6.22790975	-4.58088	-0.11397423
C	4.05510552	-5.84612058	-0.31039293
C	5.52906853	-5.92619431	0.10318187
C	6.23650406	-6.98288566	-0.74621068
C	5.61964119	-6.33181994	1.58733433
O	6.93062289	-6.23212575	2.10659315

O	6.23065898	-6.56764757	-2.09961914
O	-6.27298649	-1.39548589	-1.62268775
O	-8.11965322	1.79780751	-2.67455452
H	-0.13482354	2.40752053	-0.86010707
H	-0.30009771	-2.47456513	-0.35715405
H	-9.76416074	-0.16797203	-1.82120533
H	-11.2836985	-1.14125018	-0.13797654
H	-9.05112731	0.76791131	2.9820029
H	-7.52019816	1.72183454	1.3116188
H	-11.64063818	-0.96199537	4.55387031
H	-12.85183775	-2.00746617	2.85679176
H	-4.34335312	-1.69021338	0.02235773
H	-3.42082904	-0.30827519	0.64964199
H	-3.90067747	1.7577445	-2.46789712
H	-2.89769077	0.32735307	-2.79336
H	-5.97498085	0.31112037	0.2177397
H	-4.8013099	1.65026599	0.13732166
H	-5.52567317	-0.13001938	-3.09505765
H	-4.49752235	-1.53331882	-2.70852602
H	5.67130963	0.84640045	0.3292766
H	1.55492104	3.35902158	-0.60192288
H	3.63670493	6.55730179	0.55198921

H	3.67905912	5.13670328	1.61818106
H	7.30355405	4.4266864	1.1797214
H	5.83106332	3.96100686	2.0543313
H	5.57400214	7.67049826	1.48063621
H	5.42184272	6.43312246	2.75456767
H	7.17763019	6.44977821	-0.49862951
H	6.11120685	5.31242432	-1.340358
H	4.64501323	6.93177714	-1.56724036
H	7.57314234	7.47157465	2.52785332
H	1.352147	-3.48222767	-0.06997808
H	5.61110799	-1.09988601	0.49222755
H	7.29936921	-4.696113	0.06752682
H	6.08867099	-4.23399162	-1.14276827
H	3.5864145	-6.82873849	-0.19474383
H	3.97381165	-5.5495188	-1.36264926
H	7.25809376	-7.10442883	-0.35914368
H	5.71780621	-7.94754874	-0.62358259
H	4.91418232	-5.72539313	2.16325548
H	5.31649676	-7.38017913	1.69351355
H	7.06601199	-5.3112968	2.34911536
H	6.74820565	-7.19277206	-2.61171929
H	-6.80725146	-1.86488654	-2.2668236

H

-7.44460588

2.13855778

-3.26866812

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