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Chemical Synthesis

Supplementary Materials

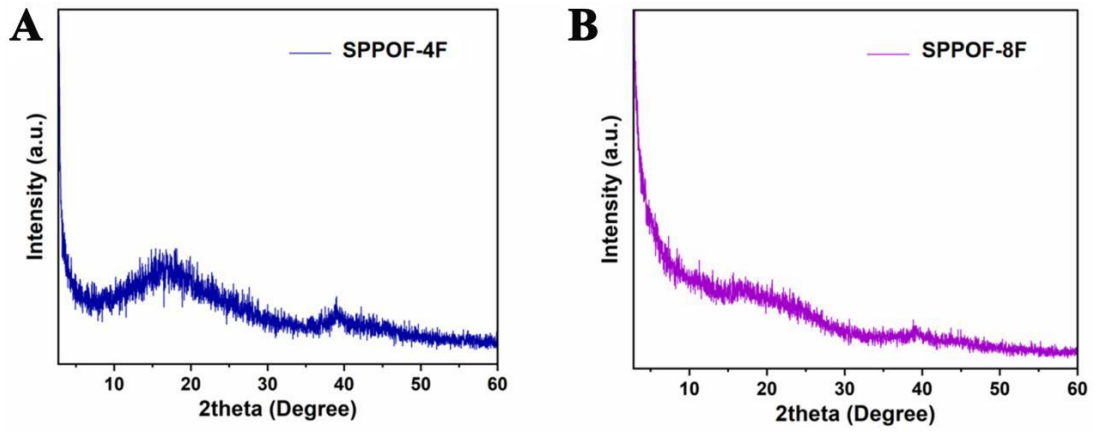
Fluorinated porous organic frameworks for C_2F_6/CF_4 gases separation

Yinhui Li, Yue Wu, Shanshan Wang, Yu Fu, Xiaoyu Li, Jiahui Zeng, Wenxiang Zhang*, Heping Ma*

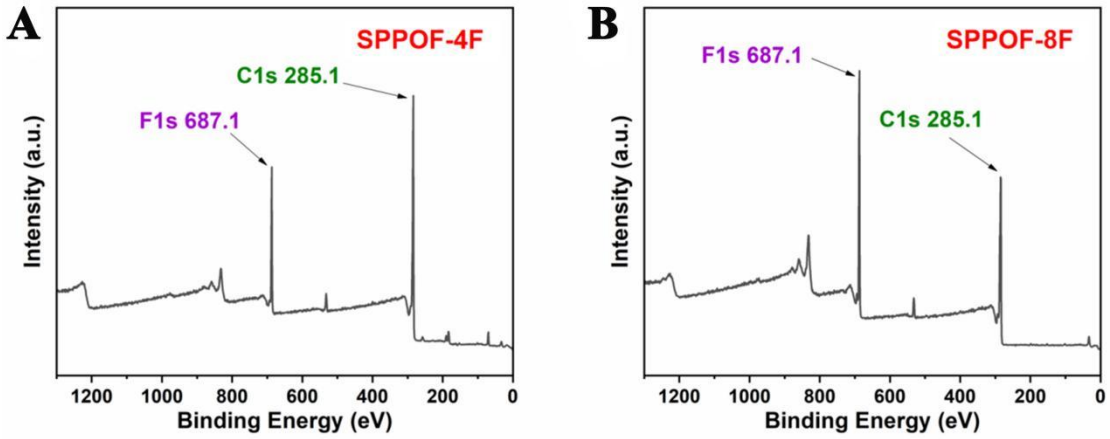
School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China.

***Correspondence to:** Dr. Wenxiang Zhang, Dr. Heping Ma, School of Chemical Engineering and Technology, Xi'an Jiaotong University, No. 28 Xianning West Road, Beilin District, Xi'an 710049, Shaanxi, China. E-mail: zhangwenxiang@xjtu.edu.cn; maheping@mail.xjtu.edu.cn

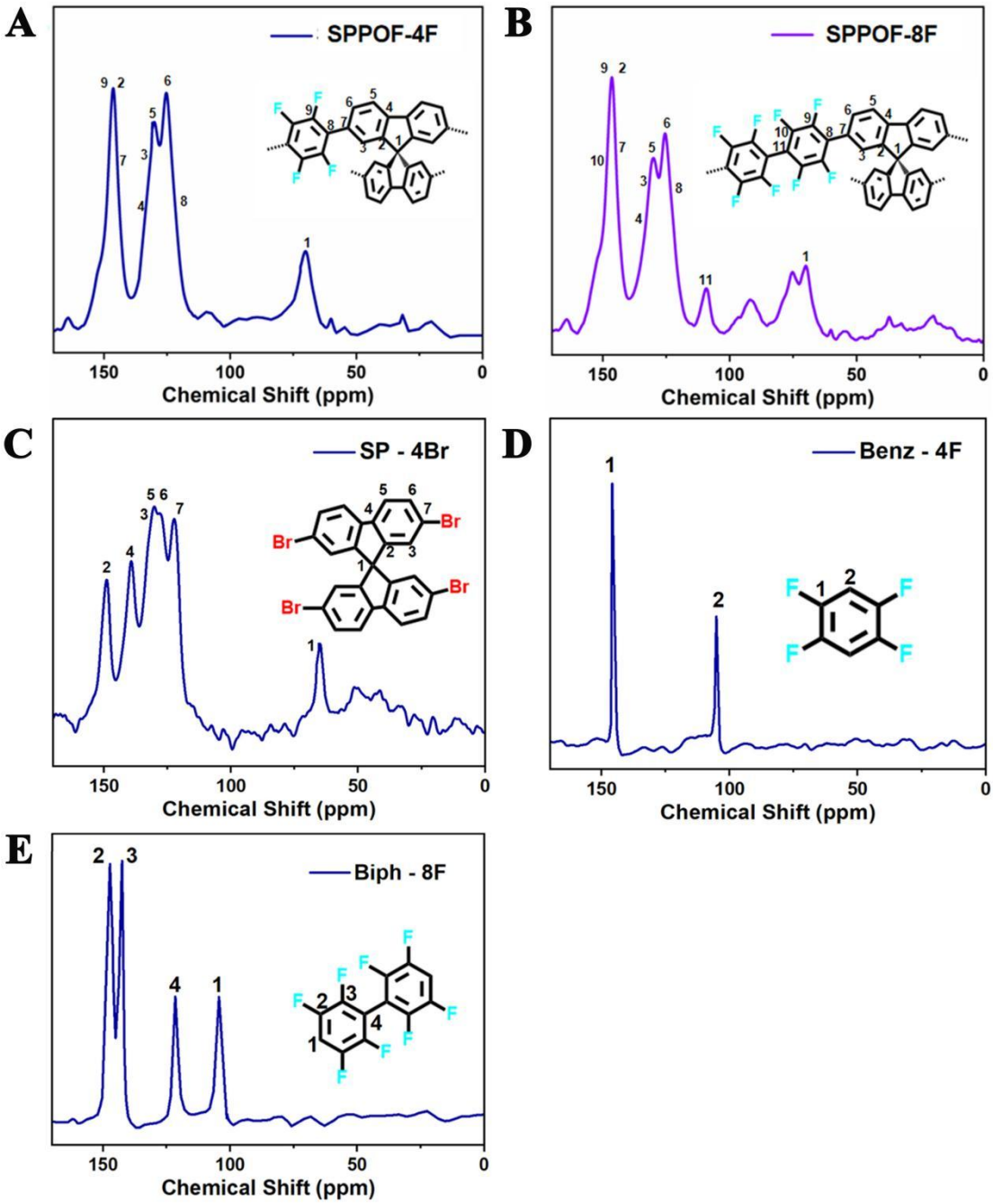
Supplementary Figures



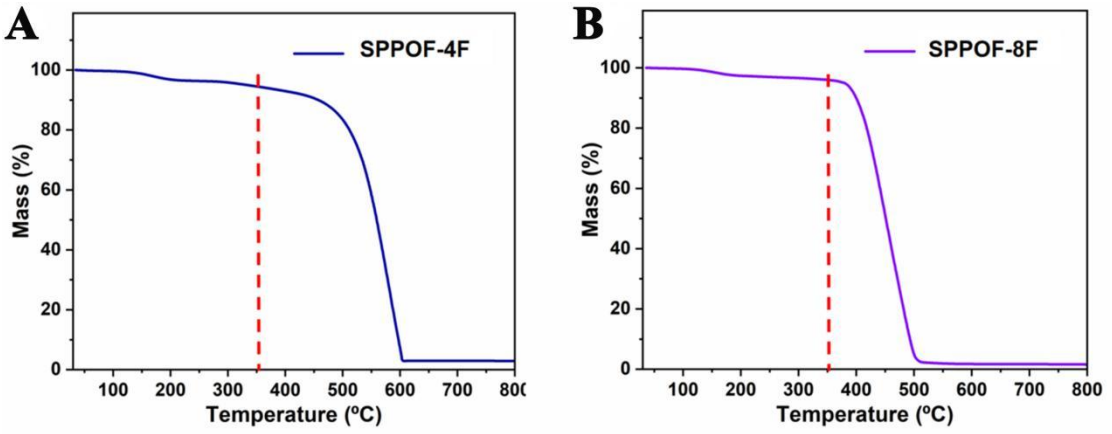
Supplementary Figure 1. Powder X-ray diffraction spectra of (A) SPPOF-4F and (B) SPPOF-8F.



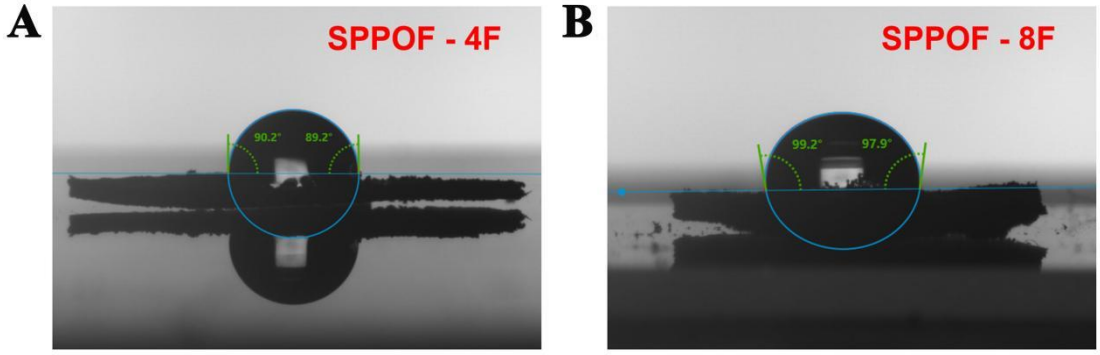
Supplementary Figure 2. XPS spectra of (A) SPPOF-4F and (B) SPPOF-8F.



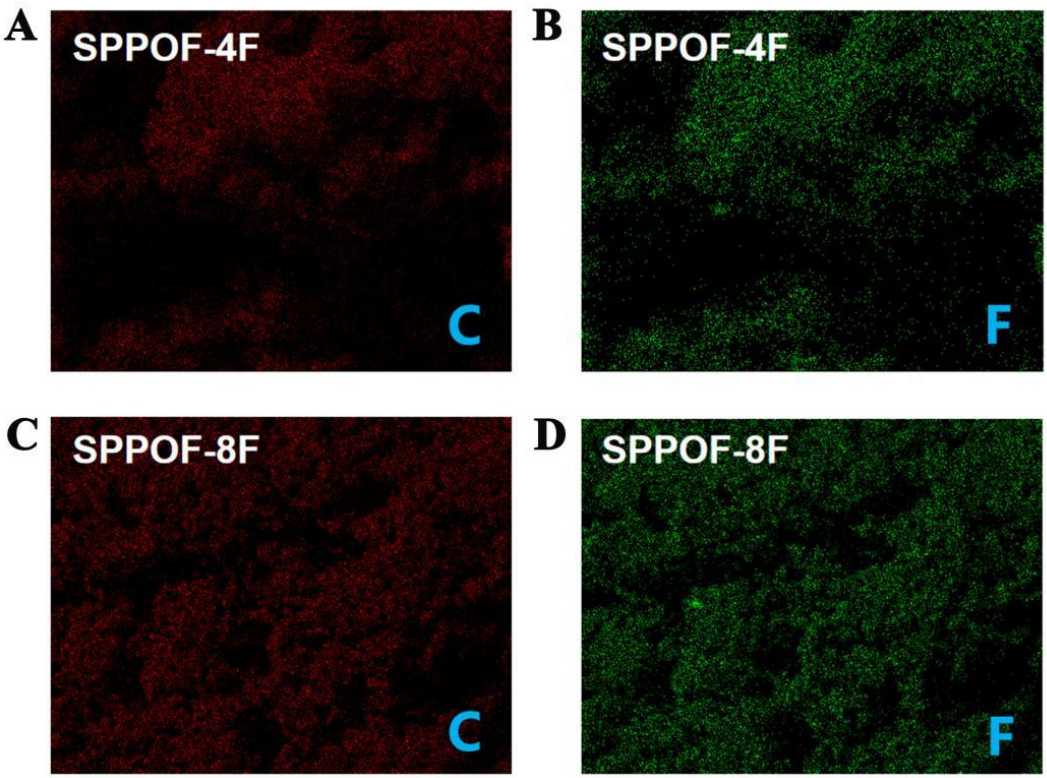
Supplementary Figure 3. Solid-state ^{13}C CP/MAS NMR spectra: (A) SPPOF-4F, (B) SPPOF-8F, (C) SP-4Br, (D) Benz-4F and (E) Biph-8F.



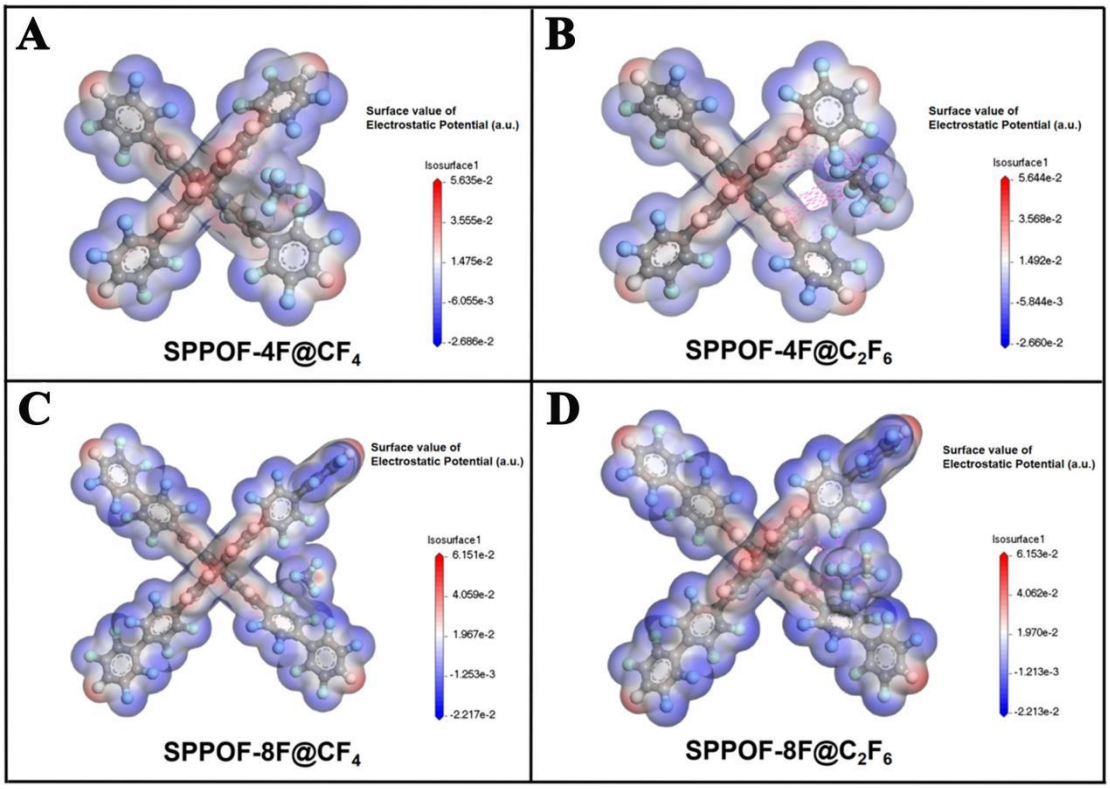
Supplementary Figure 4. TGA curves of (A) SPPOF-4F and (B) SPPOF-8F under air atmosphere.



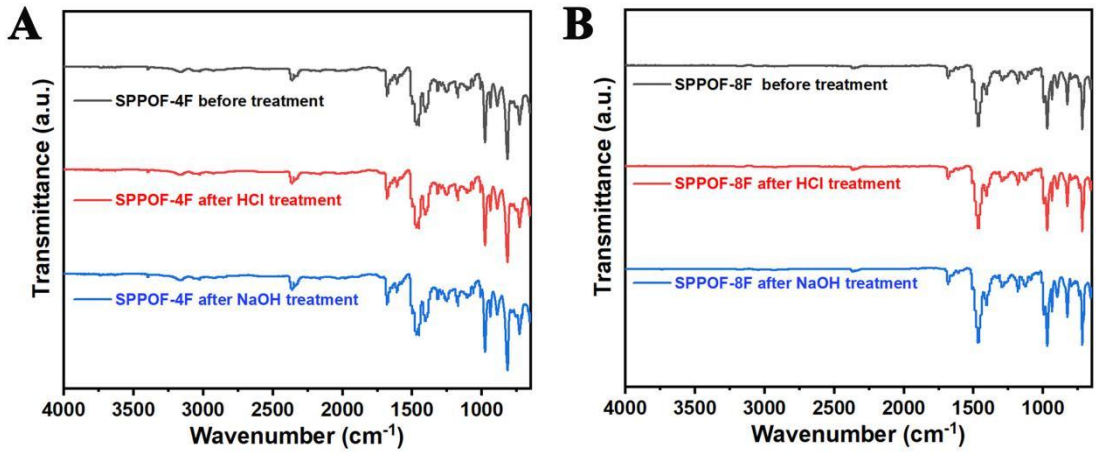
Supplementary Figure 5. Optical images of Contact Angle measurement for deionized water on the surfaces of (A) SPPOF-4F and (B) SPPOF-8F.



Supplementary Figure 6. Elemental distribution mapping images: (A) C for SPPOF-4F; (B) F for SPPOF-4F; (C) C for SPPOF-8F and (D) F for SPPOF-8F.



Supplementary Figure 7. Simulated model and the electrostatic potential maps of (A) SPPOF-4F@CF_4, (B) SPPOF-4F@C_2F_6, (C) SPPOF-8F@CF_4 and (D) SPPOF-8F@C_2F_6.



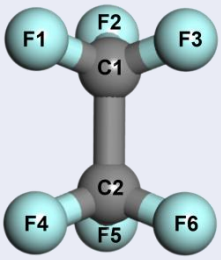
Supplementary Figure 8. Comparison of FT-IR spectra of POFs before and after HCl or NaOH treatment: (A) SPPOF-4F and (B) SPPOF-8F.

Supplementary Tables

Supplementary Table 1. C_2F_6/CF_4 adsorption compared with literature

Adsorbents	Q_{st} for C_2F_6 (kJ/mol)	Q_{st} for CF_4 (kJ/mol)	C_2F_6 uptake (mmol/g)	CF_4 uptake (mmol/g)	Ratio of uptake (C_2F_6/CF_4)	Note
SPPOF-4F (This work)	29.0	20.5	1.74	0.79	2.20	298 K, 1 bar
SPPOF-8F (This work)	28.5	11.4	1.83	0.71	2.58	298 K, 1 bar
CS400[1]	34.52	25.15	0.49	0.63	0.78	300 K, 1 bar
CS1000[1]	40.69	31.45	0.33	0.41	0.80	300 K, 1 bar
CS1000a[1]	31.17	21.86	5.4	5.3	1.02	300 K, 1 bar
Al-Fum[2]	20.3	23.4	3.3	2.1	1.57	298 K, 1 bar
MOF-303[2]	24.7	33.5	2.51	1.53	1.64	298 K, 1 bar
MIL-160[2]	17.1	17.7	1.48	0.94	1.57	298 K, 1 bar
Zeolite 13X (8-12 mesh)[3]	14.0	24.4	1.55	0.75	2.07	303 K, 1 bar
Activated Carbon (20-40 mesh)[3]	20.6	19.4	1.26	0.75	1.68	303 K, 1 bar
Activated Carbon (12-20 mesh)[3]	---	---	1.21	0.68	1.78	303 K, 1 bar
Silica gel (30-60 mesh)[3]	---	---	0.50	0.14	3.57	303 K, 1 bar
H-cage[4]	---	---	0.62	0.39	1.59	273 K, 1 bar
HF-cage[4]	---	---	0.44	0.38	1.16	273 K, 1 bar
F-cage[4]	30.9	29.2	1.78	0.93	1.91	273 K, 1 bar

Supplementary Table 2. Mulliken atomic charges distribution in C_2F_6

Mulliken atomic charges of C_2F_6				
Atomic number	**Atom**	**Mulliken atomic charges (a.u.)**		
		C_2F_6 alone	**C_2F_6 in SPPOF-4F**	**C_2F_6 in SPPOF-8F**
	C1	0.8128	0.8276	0.8292
	C2	0.8129	0.8305	0.8333
	F1	-0.2709	-0.2727	-0.2777
	F2	-0.2708	-0.2795	-0.2785
	F3	-0.2711	-0.2786	-0.2824
	F4	-0.2709	-0.2712	-0.2751
	F5	-0.2708	-0.2773	-0.2798
	F6	-0.2712	-0.2804	-0.2736
Total atomic charge		**0**	**-0.0016**	**-0.0046**

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