Supplementary Information

Computational screening of covalent organic frameworks for the capture of radioactive iodine and methyl iodide

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1. Structural properties of the 187 COFs in the database

Table S1. Structural properties of the 187 experimental COFs examined in this work

Material	PLD (Å)	LCD (Å)	S_{acc} (m^2/g)	V_{free} (cm^3/g)	φ
1. 2D-NiPc-BTDA-COF[1]	12.0	12.3	1250	0.68	0.62
2. 3D-Py-COF[2]	21.6	24.4	7229	6.62	0.93
3. 3D-Py-COF-2P[2]	12.3	13.5	7310	3.05	0.85
4. 4PE-1P[3]	23.9	24.3	2344	1.40	0.73
5. 4PE-2P[3]	32.0	32.3	2458	1.76	0.77
6. 4PE-3P[3]	38.9	39.2	2802	2.28	0.81
7. 4PE-TT[3]	27.2	27.6	2234	1.42	0.75
8. AB-COF[4]	11.1	11.6	1948	0.96	0.65
9. ACOF-1[5]	11.1	11.6	1948	0.96	0.65
10. AEM-COF-1[6]	29.1	29.3	1902	1.59	0.76
11. AEM-COF-2[6]	32.1	32.3	1316	1.22	0.72
12. ATFG-COF[4]	9.9	10.4	1517	0.70	0.62
13. AzO-COF[7]	34.3	34.5	2113	2.01	0.81
14. BDT-COF[8]	29.8	30.0	1797	1.54	0.77
15. BF-COF-1[9]	8.6	13.3	5097	1.96	0.79
16. BF-COF-2[9]	7.6	13.1	4300	1.66	0.78
17. BLP-2H-AA[10]	9.0	9.5	1115	0.56	0.50
18. BLP-2H-AB[10]	2.9	4.0	396	0.57	0.51
19. CC-TAPH-COF[11]	7.2	9.3	4355	1.53	0.75
20. COF-1[12]	3.1	4.2	0	0.56	0.51
21. COF-10[13]	31.3	31.5	1949	1.74	0.78
22. COF-102[14]	8.0	9.0	5129	1.86	0.78
23. COF-103[14]	8.5	9.7	5315	2.05	0.80
24. COF-105[14]	16.1	18.8	6645	5.17	0.91
25. COF-108[14]	19.1	27.5	6387	5.37	0.92

26. COF-11Å[15]	7.7	8.4	515	0.61	0.54
27. COF-14Å[15]	9.8	10.5	1355	0.75	0.59
28. COF-16Å[15]	12.2	12.7	1936	0.86	0.64
29. COF-18Å[15]	14.3	14.7	1705	0.89	0.66
30. COF-202[16]	5.4	9.9	4240	1.39	0.72
31. COF-300[17]	9.3	9.4	3301	1.33	0.73
32. COF-320[18]	8.3	8.5	1814	0.89	0.63
33. COF-366[19]	18.7	20.5	4107	2.24	0.81
34. COF-42-bnn[20]	16.8	17.2	2686	1.30	0.73
35. COF-42-gra[20]	5.1	6.0	2346	1.00	0.66
36. COF-43-bnn[20]	32.3	32.5	2630	2.36	0.82
37. COF-43-gra[20]	13.4	13.6	3769	1.77	0.78
38. COF-5[12]	23.4	23.7	1707	1.24	0.72
39. COF-505[21]	2.0	3.7	0	0.22	0.32
40. COF-6[13]	8.6	9.1	1128	0.53	0.53
41. COF-66[19]	21.9	22.2	1742	1.24	0.73
42. COF-8[13]	16.2	16.5	1601	0.93	0.65
43. COF-AA-H[22]	25.3	25.7	2314	1.45	0.74
44. $COF_{BTA-PDA}$[23]	16.8	17.1	2403	1.36	0.71
45. CTF-NDC[24]	3.3	4.3	0	0.26	0.35
46. COF-JLU2[25]	9.9	10.4	1368	0.67	0.60
47. COF-JLU3[26]	11.3	12.1	4393	1.70	0.75
48. COF-LZU1[27]	15.6	16.0	2172	1.24	0.71
49. COF-LZU8[28]	13.0	13.5	805	0.82	0.62
50. COF-SDU1[29]	43.1	43.3	2409	2.60	0.84
51. COF-TpAzo[30]	25.8	26.1	2081	1.56	0.78
52. CoPc-PorDBA[31]	24.7	25.5	4128	2.76	0.85
53. CPF-1[32]	23.1	24.0	5087	2.96	0.86
54. CPF-2[32]	21.6	22.5	5177	2.82	0.86

55. CS-COF[33]	20.2	20.4	1620	1.01	0.66
56. CTC-COF[34]	18.7	18.8	1513	0.91	0.65
57. CTF-0[35]	1.3	2.6	0	0.15	0.25
58. CTF-1[36]	8.4	8.9	1004	0.50	0.51
59. CTF-2-AA[37]	10.6	11.0	1251	0.61	0.55
60. CTF-2-AB[37]	3.3	4.9	443	0.61	0.55
61. CTF_FUM[24]	6.0	6.7	1045	0.50	0.52
62. CuP-Ph COF[38]	19.0	20.1	4025	2.32	0.83
63. CuP-SQ-COF[39]	11.3	12.9	3240	1.46	0.76
64. CuP-TFPh COF[40]	17.9	19.0	4439	2.07	0.83
65. DA-COF[41]	19.1	19.4	1646	1.08	0.71
66. DAAQ-TFP-COF[42]	22.0	22.2	1761	1.18	0.73
67. DBA-COF 1[43]	29.2	29.4	1965	1.59	0.76
68. DBA-COF 2[43]	34.2	34.4	2127	2.00	0.80
69. BDT-OEt-COF[8]	23.2	23.5	1851	1.18	0.72
70. 2,3-DhaTab[44]	29.1	29.3	2098	1.81	0.78
71. 2,5-DhaTab[44]	29.5	29.6	2212	1.87	0.78
72. DhaTab[45]	32.1	32.3	2130	1.99	0.79
73. 2,3-DhaTph[46]	18.2	19.2	4381	2.34	0.82
74. 2,5-DhaTph[44]	17.4	18.5	4382	2.34	0.82
75. 2,3-DhaTta[47]	29.2	29.2	2093	1.82	0.79
76. 2,3-DmaTph[46]	16.4	17.6	4206	2.14	0.81
77. D_{TP}-A_{NDI}-COF[48]	43.8	43.9	1842	2.19	0.82
78. EB-COF:Br[49]	10.0	10.6	1336	0.62	0.58
79. H_2P-COF[50]	19.2	20.3	4417	2.54	0.83
80. HAT-COF[51]	9.1	9.9	1734	0.84	0.63
81. TTF-Py-COF [52]	14.3	14.5	2054	1.10	0.69
82. HBC-COF[53]	10.6	10.8	1520	0.74	0.59
83. HCC-H_2P-COF[54]	14.4	15.7	4134	2.07	0.80

84. HO-H_2P-COF[55]	17.5	18.5	4399	2.36	0.83
85. HO_2C-H_2P-COF[55]	9.4	10.9	4927	1.90	0.79
86. HP-COF-1[56]	14.4	14.8	2003	1.06	0.67
87. HP-COF-2[56]	16.8	17.2	2429	1.35	0.72
88. HPB-COF[53]	5.8	7.6	2479	0.96	0.65
89. ICOF-1[57]	15.0	15.2	2146	1.20	0.70
90. ICOF-2[57]	16.6	17.2	2383	1.32	0.72
91. ILCOF-1-AA[58]	20.8	21.2	3865	2.57	0.83
92. ILCOF-1-AB[58]	9.4	11.1	6714	2.42	0.82
93. iPrTAPB-TFP[59]	6.5	7.5	712	0.49	0.48
94. iPrTAPB-TFPB[59]	15.4	15.9	1738	1.07	0.66
95. MPCOF[60]	9.8	10.3	1394	0.66	0.61
96. NPN-1[61]	4.1	5.3	958	0.49	0.51
97. NPN-2[61]	4.2	5.3	1125	0.56	0.54
98. NPN-3[61]	5.4	6.1	941	0.47	0.50
99. NN-TAPH-COF[11]	7.2	9.3	4435	1.53	0.75
100. NTU-COF-1[62]	18.4	18.7	1916	1.20	0.70
101. NTU-COF-2[62]	24.6	24.8	2117	1.70	0.77
102. NUS-2[63]	9.9	10.4	1368	0.67	0.60
103. NUS-3[63]	16.7	17.0	2036	0.99	0.68
104. EB-COF:Cl[49]	10.0	10.6	1490	0.69	0.59
105. OH-TAPH-COF[11]	17.5	18.5	4369	2.44	0.83
106. TpPa-Py[64]	16.0	16.3	1649	0.95	0.66
107. PC-COF[65]	41.1	41.1	3056	3.01	0.85
108. Pc-PBBA-COF[66]	16.5	16.8	1391	0.81	0.64
109. PCTF-1[67]	13.4	13.7	1872	1.07	0.68
110. PCTF-2[67]	21.4	21.5	2279	1.57	0.75
111. PCTF-3[67]	27.7	27.8	2364	1.95	0.79
112. PCTF-4[67]	17.5	17.9	1942	1.24	0.72

113. Ph-An-COF[68]	22.1	22.3	1701	1.16	0.71
114. Ph-AnCD-COF[68]	21.0	23.7	5283	2.76	0.85
115. PI-2-COF[69]	23.4	23.7	2286	1.57	0.75
116. PI-3-COF[69]	30.4	30.6	2280	2.03	0.80
117. PI-COF-4[69]	13.4	17.5	5113	3.19	0.88
118. PI-COF-4-2P[70]	7.6	8.2	5020	1.36	0.75
119. PI-COF-5[70]	22.4	26.6	6479	7.30	0.94
120. PI-COF-5-2P[70]	10.5	13.4	6543	3.42	0.88
121. Por-COF[71]	18.6	20.4	4010	2.24	0.81
122. POR-COF[72]	12.6	14.1	3548	1.54	0.77
123. PPy-COF[73]	13.3	13.7	1332	0.65	0.57
124. Py-2,2'-BPyPh-COF[74]	23.2	23.5	2251	1.64	0.77
125. Py-2,3-BPyPh-COF[74]	22.7	22.9	2243	1.62	0.76
126. Py-2,3-DHPh-COF[74]	21.0	21.5	4568	2.70	0.85
127. EB-COF:F[49]	10.0	10.6	1594	0.73	0.60
128. Py-An-COF[75]	19.2	19.5	2344	1.47	0.74
129. Py-Azine-COF[76]	12.5	13.0	2031	1.11	0.69
130. EB-COF:I[49]	9.6	10.3	1530	0.60	0.53
131. Py-COF[77]	21.6	24.4	7229	6.62	0.93
132. NUS-9 [78]	12.0	13.0	2392	1.23	0.74
133. Py-DHPh-COF[74]	19.9	20.2	4796	2.70	0.85
134. NUS-10 [78]	12.0	13.0	1959	0.95	0.70
135. Star-COF-1[79]	30.4	30.6	1371	1.22	0.71
136. Star-COF-2[79]	37.3	37.4	1496	1.51	0.75
137. Star-COF-3[79]	40.0	40.2	1602	1.72	0.77
138. T-COF 1[80]	7.6	8.2	1045	0.48	0.51

139.	T-COF 2[80]	14.6	14.9	1507	0.82	0.63
140.	T-COF 3[80]	12.4	12.7	1272	0.63	0.58
141.	TAPB-PDA COF[81]	32.1	32.3	2410	2.21	0.80
142.	TAPB-TFP[59]	11.6	12.0	1496	0.80	0.62
143.	TAPB-TFPB[59]	19.0	19.3	1973	1.32	0.71
144.	TBPB-COF[82]	16.4	16.7	1677	0.98	0.64
145.	TD-COF-5[83]	27.9	28.4	4465	3.42	0.87
146.	DAB-TFP-COF[42]	22.0	22.3	1739	1.20	0.73
147.	TfpBDH[84]	36.2	36.3	2102	2.08	0.81
148.	TFPT-COF[85]	34.2	34.4	2131	2.02	0.80
149.	TH-COF-1[86]	11.7	12.1	1561	0.65	0.60
150.	Tp-Azo[87]	25.5	25.7	1829	1.36	0.75
151.	TP-COF[88]	28.5	28.7	1758	1.42	0.75
152.	Tp-Por-COF-AA[89]	41.1	41.2	1907	2.10	0.81
153.	Tp-Por-COF-AB[89]	19.9	20.1	2880	1.73	0.78
154.	Tp-Stb[87]	22.3	22.5	1987	1.33	0.73
155.	TpBD-$2NO_2$[90]	21.5	21.7	1638	1.13	0.71
156.	TPBD-ME_2[90]	21.6	21.6	1523	1.03	0.68
157.	TpBD-N_{H2}[91]	22.1	22.2	1705	1.20	0.72
158.	TpBD-$NHCOCH_3$[91]	17.7	18.1	1335	0.85	0.64
159.	TpBD-NO_2[90]	21.2	21.4	1517	0.98	0.69
160.	TpBD-$(OMe)_2$[90]	19.9	20.3	2149	1.34	0.73
161.	TpBD[92]	22.6	22.9	1717	1.20	0.71
162.	TpBDH[93]	21.9	22.2	1504	1.04	0.71
163.	TpPa-1-F_2[90]	15.3	15.6	1359	0.77	0.64
164.	TpPa-1[94]	15.8	16.1	1643	0.93	0.66
165.	TpPa-2[94]	13.4	13.8	1586	0.78	0.61
166.	TpPa-F_4[90]	14.6	14.9	1084	0.59	0.60

167.	TpPA-NO_2[90]	11.1	11.4	1281	0.61	0.58
168.	TpPa-SO_3H-Py[95]	16.0	16.3	1523	0.83	0.64
169.	TpPa-SO_3H[90]	12.2	12.5	1289	0.63	0.59
170.	TPT-COF-1[96]	21.6	21.9	2122	1.38	0.74
171.	TPT-COF-2[96]	33.8	33.9	2468	2.18	0.81
172.	TpTG-Br[97]	2.6	3.2	0	0.20	0.35
173.	TpTG-Cl[97]	2.8	3.4	0	0.23	0.36
174.	TpTG-I[97]	2.4	3.0	0	0.17	0.34
175.	TRIPTA[98]	11.9	12.4	1503	0.79	0.62
176.	TT-COF[99]	26.1	26.3	1610	1.30	0.74
177.	TTF-COF[100]	18.1	18.6	3391	1.92	0.79
178.	TThPP[101]	16.7	17.8	3780	2.08	0.81
179.	ZnP-COF[50]	17.9	19.0	4000	2.27	0.82
180.	ZnPc-COF[102]	16.6	17.0	1409	0.85	0.66
181.	ZnPc-DPB[102]	26.6	26.8	1798	1.39	0.76
182.	ZnPc-NDI[102]	27.0	27.2	1428	1.20	0.73
183.	ZnPc-PPE[102]	32.1	32.2	2060	1.84	0.79
184.	ZnPc-Py[102]	18.3	18.5	1312	0.85	0.66
185.	N3-COF[103]	18.2	18.5	1885	1.23	0.71
186.	TTI-COF[104]	18.2	18.5	1959	1.26	0.71
187.	NUS-14[105]	40.7	40.8	2537	2.71	0.84

PLD and LCD represent the pore limiting diameter and largest cavity diameter, respectively. Accessible surface area (S_{acc}) of each material was calculated by a probe molecule with a size equal to the kinetic diameter of N_2 (3.68 Å), while a probe size of 0.0 Å was applied to calculate the free volume (V_{free}) which is the absolute amount of volume not occupied by the framework atoms. The void fraction (φ) was determined from the ratio of free volume to the total volume of the cell.

2. Force field parameters and models

Table S2. Potential parameters iodine[106] and methyl iodide[107] used in this work

Atomic type	σ **(Å)**	ε/k_B **(K)**	q **(e)**
Iodine			
I_2-united	4.98	550.0	0.0
Methyl iodide			
CH_3I_H	2.20	10.01	0.052
CH_3I_C	3.40	51.22	-0.020
CH_3I_I	4.12	324.06	-0.137

Table S3. Potential parameters for the framework atoms of COFs[108]

Atomic type	σ **(Å)**	ε/k_B **(K)**
H	2.57	22.14
B	3.64	90.58
C	3.43	52.84
N	3.26	34.72
O	3.12	30.20
F	3.00	25.16
Si	3.83	202.31
P	3.70	153.50
S	3.60	137.89
Cl	3.52	114.24
Br	3.73	126.32
I	4.01	170.60
Zn	2.46	62.40
Cu	3.11	2.52
Ni	2.52	7.55

Table S4. Comparison of the I_2 uptakes calculated using UFF and DREIDING force fields

Material	**I_2 uptake** (g/g)	
	UFF	**DREIDING**[109]
COF-108	13.59	13.81
COF-105	12.67	13.04
Ph-AnCD-COF	6.85	7.12
H_2P-COF	5.43	5.73
COF-103	4.98	5.27
COF-10	3.99	4.10
POR-COF	3.32	3.46
COF-202	2.83	2.92
COF-LZU1	2.10	2.20
COF-6	1.11	1.12

To justify the use of UFF force field for the COFs, we arbitrarily selected 10 different COFs and performed GCMC simulations to examine their I_2 uptakes at 423 K and 1 bar using the DREIDING force field[109], which is another popular force field that have been widely adopted in the studies of MOFs and COFs. As can been seen from the results shown in Table S4, the I_2 uptakes of these COFs are respectively very similar to those obtained using the UFF force field. Considering that the UFF one has been validated for I_2 adsorption in MOFs, it was also adopted in current study and the potential parameters are given in Table S3.

3. I_2 adsorption properties of the top 10 existing COFs and the designed material

Table S5. Structural features and the uptakes of the top 10 COFs identified for I_2 adsorption

Material	Dimension	Topology/ pore shape	I_2 uptake (g/g)	LCD (Å)	S_{acc} (m^2/g)	φ
3D-Py-COF	3D	**pts**	16.7	24.4	7229	0.93
COF-108	3D	**bor**	13.8	27.5	6386	0.92
COF-105	3D	**ctn**	13.0	18.8	6644	0.91
PI-COF-5-2P	3D	**dia**	8.7	13.4	6542	0.88
TD-COF-5	2D	**hexagonal**	8.7	28.4	4464	0.87
3D-Py-COF-2P	3D	**pts**	8.1	13.5	7309	0.85
PI-COF-4	3D	**dia**	7.8	17.5	5113	0.88
Ph-AnCD-COF	2D	**hexagonal**	7.1	23.7	5283	0.85
CPF-1	2D	**square**	6.9	24.0	5086	0.86
CoPc-PorDBA	2D	**square**	6.5	25.5	4128	0.85

Table S6. Fractional atomic coordinates for the designed 3D-Py-COF-TANM in this work

3D-Py-COF-TANM							
Cubic, P42/MMC a=b=28.198 c=39.256							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
H1	0.2132	0.5000	0.1035	**C20**	0.5000	0.3551	0.2936
H2	0.0468	0.5000	0.1492	**C21**	0.5000	0.3617	0.2574
H3	0.1132	0.5000	0.1890	**C22**	0.5000	0.3942	0.3156
C4	0.0463	0.5000	0.0757	**C23**	0.5000	0.4091	0.2451
H5	0.1483	0.5000	0.0634	**C24**	0.5000	0.4400	0.3021
C6	0.9566	0.5000	0.0386	**C25**	0.5000	0.4502	0.2667
C7	0.9167	0.5000	0.0176	**C26**	0.5000	0.2756	0.2496
C8	0.9127	0.5000	0.0997	**H27**	0.5000	0.3885	0.3444
C9	0.8246	0.5000	0.1138	**H28**	0.5000	0.4720	0.3198
C10	0.8317	0.5000	0.1491	**H29**	0.5000	0.4161	0.2165
C11	0.7904	0.5000	0.1690	**C30**	0.5000	0.6782	0.2349
N12	0.7776	0.5000	0.2025	**H31**	0.5000	0.3041	0.3365
C13	0.1368	0.5000	0.0912	**H32**	0.5000	0.2438	0.2317
C14	0.1212	0.5000	0.1605	**H33**	0.5000	0.6725	0.2061
H15	0.8797	0.5000	0.0293	**C34**	0.0000	0.5000	0.0190
C16	0.0833	0.5000	0.1367	**C35**	0.0000	0.5000	0.0901
H17	0.7541	0.5000	0.1562	**H36**	0.0000	0.5000	0.1190
C18	0.5000	0.2683	0.2857	**C37**	0.5000	0.5000	0.2500
C19	0.5000	0.3090	0.3077				

4. Properties of 12 MOFs with pts topology for I_2 adsorption

Table S7. Structural features and I_2 uptakes (423 K and 1 bar) of 12 MOFs with **pts** topology

Material[a]	LCD (Å)	S_{acc} (m^2/g)	φ	I_2 uptake (g/g)
FEBXIV	15.9	5216	0.88	7.1
FEBXOB	13.0	5353	0.84	5.8
FEBXER	12.5	5124	0.85	5.8
EFAYEQ	10.5	4647	0.78	3.8
EFAYIU	10.4	4679	0.78	3.8
SUKYON	10.8	4826	0.76	3.1
ENITAX	10.1	4033	0.78	3.0
PUWDAM	9.4	3743	0.75	2.9
SUKYIH	9.6	3743	0.75	2.8
DAKVOC	10.8	2349	0.72	2.4
DAKVUI	10.8	2213	0.71	2.3
IVETOT	9.2	2298	0.65	2.1

[a] Names of MOFs were denoted using the refcodes in the Cambridge Structural Database (CSD).

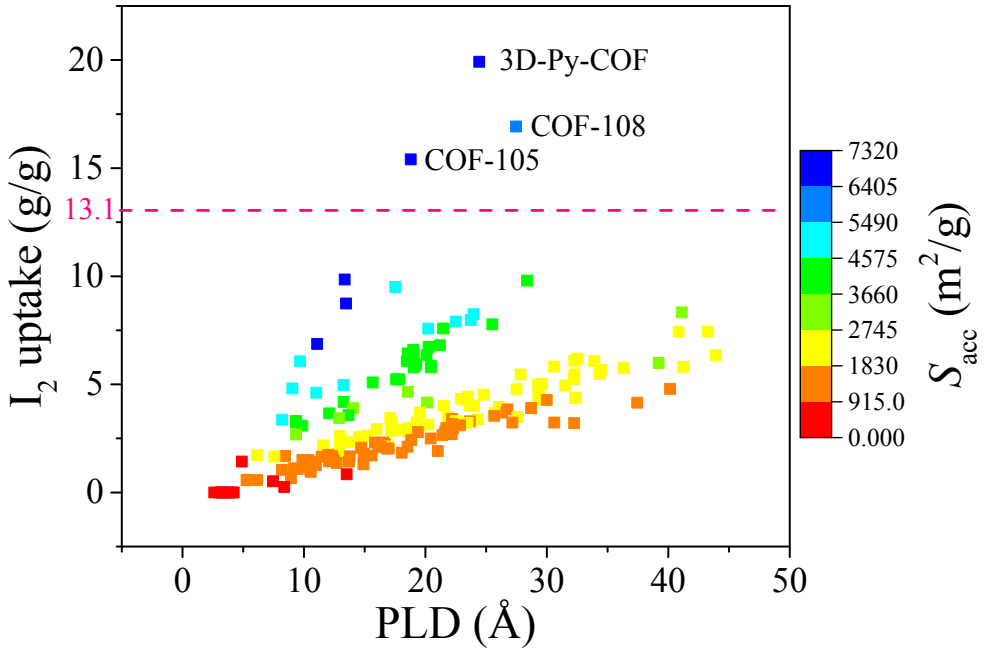

Fig. S1. Performance of the 187 COFs for I_2 adsorption at 298 K and 1 bar. The horizontal dashed line represents the I_2 uptake of the best MOF (NU-110) reported so far.

5. Properties of top 10 existing COFs and other adsorbents for CH_3I adsorption

Table S8. Structural features and the CH_3I uptakes of the top 10 COFs

Material	Dimension	Topology	CH_3I uptake (g/g)	LCD (Å)	S_{acc} (m^2/g)	φ
COF-103	3D	**ctn**	2.8	9.7	5315	0.80
COF-102	3D	**ctn**	2.6	9.0	5129	0.78
BF-COF-1	3D	**ctn**	2.1	8.2	5175	0.78
BF-COF-2	3D	**ctn**	1.8	8.0	4485	0.76
COF-202	3D	**ctn**	1.7	9.9	4240	0.72
PI-COF-4-2P	3D	**dia**	1.6	8.2	5020	0.75
COF-300	3D	**dia**	1.4	9.4	3301	0.73
POR-COF	2D	**square**	1.2	14.1	3548	0.77
RT-COF-1	2D	**hexagonal**	1.1	12.3	1724	0.61
TTF-Py-COF	2D	**square**	1.1	14.5	2054	0.69

Table S9. Comparison of the CH_3I adsorption performance between the top 3 COFs and other adsorbents.

Material	CH_3I uptake (g/g)	Temperature (K)	Ref.
Zeolite (NaX)	0.10	373	110
Zeocarbon	0.10	>323	111
Activated carbon (AC)	0.32	>323	111
Silver-Exchanged Zeolite (AgX)	0.25	373	111
Silver-impregnated alumina (Ag-A)	0.22	>373	111
TEDA-Impregnated AC	0.47	303	112
COF-103	2.78	423	This work
COF-102	2.58	423	This work
BF-COF-1	2.05	423	This work

References

1 X. Ding, L. Chen, Y. Honsho, X. Feng, O. Saengsawang, J. Guo, A. Saeki, S. Seki, S. Irle, S. Nagase, V. Parasuk and D. Jiang, *J. Am. Chem. Soc.*, 2011, 133, 14510.

2 G. Lin, H. Ding, D.Yuan, B. Wang and C. Wang, *J. Am. Chem. Soc.*, 2016, 138, 302.

3 L. Ascherl, T. Sick, J. T. Margraf, S. H. Lapidus, M. Calik, C. Hettstedt, K. Karaghiosoff, M. Döblinger, T. Clark, K. W. Chapman, F. Auras and T. Bein, *Nat. Chem.*, 2016, 8, 310.

4 L. Stegbauer, M. W. Hahn, A. Jentys, G. Savasci, C. Ochsenfeld, J. A. Lercher and B. V. Lotsch, *Chem. Mater.*, 2015, 27, 7874.

5 Z. Li, X. Feng, Y. Zou, Y. Zhang, H. Xia, X. Liu and Y. Mu, *Chem. Commun.*, 2014, **50**, 13825.

6 H. Yang, Y. Du, S. Wan, G. D. Trahan, Y. Jin and W. Zhang, *Chem. Sci.*, 2015, **6**, 4049.

7 J. Zhang, L. Wang, N. Li, J. Liu, W. Zhang, Z. Zhang, N. Zhou and X. Zhu, *CrystEngComm*, 2014, **16**, 6547.

8 M. S. Lohse, J. M. Rotter, J. T. Margraf, V. Werner, M. Becker, S. Herbert, P. Knochel, T. Clark, T. Bein and D. D. Medina, *CrystEngComm*, 2016, **18**, 4295-4302.

9 Q. Fang, S. Gu, J. Zheng, Z. Zhuang, S. Qiu and Y. Yan, *Angew. Chem. Int. Ed.*, 2014, **53**, 2878.

10 K. T. Jackson, T. E. Reich and H. M. El-Kaderi, *Chem. Commun.*, 2012, **48**, 8823.

11 S. Zhao, B. Dong, R. Ge, C. Wang, X. Song, W. Ma, Y. Wang, C. Hao, X. Guo and Y. Gao, *RSC Adv.* 2016, **6**, 38774.

12 A. P. Cote, A. I. Benin, N. W. Ockwig, M. O'Keeffe, A. J. Matzger and O. M. Yaghi, *Science* 2005, **310**, 1166.

13 A. P. Côté, H. M. El-Kaderi, H. Furukawa, J. R. Hunt and O. M. Yaghi, *J. Am. Chem. Soc.*, 2007, **129**, 12914.

14 H. M. El-Kaderi, J. R. Hunt, J. L. Mendoza-Cortes, A. P. Cote, R. E. Taylor, M. O'Keeffe and O. M. Yaghi, *Science*, 2007, **316**, 268-272.

15 R. W. Tilford, S. J. Mugavero, P. J. Pellechia and J. J. Lavigne, *Adv. Mater.*, 2008, **20**, 2741-2746.

16 J. R. Hunt, C. J. Doonan, J. D. LeVangie, A. P. Côté and O. M. Yaghi, *J. Am. Chem. Soc.*, 2008, **130**, 11872.

17 F. J. Uribe-Romo, J. R. Hunt, H. Furukawa, C. O. Klöck, M. Keeffe and O. M. Yaghi, *J. Am. Chem. Soc.*, 2009, **131**, 4570.

18 Y. Zhang, J. Su, H. Furukawa, Y. Yun, F. Gándara, A. Duong, X. Zou and O. M. Yaghi, *J. Am. Chem. Soc.* 2013, **135**, 16336.

19 S. Wan, F. Gándara, A. Asano, H. Furukawa, A. Saeki, S. K. Dey, L. Liao, M. W. Ambrogio, Y. Y. Botros, X. Duan, S. Seki, J. F. Stoddart and O. M. Yaghi, *Chem. Mater.*, 2011, 23, 4094.

20 F. J. Uribe-Romo, C. J. Doonan, H. Furukawa, K. Oisaki and O. M. Yaghi, *J. Am. Chem. Soc.*, 2011, **133**, 11478.

21 D. Guo, R. Shibuya, C. Akiba, S. Saji, T. Kondo and J. Nakamura, *Science*, 2016, **351**, 361.

22 T. Zhou, S. Xu, Q. Wen, Z. Pang and X. Zhao, *J. Am. Chem. Soc.*, 2014, **136**, 15885.

23 L. Xu, X. Zhou, W. Q. Tian, T. Gao, Y. F. Zhang, S. Lei and Z. F. Liu, *Angew. Chem. Int. Ed.*, 2014, **53**, 9564.

24 K. Wang, H. Huang, D. Liu, C. Wang, J. Li and C. Zhong, *Environ. Sci. Tech.*, 2016, **50**, 4869.

25 Z. Li, Y. Zhi, X. Feng, X. Ding, Y. Zou, X. Liu and Y. Mu, *Chem. Eur. J.*, 2015, **21**, 12079.

26 Z. Li, Y. Zhang, H. Xia, Y. Mu and X. Liu, *Chem. Commun.*, 2016, **52**, 6613.

27 S. Ding, J. Gao, Q. Wang, Y. Zhang, W. Song, C. Su and W. Wang, *J. Am. Chem. Soc.*, 2011, **133**, 19816.

28 S. Ding, M. Dong, Y. Wang, Y. Chen, H. Wang, C. Su and W. Wang, *J. Am. Chem. Soc.*, 2016, **138**, 3031.

29 S. Lin, X. Y. Hou, X. Deng, H. L. Wang, S. Z. Sun and X. M. Zhang, *RSC Adv.*, 2015, **5**, 41017.

30 R. Ge, D. Hao, Q. Shi, B. Dong, W. Leng, C. Wang and Y. Gao, *J. Chem. Eng. Data.*, 2016, **61**, 1904.

31 V. S. P. K. Neti, X. Wu, M. Hosseini, R. A. Bernal, S. Deng and L. Echegoyen, *CrystEngComm*, 2013, **15**, 7157.

32 W. Zhang, P. Jiang, Y. Wang, J. Zhang and P. Zhang, *Catal. Sci. Technol.*, 2015, **5**, 101.

33 J. Guo, Y. Xu, S. Jin, L. Chen, T. Kaji, Y. Honsho, M. A. Addicoat, J. Kim, A. Saeki, H. Ihee, S. Seki, S. Irle, M. Hiramoto, J. Gao and D. Jiang, *Nat. Commun.*, 2013, **4**.

34 J. Yu, Z. Chen, J. Sun, Z. Huang and Q. Zheng, *J. Mater. Chem.*, 2012, 22, 5369.

35 P. Katekomol, J. Roeser, M. Bojdys, J. Weber and A. Thomas, *Chem. Mater.*, 2013, 25, 1542.

36 P. Kuhn, M. Antonietti and A. Thomas, *Angew. Chem. Int. Ed.*, 2008, **47**, 3450.

37 M. J. Bojdys, J. Jeromenok, A. Thomas and M. Antonietti, *Adv. Mater.*, 2010, **22**, 2202.

38 X. Chen, M. Addicoat, S. Irle, A. Nagai and D. Jiang, *J. Am. Chem. Soc.*, 2013, **135**, 546-549.

39 A. Nagai, X. Chen, X. Feng, X. Ding, Z. Guo and D. Jiang, *Angew. Chem. Int. Ed.*, 2013, **52**, 3770.

40 X. Chen, M. Addicoat, S. Irle, A. Nagai and D. Jiang, *J. Am. Chem. Soc.*, 2013, **135**, 546.

41 X. Feng, L. Chen, Y. Honsho, O. Saengsawang, L. Liu, L. Wang, A. Saeki, S. Irle, S. Seki, Y. Dong and D. Jiang, *Adv. Mater.*, 2012, **24**, 3026.

42 C. R. DeBlase, K. E.Silberstein, T. Truong, H. D. Abruña and W. R. Dichtel, *J. Am. Chem. Soc.*, 2013, **135**, 16821.

43 L. A. Baldwin, J. W. Crowe, M. D. Shannon, C. P. Jaroniec and P. L. McGrier, *Chem. Mater.*, 2015, **27**, 6169.

44 B. P. Biswal, S. Kandambeth, S. Chandra, D. B. Shinde, S. Bera, S. Karak, B. Garai, U. K. Kharul and R. Banerjee, *J. Mater. Chem. A*, 2015, **3**, 23664.

45 S. Kandambeth, V. Venkatesh, D. B. Shinde, S. Kumari, A. Halder, S. Verma and R. Banerjee, *Nat. Commun.*, 2015, **6**, 6786.

46 D. B. Shinde, S. Kandambeth, P. Pachfule, R. R. Kumar and R. Banerjee, *Chem. Commun.*, 2015, **51**, 310.

47 A. Halder, S. Kandambeth, B. P. Biswal, G. Kaur, N. C. Roy, M. Addicoat, J. K. Salunke, S. Banerjee, K. Vanka, T. Heine, S. Verma and R. Banerjee, *Angew. Chem. Int. Ed.*, 2016, **55**, 806.

48 S. Jin, K. Furukawa, M. Addicoat, L. Chen, S. Takahashi, S. Irle, T. Nakamura and D. Jiang, *Chem. Sci.*, 2013, **4**, 4505.

49 H. Ma, B. Liu, B. Li, L. Zhang, Y. Li, H. Tan, H. Zang and G. Zhu, *J. Am. Chem. Soc.*, 2016, **138**, 5897.

50 X. Feng, L. Liu, Y. Honsho, A. Saeki, S. Seki, S. Irle, Y. Dong, A. Nagai and D. Jiang, *Angew. Chem. Int. Ed.*, 2012, **51**, 2618.

51 S.Xu, T. Zhan, Q. Wen, Z. Pang and X. Zhao, *ACS Macro Letters*, 2016, **5**, 99.

52 S. Jin, T. Sakurai, T. Kowalczyk, S. Dalapati, F. Xu, H. Wei, X. Chen, J. Gao, S. Seki, S. Irle and D. Jiang, *Chem. Eur. J.*, 2014, **20**, 14608.

53 S. Dalapati, M. Addicoat, S. Jin, T. Sakurai, J. Gao, H. Xu, S. Irle, S. Seki and D. Jiang, *Nat. Commun.*, 2015, **6**, 7786.

54 N. Huang, R. Krishna and D. Jiang, *J. Am. Chem. Soc.*, 2015, **137**, 7079.

55 N. Huang, X. Chen, R. Krishna and D. Jiang, *Angew. Chem. Int. Ed.*, 2015, **54**, 2986.

56 Y. Zhu, S. Wan, Y. Jin and W. Zhang, *J. Am. Chem. Soc.*, 2015, **137**, 13772.

57 Y. Du, H. Yang, J. M. Whiteley, S. Wan, Y. Jin, S. Lee and W. Zhang, *Angew. Chem. Int. Ed.*, 2016, **55**, 1737.

58 M. G. Rabbani, A. K. Sekizkardes, Z. Kahveci, T. E. Reich, R. Ding and H. M. El-Kaderi, *Chem. Eur. J.*, 2013, **19**, 3324.

59 D. Kaleeswaran, P. Vishnoi and R. Murugavel, *J. Mater. Chem. C*, 2015, **3**, 7159.

60 S. Zhang, X. Zhao, B. Li, C. Bai, Y. Li, L. Wang, R. Wen, M. Zhang, L. Ma and S. Li, *J. Hazard. Mater.*, 2016, **314**, 95.

61 D. Beaudoin, T. Maris and J. D. Wuest, *Nat. Chem.*, 2013, **5**, 830.

62 Y. Zeng, R. Zou, Z. Luo, H. Zhang, X. Yao, X. Ma, R. Zou and Y. Zhao, *J. Am. Chem. Soc.*, 2015, **137**, 1020.

63 Z. Kang, Y. Peng, Y. Qian, D. Yuan, M. A. Addicoat, T. Heine, Z. Hu, L. Tee, Z. Guo and D. Zhao, *Chem. Mater.*, 2016, **28**, 1277.

64 S. Chandra, T. Kundu, K. Dey, M. Addicoat, T. Heine and R. Banerjee, *Chem. Mater.*, 2016, **28**, 1489.

65 S. Yu, H. Lyu, J. Tian, H. Wang, D. Zhang, Y. Liu and Z. Li, *Polym. Chem.*, 2016, **7**, 3392.

66 E. L. Spitler and W. R. Dichtel, *Nat. Chem.*, 2010, **2**, 672.

67 A. Bhunia, V. Vasylyeva and C. Janiak, *Chem. Commun.*, 2013, **49**, 3961.

68 N. Huang, X. Ding, J. Kim, H. Ihee and D. Jiang, *Angew. Chem. Int. Ed.*, 2015, **54**, 8704.

69 L. Y. Bai, S. Z. F. Phua, W. Q. Lim, A. Jana, Z. Luo, H. P. Tham, L. Z. Zhao, Q. Gao and Y. L. Zhao, *Chem. Commun.*, 2016, **52**, 4128.

70 Q. Fang, J. Wang, S. Gu, R. B. Kaspar, Z. Zhuang, J. Zheng, H. Guo and S. Qiu, Y. Yan, *J. Am. Chem. Soc.*, 2015, **137**, 8352.

71 H. Liao, H. Wang, H. Ding, X. Meng, H. Xu, B. Wang, X. Ai and C. Wang, *J. Mater. Chem. A* , 2016, **4**, 7416.

72 B. Nath, W. Li, J. Huang, G. Wang, Z. Fu, M. Yao and G. Xu, *CrystEngComm*, 2016, **18**, 4259.

73 S. Wan, J. Guo, J. Kim, H. Ihee and D. Jiang, *Angew. Chem. Int. Ed.*, 2009, **48**, 5439.

74 X. Chen, N. Huang, J. Gao, H. Xu, F. Xu and D. Jiang, *Chem. Commun.*, 2014, **50**, 6161.

75 Y. Wu, H. Xu, X. Chen, J. Gao and D. Jiang, *Chem. Commun.*, 2015, **51**, 10096.

76 S. Dalapati, S. Jin, J. Gao, Y. Xu, A. Nagai and D. Jiang, *J. Am. Chem. Soc.*, 2013, **135**, 17310.

77 E. L. Spitler, J. W. Colson, F. J. Uribe-Romo, A. R. Woll, M. R. Giovino, A. Saldivar and W. R. Dichtel, *Angew. Chem. Int. Ed.*, 2012, **51**, 2623.

78 Y. Peng, G. Xu, Z. Hu, Y. Cheng, C. Chi, D. Yuan, H. Cheng and D. Zhao, *ACS App. Mater. Inter.,* 2016, **8**, 18505.

79 X. Feng, Y. Dong and D. Jiang, *CrystEngComm*., 2013, **15**, 1508.

80 G. H. V. Bertrand, V. K. Michaelis, T. C. Ong, R. G. Griffin and M. Dinca, *Proc. Natl. Acad. Sci.*, 2013, **110**, 4923.

81 B. J. Smith, A. C. Overholts, N. Hwang and W. R. Dichtel, *Chem. Commun.*, 2016, **52**, 3690.

82 M. O. Blunt, J. C. Russell, N. R. Champness and P. H. Beton, *Chem. Commun.*, 2010, **46**, 7157.

83 Z. Kahveci, T. Islamoglu, G. A. Shar, R. Ding and H. M. El-Kaderi, *CrystEngComm*, 2013, **15**, 1524.

84 G. Das, B. P. Biswal, S. Kandambeth, V. Venkatesh, G. Kaur, M. Addicoat, T. Heine, S. Verma and R. Banerjee, *Chem. Sci.*, 2015, **6**, 3931.

85 L. Stegbauer, K. Schwinghammer and B. V. Lotsch, *Chem. Sci.*, 2014, **5**, 2789.

86 L. Wang, B. Dong, R. Ge, F. Jiang, J. Xiong, Y. Gao and J. Xu, *Microporous and Mesoporous Materials*, 2016, **224**, 95.

87 S. Chandra, T. Kundu, S. Kandambeth, R. BabaRao, Y. Marathe, S. M. Kunjir and R. Banerjee, *J. Am. Chem. Soc.*, 2014, **136**, 6570.

88 S. Wan, J. Guo, J. Kim, H. Ihee and D. Jiang, *Angew. Chem. Int. Ed.*, 2008, **47**, 8826.

89 M. Calik, F. Auras, L. M. Salonen, K. Bader, I. Grill, M. Handloser, D. D. Medina, M. Dogru, F. Löbermann, D. Trauner, A. Hartschuh and T. Bein, *J. Am. Chem. Soc.*, 2014, **136**, 17802.

90 S. Chandra, S. Kandambeth, B. P. Biswal, B. Lukose, S. M. Kunjir, M. Chaudhary, R. Babarao, T. Heine and R. Banerjee, *J. Am. Chem. Soc.*, 2013, **135**, 17853.

91 M. S. Lohse, T. Stassin, G. Naudin, S. Wuttke, R. Ameloot, D. De Vos, D. D. Medina and T. Bein, *Chem. Mater.*, 2016, **28**, 626.

92 B. P. Biswal, S. Chandra, S. Kandambeth, B. Lukose, T. Heine and R. Banerjee, *J. Am. Chem. Soc.*, 2013, **135**, 5328.

93 G. Das, B. P. Biswal, S. Kandambeth, V. Venkatesh, G. Kaur, M. Addicoat, T. Heine, S. Verma and R. Banerjee, *Chem. Sci.*, 2015, **6**, 3931.

94 S. Kandambeth, A. Mallick, B. Lukose, M. V. Mane, T. Heine and R. Banerjee, *J. Am. Chem. Soc.*, 2012, **134**, 19524.

95 S. Chandra, T. Kundu, K. Dey, M. Addicoat, T. Heine and R. Banerjee, *Chem. Mater.*, 2016, **28**, 1489.

96 L. Xu, S. Ding, J. Liu, J. Sun, W. Wang and Q. Zheng, *Chem. Commun.*, 2016, **52**, 4706.

97 S. Mitra, S. Kandambeth, B. P. Biswal, M. A. Khayum, C. K. Choudhury, M. Mehta, G. Kaur, S. Banerjee, A. Prabhune, S. Verma, S. Roy, U. K. Kharul and R. Banerjee, *J. Am. Chem. Soc.*, 2016, **138**, 2823.

98 R. Gomes and A. Bhaumik, *RSC Adv.*, 2016, *6*, 28047.

99 M. Dogru, M. Handloser, F. Auras, T. Kunz, D. Medina, A. Hartschuh, P. Knochel and T. Bein, *Angew. Chem. Int. Ed.*, 2013, **52**, 2920.

100 S. Cai, Y. Zhang, A. B. Pun, B. He, J. Yang, F. M. Toma, I. D. Sharp, O. M. Yaghi, J. Fan, S. Zheng, W. Zhang and Y. Liu, *Chem. Sci.*, 2014, **5**, 4693.

101 H. Yang, S. Zhang, L. Han, Z. Zhang, Z. Xue, J. Gao, Y. Li, C. Huang, Y. Yi, H. Liu and Y. Li, *ACS App. Mater. Inter.* 2016, 8, (8), 5366.

102 E. L. Spitler, J. W. Colson, F. J. Uribe-Romo, A. R. Woll, M. R. Giovino, A. Saldivar and W. R. Dichtel, *Angew. Chem. Int. Ed.*, 2012, **51**, 2623.

103 L. Bai, Q. Gao and Y. Zhao, *J. Mater. Chem. A*, 2016, **4**, 14106.

104 V. S. Vyas, M. Vishwakarma, I. Moudrakovski, F. Haase, G. Savasci, C. Ochsenfeld, J. P. Spatz and B.V. Lotsch, *Adv. Mater.*, 2016, **28**, 8749.

105 Y. Peng, W. K. Wong, Z. Hu, Y. Cheng, D. Yuan, S. A. Khan and D. Zhao, *Chem.f Mater.*, 2016, **28**, 5095.

106 J. O. Hirschfelder, C. F. Curtiss, R. B. Bird and M. G. Mayer, Molecular theory of gases and liquids, Wiley, New York, 1954.

107 H. Crone-Munzebrock and G. Doge, *Ber. Bunsenges. Phys. Chem.*, 1990, **94**, 297.

108 A. K. Rappe, C. J. Casewit, K. S. Colwell, W. A. GoddardIII, W. M. Skiff, *J. Am. Chem. Soc.* 1992, **114**, 10024.

109 S. L. Mayo, B. D. Olafson, W. A. Goddard, *J. Phys. Chem. C*, **1990**, **94**, 8897.

110 G. Ii Park, B.S. Choi II, H. Cho, J.H. Kim, *J. Korean Nucl. Soc.* 2000, ***32***, 504.

111 T. Fukasawa, K. Funabashi, Y. Kondo, *J. Nucl. Sci. Technol*. 1994, **31**, 1073.

112 G. Park, I. Kim, J. K. Lee, S. K. Ryu and J. H. Kim, Carbon Science, 2001, **2**, 9