**Supplementary Materials For**

Exploring the Structure-Property Relationships of Covalent Organic Frameworks for Noble Gas Separations

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**1.** **Database of COF structures**

**Table S1**. Structural features of 187 experimental COFs

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| COF name | PLD  (Å) | LCD  (Å) | *Sacc* (m2/g) | *Vfree* (cm3/g) | *φ* |
| 1. 2D-NiPc-BTDA-COF1 | 12.0 | 12.3 | 1250 | 0.68 | 0.62 |
| 1. 3D-Py-COF2 | 21.6 | 24.4 | 7229 | 6.62 | 0.93 |
| 1. 3D-Py-COF-2P2 | 12.3 | 13.5 | 7310 | 3.05 | 0.85 |
| 1. 4PE-1P3 | 23.9 | 24.3 | 2344 | 1.40 | 0.73 |
| 1. 4PE-2P3 | 32.0 | 32.3 | 2458 | 1.76 | 0.77 |
| 1. 4PE-3P3 | 38.9 | 39.2 | 2802 | 2.28 | 0.81 |
| 1. 4PE-TT3 | 27.2 | 27.6 | 2234 | 1.42 | 0.75 |
| 1. AB-COF4 | 11.1 | 11.6 | 1948 | 0.96 | 0.65 |
| 1. ACOF-15 | 11.1 | 11.6 | 1948 | 0.96 | 0.65 |
| 1. AEM-COF-16 | 29.1 | 29.3 | 1902 | 1.59 | 0.76 |
| 1. AEM-COF-26 | 32.1 | 32.3 | 1316 | 1.22 | 0.72 |
| 1. ATFG-COF4 | 9.9 | 10.4 | 1517 | 0.70 | 0.62 |
| 1. AzO-COF7 | 34.3 | 34.5 | 2113 | 2.01 | 0.81 |
| 1. BDT-COF8 | 29.8 | 30.0 | 1797 | 1.54 | 0.77 |
| 1. BF-COF-19 | 8.6 | 13.3 | 5097 | 1.96 | 0.79 |
| 1. BF-COF-29 | 7.6 | 13.1 | 4300 | 1.66 | 0.78 |
| 1. BLP-2H-AA10 | 9.0 | 9.5 | 1115 | 0.56 | 0.50 |
| 1. BLP-2H-AB10 | 2.9 | 4.0 | 396 | 0.57 | 0.51 |
| 1. CC-TAPH-COF11 | 7.2 | 9.3 | 4355 | 1.53 | 0.75 |
| 1. COF-112 | 3.1 | 4.2 | 0 | 0.56 | 0.51 |
| 1. COF-1013 | 31.3 | 31.5 | 1949 | 1.74 | 0.78 |
| 1. COF-10214 | 8.0 | 9.0 | 5129 | 1.86 | 0.78 |
| 1. COF-10314 | 8.5 | 9.7 | 5315 | 2.05 | 0.80 |
| 1. COF-10514 | 16.1 | 18.8 | 6645 | 5.17 | 0.91 |
| 1. COF-10814 | 19.1 | 27.5 | 6387 | 5.37 | 0.92 |
| 1. COF-11Å15 | 7.7 | 8.4 | 515 | 0.61 | 0.54 |
| 1. COF-14Å15 | 9.8 | 10.5 | 1355 | 0.75 | 0.59 |
| 1. COF-16Å15 | 12.2 | 12.7 | 1936 | 0.86 | 0.64 |
| 1. COF-18Å15 | 14.3 | 14.7 | 1705 | 0.89 | 0.66 |
| 1. COF-20216 | 5.4 | 9.9 | 4240 | 1.39 | 0.72 |
| 1. COF-30017 | 9.3 | 9.4 | 3301 | 1.33 | 0.73 |
| 1. COF-32018 | 8.3 | 8.5 | 1814 | 0.89 | 0.63 |
| 1. COF-36619 | 18.7 | 20.5 | 4107 | 2.24 | 0.81 |
| 1. COF-42-bnn20 | 16.8 | 17.2 | 2686 | 1.30 | 0.73 |
| 1. COF-42-gra20 | 5.1 | 6.0 | 2346 | 1.00 | 0.66 |
| 1. COF-43-bnn20 | 32.3 | 32.5 | 2630 | 2.36 | 0.82 |
| 1. COF-43-gra20 | 13.4 | 13.6 | 3769 | 1.77 | 0.78 |
| 1. COF-512 | 23.4 | 23.7 | 1707 | 1.24 | 0.72 |
| 1. COF-50521 | 2.0 | 3.7 | 0 | 0.22 | 0.32 |
| 1. COF-613 | 8.6 | 9.1 | 1128 | 0.53 | 0.53 |
| 1. COF-6619 | 21.9 | 22.2 | 1742 | 1.24 | 0.73 |
| 1. COF-813 | 16.2 | 16.5 | 1601 | 0.93 | 0.65 |
| 1. COF-AA-H22 | 25.3 | 25.7 | 2314 | 1.45 | 0.74 |
| 1. COFBTA-PDA23 | 16.8 | 17.1 | 2403 | 1.36 | 0.71 |
| 1. CTF-NDC24 | 3.3 | 4.3 | 0 | 0.26 | 0.35 |
| 1. COF-JLU225 | 9.9 | 10.4 | 1368 | 0.67 | 0.60 |
| 1. COF-JLU326 | 11.3 | 12.1 | 4393 | 1.70 | 0.75 |
| 1. COF-LZU127 | 15.6 | 16.0 | 2172 | 1.24 | 0.71 |
| 1. COF-LZU828 | 13.0 | 13.5 | 805 | 0.82 | 0.62 |
| 1. COF-SDU129 | 43.1 | 43.3 | 2409 | 2.60 | 0.84 |
| 1. COF-TpAzo30 | 25.8 | 26.1 | 2081 | 1.56 | 0.78 |
| 1. CoPc-PorDBA31 | 24.7 | 25.5 | 4128 | 2.76 | 0.85 |
| 1. CPF-132 | 23.1 | 24.0 | 5087 | 2.96 | 0.86 |
| 1. CPF-232 | 21.6 | 22.5 | 5177 | 2.82 | 0.86 |
| 1. CS-COF33 | 20.2 | 20.4 | 1620 | 1.01 | 0.66 |
| 1. CTC-COF34 | 18.7 | 18.8 | 1513 | 0.91 | 0.65 |
| 1. CTF-035 | 1.3 | 2.6 | 0 | 0.15 | 0.25 |
| 1. CTF-136 | 8.4 | 8.9 | 1004 | 0.50 | 0.51 |
| 1. CTF-2-AA37 | 10.6 | 11.0 | 1251 | 0.61 | 0.55 |
| 1. CTF-2-AB37 | 3.3 | 4.9 | 443 | 0.61 | 0.55 |
| 1. CTF\_FUM24 | 6.0 | 6.7 | 1045 | 0.50 | 0.52 |
| 1. CuP-Ph COF38 | 19.0 | 20.1 | 4025 | 2.32 | 0.83 |
| 1. CuP-SQ-COF39 | 11.3 | 12.9 | 3240 | 1.46 | 0.76 |
| 1. CuP-TFPh COF40 | 17.9 | 19.0 | 4439 | 2.07 | 0.83 |
| 1. DA-COF41 | 19.1 | 19.4 | 1646 | 1.08 | 0.71 |
| 1. DAAQ-TFP-COF42 | 22.0 | 22.2 | 1761 | 1.18 | 0.73 |
| 1. DBA-COF 143 | 29.2 | 29.4 | 1965 | 1.59 | 0.76 |
| 1. DBA-COF 243 | 34.2 | 34.4 | 2127 | 2.00 | 0.80 |
| 1. BDT-OEt-COF8 | 23.2 | 23.5 | 1851 | 1.18 | 0.72 |
| 1. 2,3-DhaTab44 | 29.1 | 29.3 | 2098 | 1.81 | 0.78 |
| 1. 2,5-DhaTab44 | 29.5 | 29.6 | 2212 | 1.87 | 0.78 |
| 1. DhaTab45 | 32.1 | 32.3 | 2130 | 1.99 | 0.79 |
| 1. 2,3-DhaTph46 | 18.2 | 19.2 | 4381 | 2.34 | 0.82 |
| 1. 2,5-DhaTph44 | 17.4 | 18.5 | 4382 | 2.34 | 0.82 |
| 1. 2,3-DhaTta47 | 29.2 | 29.2 | 2093 | 1.82 | 0.79 |
| 1. 2,3-DmaTph46 | 16.4 | 17.6 | 4206 | 2.14 | 0.81 |
| 1. DTP-ANDI-COF48 | 43.8 | 43.9 | 1842 | 2.19 | 0.82 |
| 1. EB-COF:Br49 | 10.0 | 10.6 | 1336 | 0.62 | 0.58 |
| 1. H2P-COF50 | 19.2 | 20.3 | 4417 | 2.54 | 0.83 |
| 1. HAT-COF51 | 9.1 | 9.9 | 1734 | 0.84 | 0.63 |
| 1. TTF-Py-COF 52 | 14.3 | 14.5 | 2054 | 1.10 | 0.69 |
| 1. HBC-COF53 | 10.6 | 10.8 | 1520 | 0.74 | 0.59 |
| 1. HCC-H2P-COF54 | 14.4 | 15.7 | 4134 | 2.07 | 0.80 |
| 1. HO-H2P-COF55 | 17.5 | 18.5 | 4399 | 2.36 | 0.83 |
| 1. HO2C-H2P-COF55 | 9.4 | 10.9 | 4927 | 1.90 | 0.79 |
| 1. HP-COF-156 | 14.4 | 14.8 | 2003 | 1.06 | 0.67 |
| 1. HP-COF-256 | 16.8 | 17.2 | 2429 | 1.35 | 0.72 |
| 1. HPB-COF53 | 5.8 | 7.6 | 2479 | 0.96 | 0.65 |
| 1. ICOF-157 | 15.0 | 15.2 | 2146 | 1.20 | 0.70 |
| 1. ICOF-257 | 16.6 | 17.2 | 2383 | 1.32 | 0.72 |
| 1. ILCOF-1-AA58 | 20.8 | 21.2 | 3865 | 2.57 | 0.83 |
| 1. ILCOF-1-AB58 | 9.4 | 11.1 | 6714 | 2.42 | 0.82 |
| 1. iPrTAPB-TFP59 | 6.5 | 7.5 | 712 | 0.49 | 0.48 |
| 1. iPrTAPB-TFPB59 | 15.4 | 15.9 | 1738 | 1.07 | 0.66 |
| 1. MPCOF60 | 9.8 | 10.3 | 1394 | 0.66 | 0.61 |
| 1. NPN-161 | 4.1 | 5.3 | 958 | 0.49 | 0.51 |
| 1. NPN-261 | 4.2 | 5.3 | 1125 | 0.56 | 0.54 |
| 1. NPN-361 | 5.4 | 6.1 | 941 | 0.47 | 0.50 |
| 1. NN-TAPH-COF11 | 7.2 | 9.3 | 4435 | 1.53 | 0.75 |
| 1. NTU-COF-162 | 18.4 | 18.7 | 1916 | 1.20 | 0.70 |
| 1. NTU-COF-262 | 24.6 | 24.8 | 2117 | 1.70 | 0.77 |
| 1. NUS-263 | 9.9 | 10.4 | 1368 | 0.67 | 0.60 |
| 1. NUS-363 | 16.7 | 17.0 | 2036 | 0.99 | 0.68 |
| 1. EB-COF:Cl49 | 10.0 | 10.6 | 1490 | 0.69 | 0.59 |
| 1. OH-TAPH-COF11 | 17.5 | 18.5 | 4369 | 2.44 | 0.83 |
| 1. TpPa-Py64 | 16.0 | 16.3 | 1649 | 0.95 | 0.66 |
| 1. PC-COF65 | 41.1 | 41.1 | 3056 | 3.01 | 0.85 |
| 1. Pc-PBBA-COF66 | 16.5 | 16.8 | 1391 | 0.81 | 0.64 |
| 1. PCTF-167 | 13.4 | 13.7 | 1872 | 1.07 | 0.68 |
| 1. PCTF-267 | 21.4 | 21.5 | 2279 | 1.57 | 0.75 |
| 1. PCTF-367 | 27.7 | 27.8 | 2364 | 1.95 | 0.79 |
| 1. PCTF-467 | 17.5 | 17.9 | 1942 | 1.24 | 0.72 |
| 1. Ph-An-COF68 | 22.1 | 22.3 | 1701 | 1.16 | 0.71 |
| 1. Ph-AnCD-COF68 | 21.0 | 23.7 | 5283 | 2.76 | 0.85 |
| 1. PI-2-COF69 | 23.4 | 23.7 | 2286 | 1.57 | 0.75 |
| 1. PI-3-COF69 | 30.4 | 30.6 | 2280 | 2.03 | 0.80 |
| 1. PI-COF-469 | 13.4 | 17.5 | 5113 | 3.19 | 0.88 |
| 1. PI-COF-4-2P70 | 7.6 | 8.2 | 5020 | 1.36 | 0.75 |
| 1. PI-COF-570 | 22.4 | 26.6 | 6479 | 7.30 | 0.94 |
| 1. PI-COF-5-2P70 | 10.5 | 13.4 | 6543 | 3.42 | 0.88 |
| 1. Por-COF71 | 18.6 | 20.4 | 4010 | 2.24 | 0.81 |
| 1. POR-COF72 | 12.6 | 14.1 | 3548 | 1.54 | 0.77 |
| 1. PPy-COF73 | 13.3 | 13.7 | 1332 | 0.65 | 0.57 |
| 1. Py-2,2'-BPyPh-COF74 | 23.2 | 23.5 | 2251 | 1.64 | 0.77 |
| 1. Py-2,3-BPyPh-COF74 | 22.7 | 22.9 | 2243 | 1.62 | 0.76 |
| 1. Py-2,3-DHPh-COF74 | 21.0 | 21.5 | 4568 | 2.70 | 0.85 |
| 1. EB-COF:F49 | 10.0 | 10.6 | 1594 | 0.73 | 0.60 |
| 1. Py-An-COF75 | 19.2 | 19.5 | 2344 | 1.47 | 0.74 |
| 1. Py-Azine-COF76 | 12.5 | 13.0 | 2031 | 1.11 | 0.69 |
| 1. EB-COF:I49 | 9.6 | 10.3 | 1530 | 0.60 | 0.53 |
| 1. Py-COF77 | 21.6 | 24.4 | 7229 | 6.62 | 0.93 |
| 1. NUS-9 78 | 12.0 | 13.0 | 2392 | 1.23 | 0.74 |
| 1. Py-DHPh-COF74 | 19.9 | 20.2 | 4796 | 2.70 | 0.85 |
| 1. NUS-10 78 | 12.0 | 13.0 | 1959 | 0.95 | 0.70 |
| 1. Star-COF-179 | 30.4 | 30.6 | 1371 | 1.22 | 0.71 |
| 1. Star-COF-279 | 37.3 | 37.4 | 1496 | 1.51 | 0.75 |
| 1. Star-COF-379 | 40.0 | 40.2 | 1602 | 1.72 | 0.77 |
| 1. T-COF 180 | 7.6 | 8.2 | 1045 | 0.48 | 0.51 |
| 1. T-COF 280 | 14.6 | 14.9 | 1507 | 0.82 | 0.63 |
| 1. T-COF 380 | 12.4 | 12.7 | 1272 | 0.63 | 0.58 |
| 1. TAPB-PDA COF81 | 32.1 | 32.3 | 2410 | 2.21 | 0.80 |
| 1. TAPB-TFP59 | 11.6 | 12.0 | 1496 | 0.80 | 0.62 |
| 1. TAPB-TFPB59 | 19.0 | 19.3 | 1973 | 1.32 | 0.71 |
| 1. TBPB-COF82 | 16.4 | 16.7 | 1677 | 0.98 | 0.64 |
| 1. TD-COF-583 | 27.9 | 28.4 | 4465 | 3.42 | 0.87 |
| 1. DAB-TFP-COF42 | 22.0 | 22.3 | 1739 | 1.20 | 0.73 |
| 1. TfpBDH84 | 36.2 | 36.3 | 2102 | 2.08 | 0.81 |
| 1. TFPT-COF85 | 34.2 | 34.4 | 2131 | 2.02 | 0.80 |
| 1. TH-COF-186 | 11.7 | 12.1 | 1561 | 0.65 | 0.60 |
| 1. Tp-Azo87 | 25.5 | 25.7 | 1829 | 1.36 | 0.75 |
| 1. TP-COF88 | 28.5 | 28.7 | 1758 | 1.42 | 0.75 |
| 1. Tp-Por-COF-AA89 | 41.1 | 41.2 | 1907 | 2.10 | 0.81 |
| 1. Tp-Por-COF-AB89 | 19.9 | 20.1 | 2880 | 1.73 | 0.78 |
| 1. Tp-Stb87 | 22.3 | 22.5 | 1987 | 1.33 | 0.73 |
| 1. TpBD-2NO290 | 21.5 | 21.7 | 1638 | 1.13 | 0.71 |
| 1. TPBD-ME290 | 21.6 | 21.6 | 1523 | 1.03 | 0.68 |
| 1. TpBD-NH291 | 22.1 | 22.2 | 1705 | 1.20 | 0.72 |
| 1. TpBD-NHCOCH391 | 17.7 | 18.1 | 1335 | 0.85 | 0.64 |
| 1. TpBD-NO290 | 21.2 | 21.4 | 1517 | 0.98 | 0.69 |
| 1. TpBD-(OMe)290 | 19.9 | 20.3 | 2149 | 1.34 | 0.73 |
| 1. TpBD92 | 22.6 | 22.9 | 1717 | 1.20 | 0.71 |
| 1. TpBDH93 | 21.9 | 22.2 | 1504 | 1.04 | 0.71 |
| 1. TpPa-1-F290 | 15.3 | 15.6 | 1359 | 0.77 | 0.64 |
| 1. TpPa-194 | 15.8 | 16.1 | 1643 | 0.93 | 0.66 |
| 1. TpPa-294 | 13.4 | 13.8 | 1586 | 0.78 | 0.61 |
| 1. TpPa-F490 | 14.6 | 14.9 | 1084 | 0.59 | 0.60 |
| 1. TpPA-NO290 | 11.1 | 11.4 | 1281 | 0.61 | 0.58 |
| 1. TpPa-SO3H-Py95 | 16.0 | 16.3 | 1523 | 0.83 | 0.64 |
| 1. TpPa-SO3H90 | 12.2 | 12.5 | 1289 | 0.63 | 0.59 |
| 1. TPT-COF-196 | 21.6 | 21.9 | 2122 | 1.38 | 0.74 |
| 1. TPT-COF-296 | 33.8 | 33.9 | 2468 | 2.18 | 0.81 |
| 1. TpTG-Br97 | 2.6 | 3.2 | 0 | 0.20 | 0.35 |
| 1. TpTG-Cl97 | 2.8 | 3.4 | 0 | 0.23 | 0.36 |
| 1. TpTG-I97 | 2.4 | 3.0 | 0 | 0.17 | 0.34 |
| 1. TRIPTA98 | 11.9 | 12.4 | 1503 | 0.79 | 0.62 |
| 1. TT-COF99 | 26.1 | 26.3 | 1610 | 1.30 | 0.74 |
| 1. TTF-COF100 | 18.1 | 18.6 | 3391 | 1.92 | 0.79 |
| 1. TThPP101 | 16.7 | 17.8 | 3780 | 2.08 | 0.81 |
| 1. ZnP-COF50 | 17.9 | 19.0 | 4000 | 2.27 | 0.82 |
| 1. ZnPc-COF102 | 16.6 | 17.0 | 1409 | 0.85 | 0.66 |
| 1. ZnPc-DPB102 | 26.6 | 26.8 | 1798 | 1.39 | 0.76 |
| 1. ZnPc-NDI102 | 27.0 | 27.2 | 1428 | 1.20 | 0.73 |
| 1. ZnPc-PPE102 | 32.1 | 32.2 | 2060 | 1.84 | 0.79 |
| 1. ZnPc-Py102 | 18.3 | 18.5 | 1312 | 0.85 | 0.66 |
| 1. N3-COF103 | 18.2 | 18.5 | 1885 | 1.23 | 0.71 |
| 1. TTI-COF104 | 18.2 | 18.5 | 1959 | 1.26 | 0.71 |
| 1. NUS-14105 | 40.7 | 40.8 | 2537 | 2.71 | 0.84 |

\*Accessible surface area (*Sacc*) of each material was calculated by a probe molecule with a size equal to the kinetic diameter of N2 (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.

The COFs provided in the database can be divided into two categories. One is those with the structures that are constructed according to the specific atomic coordinate files reported by the experimental studies. The other is those reported without atomic coordinate files but they are all the ones with the topologies already known. Thus, based on the experimental information, the starting structure of each of these COFs was built by: (i) selecting one existing COF structure with the same topology; (ii) replacing the building blocks of this structure with the specific ones that correspond to the monomer molecules for synthesizing the targeted material; (iii) imposing the unit cell parameters determined experimentally (if available) or initially arranging appropriate ones. Then, molecular mechanism (MM) approach combined with DREIDIND force field was first employed to optimize these initial models (for the structures without cell parameters available, both the lattice parameters and atomic positions were also allowed to fully relax), using the Forcite module implemented in Material Studio software. Finally, periodic density functional theory calculations combined with Grimme’s dispersion correction were performed to further refine these structures. These DFT-D2 calculations were carried out using the Dmol3 code implemented in the Material Studio software.

For the experimentally reported COFs structures that contain solvents or disorder atoms, the structures were cleaned and fixed manually followed by optimization. The optimization methods are similar to the procedures mentioned above for those COFs without experimentally atomic positions, except that the experimental lattice parameters were fixed.

**2. Validation of the force fields**

**Table S2**. Lennard-Jones parameters for the framework atoms of the COFs

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Atoms | C | O | H | N | F | B | Si | S | P | Zn | Cu | Ni*a* |
| *σ* (Å) | 3.47 | 3.03 | 2.85 | 3.26 | 3.09 | 3.58 | 3.80 | 3.59 | 3.70 | 4.04 | 3.11 | 2.52 |
| *ε/kB* (K) | 47.86 | 48.16 | 7.650 | 38.95 | 36.48 | 47.81 | 156.0 | 173.1 | 161.0 | 27.68 | 2.52 | 7.55 |

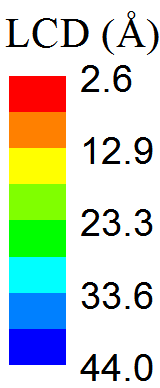
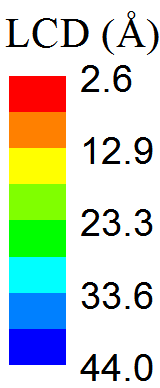
a Taken from the UFF force field108 (they are missing in the Dreiding force field).



**Fig. S1** Comparison of the simulated adsorption isotherms of Ar in COFs with the corresponding experimental data109 (red squares: simulation results; black circles: experimental data).

**3. Structure-property relationships**

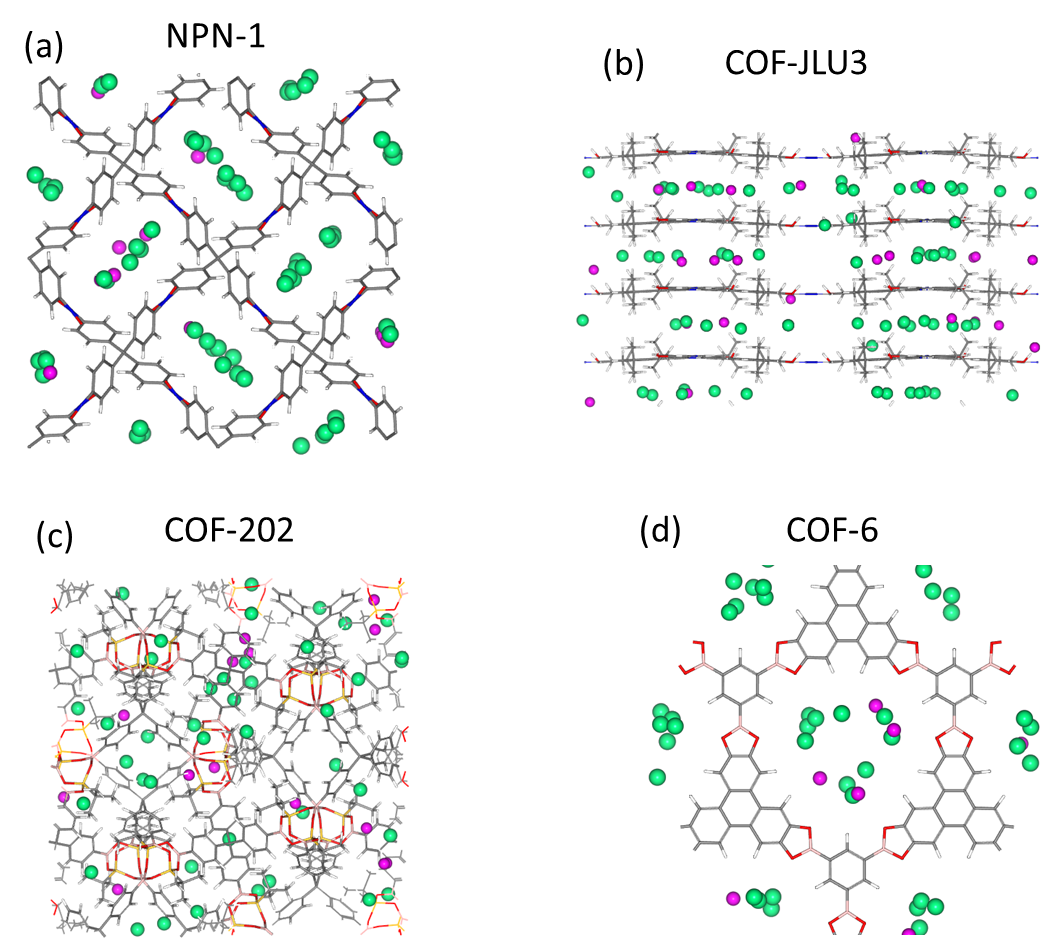
* **Kr/Ar separation**



**Fig. S2** Relationships between the isosteric heat of adsorption of Kr (*Q*st,Kr) at adsorption pressure of COFs and adsorption figure of merit (AFM) for Kr/Ar separation under the conditions of VSA and PSA processes.

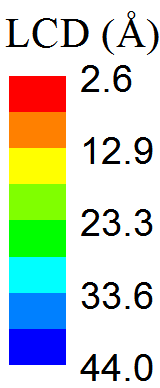
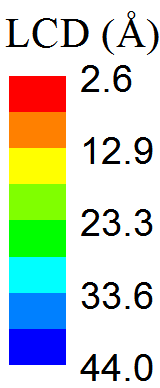
 

**Fig. S3** Relationships between the largest cavity diameter (LCD) of COFs and adsorption figure of merit (AFM) for Kr/Ar separation under the conditions of VSA and PSA processes.



**Fig. S4** Adsorption configurations of Kr/Ar mixture in (a) 3D NPN-1with interpenetrated framework, (b) 2D COF-JLU3 with slit-like pore, (c) 3D COF-202 with **ctn** topology, (d) 2D COF-6 with simple 1D pore channel. (Kr and Ar are respectively represented as green and magenta balls. Atoms of COF: B: pink; O, red; C, gray; N, blue and H, white)

* **Xe/Kr separation**



**Fig. S5** Relationships between the isosteric heat of adsorption of Xe (*Q*st,Xe) at adsorption pressure of COFs and adsorption figure of merit (AFM) for Xe/Kr separation under the conditions of VSA and PSA processes.

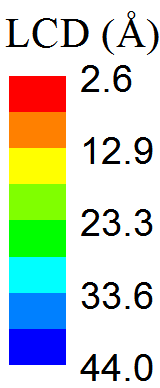
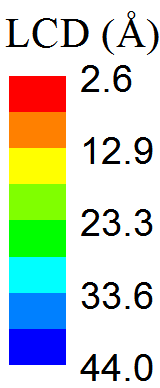
 

**Fig. S6** Relationships between the Xe/Kr selectivity and pore morphology of COFs. The LCD (largest cavity diameter) / PLD (pore limiting diameter) ratio of 1 means that the pore shape is cylinder-like, while the higher ratio means that the structure resembles a network consisted of large cavities with narrow channels or windows.



**Fig. S7** Relationships between the largest cavity diameter (LCD) of COFs and the adsorption figure of merit (AFM) for Xe/Kr separation under the conditions of VSA and PSA processes.

* **Rn/Xe separation**



**Fig. S8** Relationships between the isosteric heat of adsorption of Rn (*Q*st,Rn) at adsorption pressure of COFs and adsorption figure of merit (AFM) for Rn/Xe separation under the conditions of VSA and PSA processes.



**Fig. S9** Relationships between the largest cavity diameter (LCD) of COFs and the adsorption figure of merit (AFM) for Rn/Xe separation under the conditions of VSA and PSA processes.

**References**

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