Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

Zr-MOFs for CF_4/CH_4, CH_4/H_2, and CH_4/N_2 Separation: Towards the Goal of Discovering Stable and Effective Adsorbents

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Submitted to *MSDE*

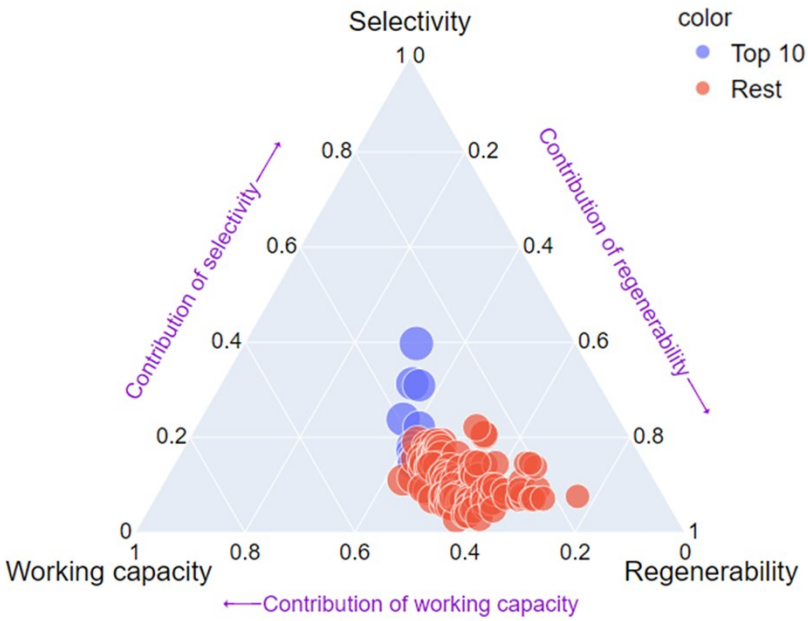

Figure S1. Ternary plot of CH_4/H_2 separation performance metrics showing their contribution to overall separation performance score.

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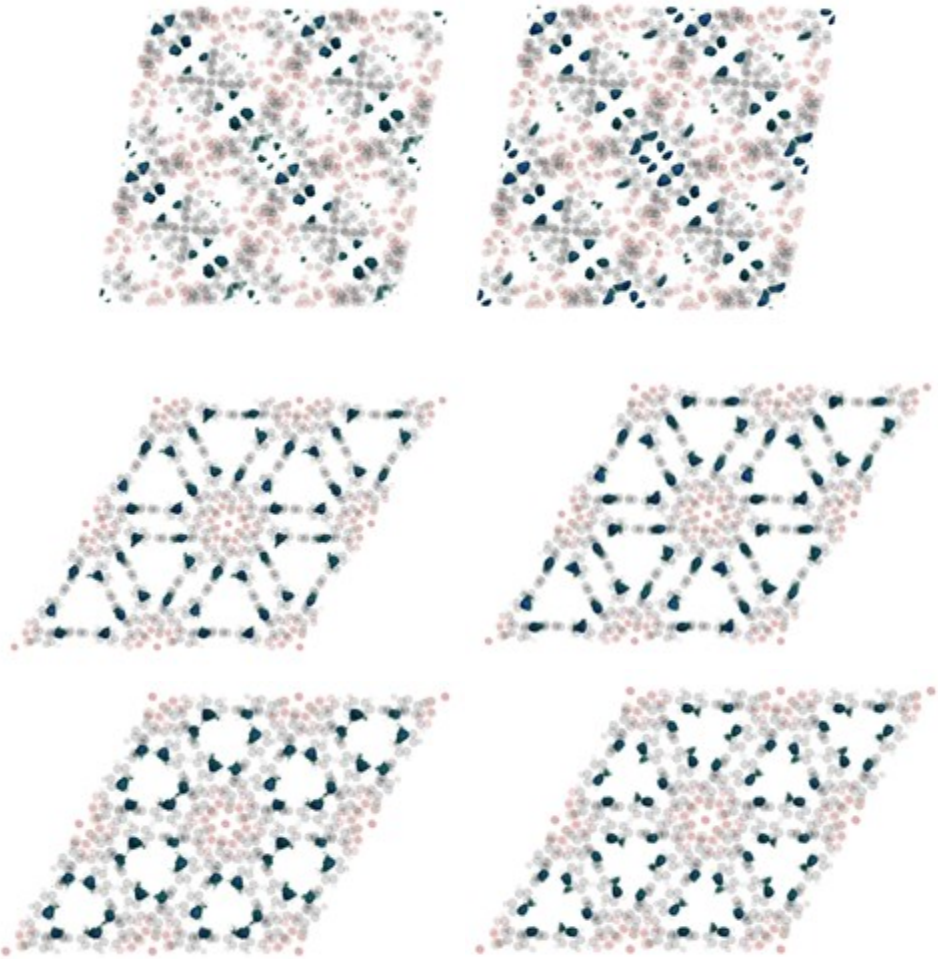

Figure S2. CH_4 density profiles determined for CH_4/H_2 mixture in MOF-812 (top), BUT-67 (center), and BUT-66 (bottom) at 1 (left) and 10 (right) bar at 298 K.

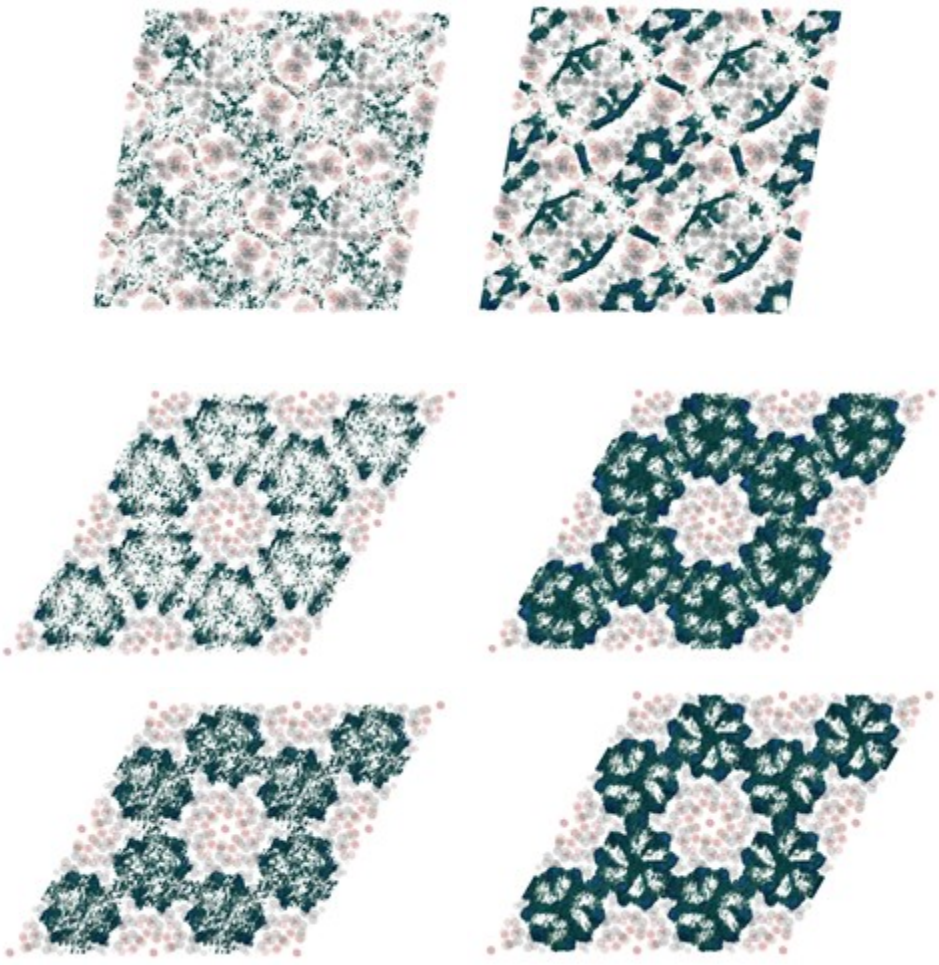

Figure S3. H_2 density profiles determined for CH_4/H_2 mixture in MOF-812 (top), BUT-67 (center), and BUT-66 (bottom) at 1 (left) and 10 (right) bar at 298 K.

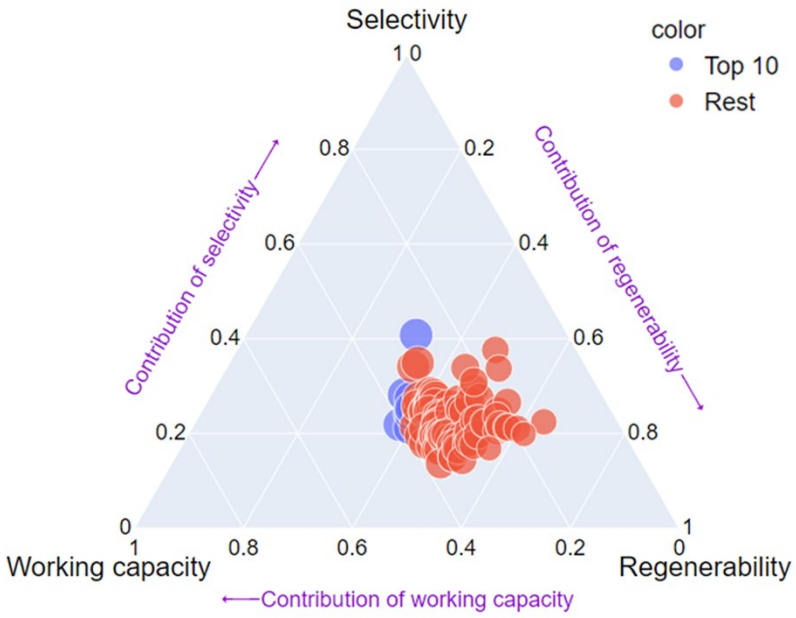

Figure S4. Ternary plot of CH_4/N_2 separation performance metrics (according to PACMOF charges) showing their contribution to overall separation performance score.

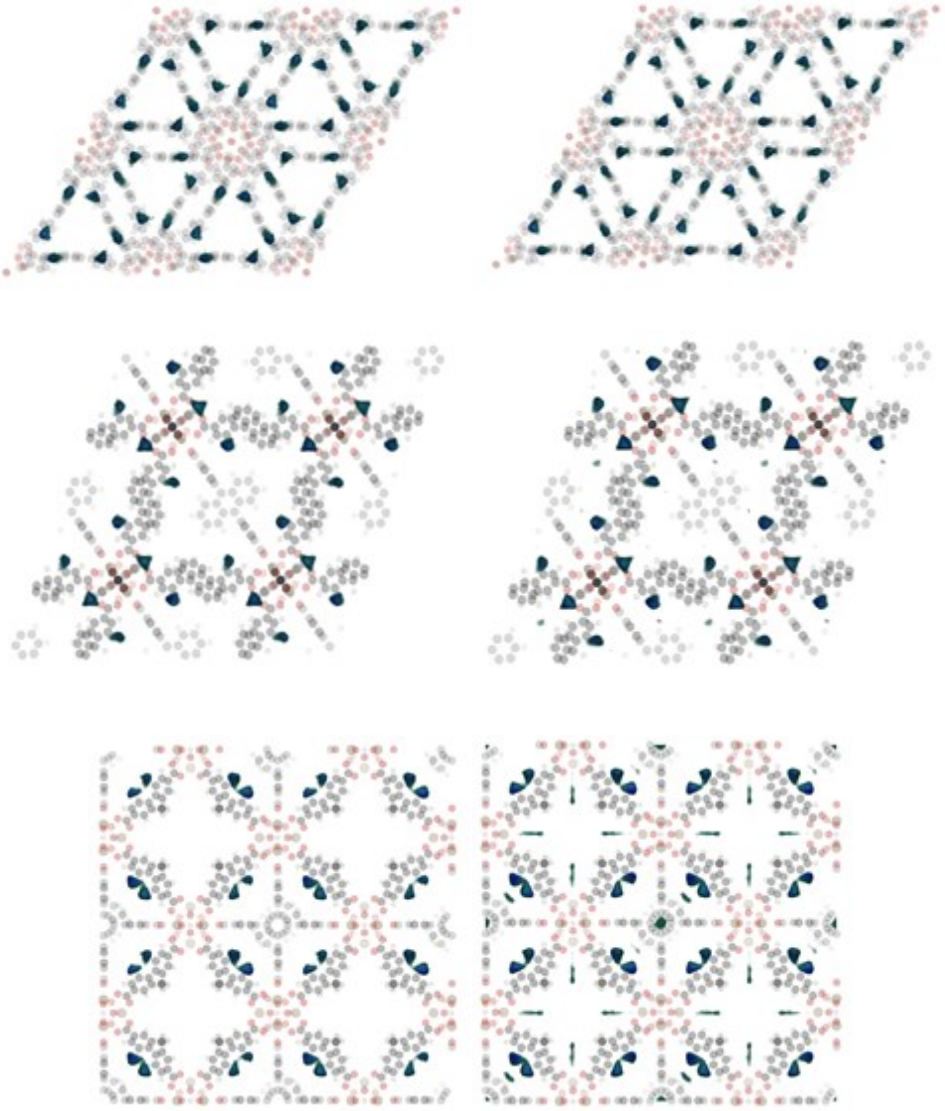

Figure S5. CH_4 density profiles determined for CH_4/N_2 mixture in BUT-67 (top), Zr-AbBA (center), and PCN-702 (bottom) at 1 (left) and 10 (right) bar at 298 K.

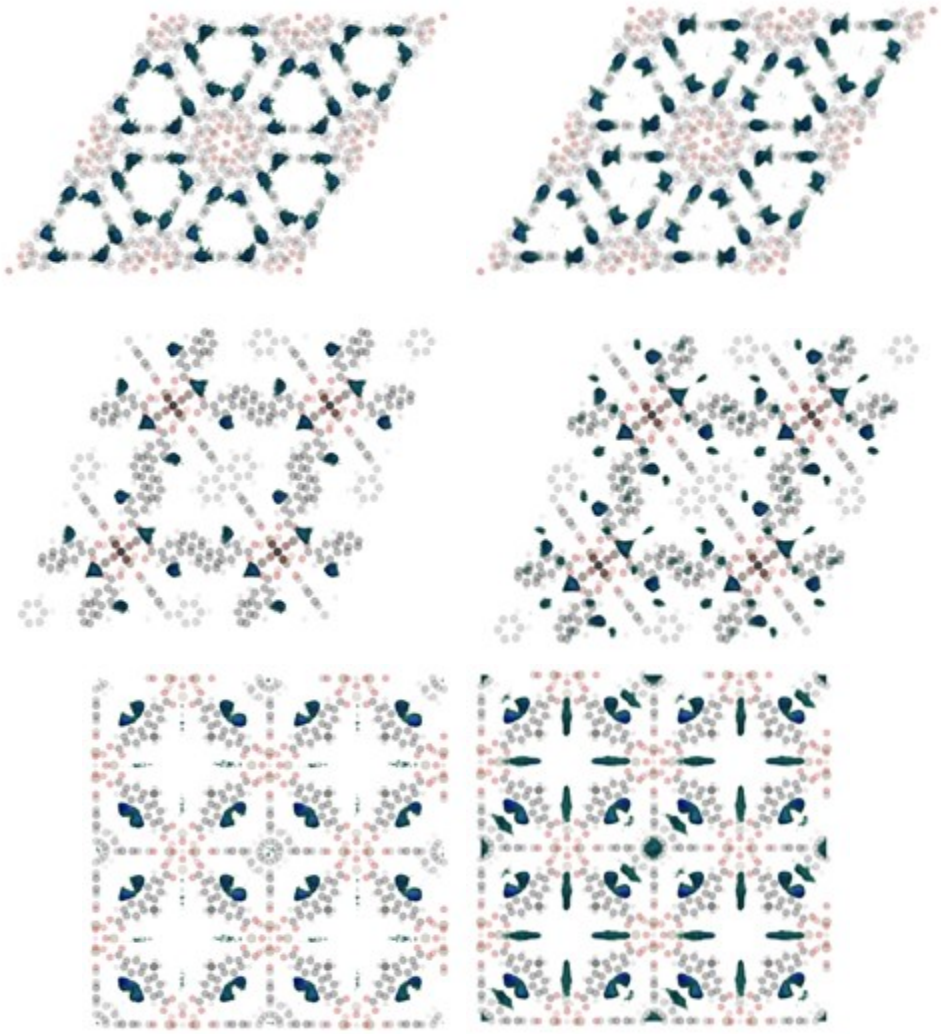

Figure S6. N_2 density profiles determined for CH_4/N_2 mixture in BUT-67 (top), Zr-AbBA (center), and PCN-702 (bottom) at 1 (left) and 10 (right) bar at 298 K.

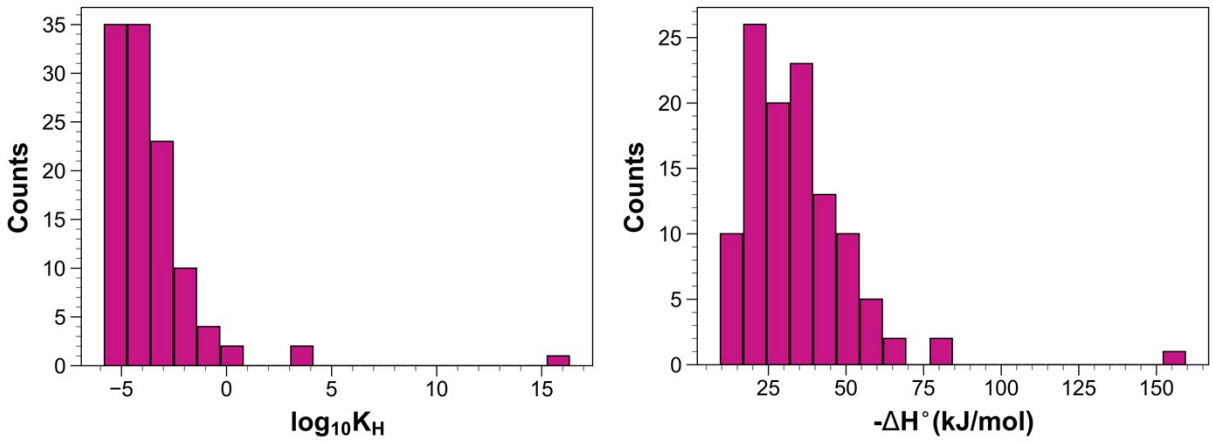

Figure S7. Histograms of K_H (left) and -ΔH° (right) of H_2O in the Zr-MOFs calculated at 298 K with PACMOF charges.

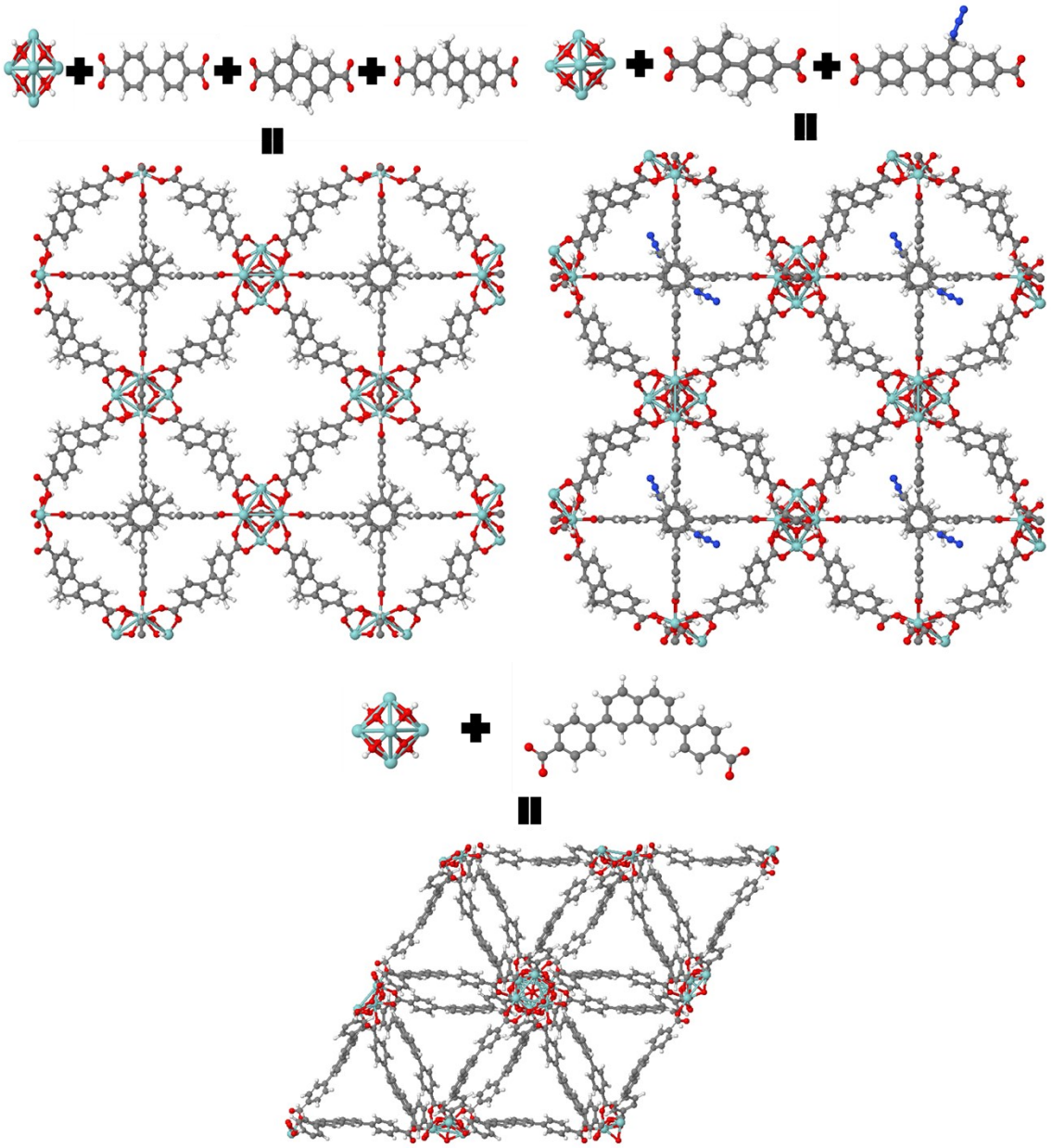

Figure S8. Representations of the top three Zr-MOFs for the CF_4/CH_4 separation. (PCN-700-BPDC-TPDC (top left), LIFM-90 (top right), and BUT-67 (bottom)) (H, C, O, N and Zr atoms are shown in white, grey, red, blue and cyan, respectively) (constituents of the linkers are shown on the same plane when possible)

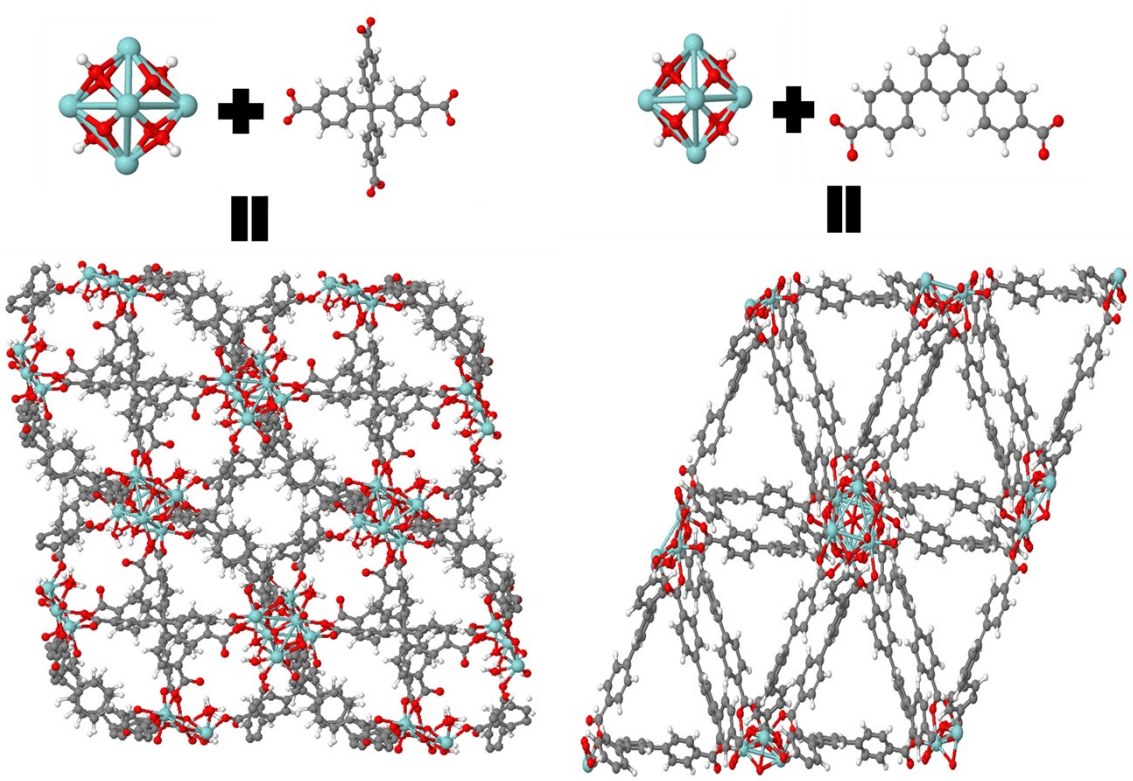

Figure S9. Depictions of the first and third ranked Zr-MOFs for the CH_4/H_2 separation. (MOF-812 (left), and BUT-66 (right)) (H, C, O, and Zr atoms are shown in white, grey, red, and cyan, successively) (constituents of the linkers are shown on the same plane when possible)

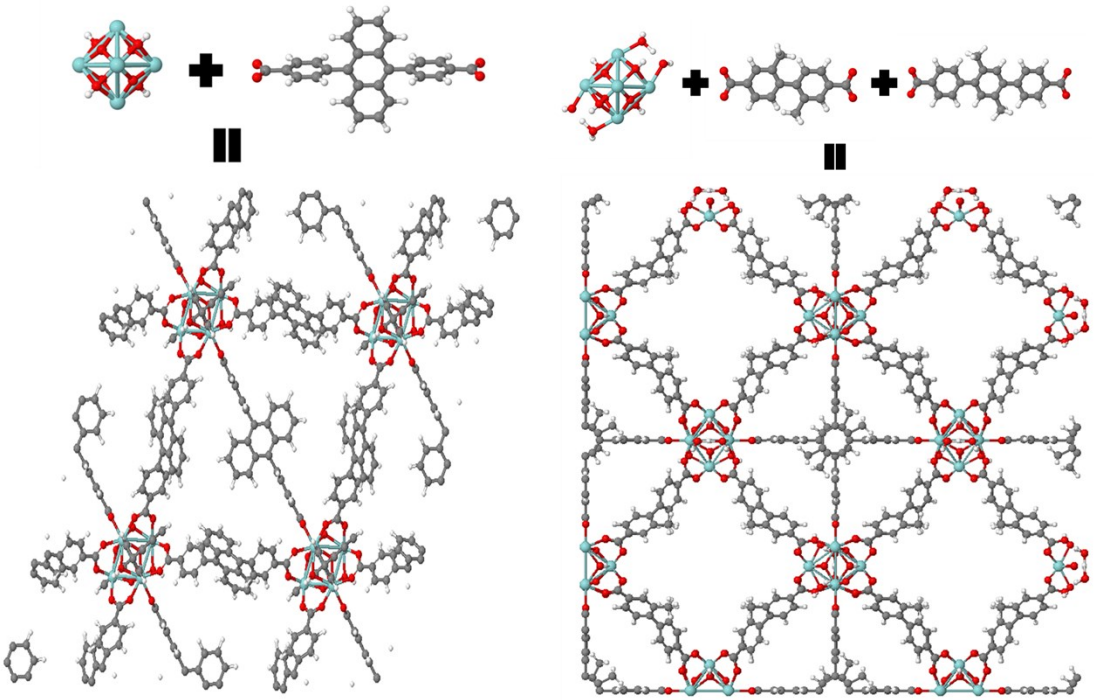

Figure S10. Illustration of the second and third best Zr-MOFs for the CH_4/N_2 separation. (Zr-AbBA (left), and PCN-702 (right)) (H, C, O, and Zr atoms are shown in white, gray, red, and cyan, respectively) (constituents of the linkers are shown on the same plane when possible)

Table S1. Separation performance metrics and structural features of the ranked Zr-MOFs for the separation of CF_4/CH_4 gas mixture.

Structure	S_{CF_4/CH_4}	ΔN_{CF_4} (mol/kg)	R_{CF_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
PCN-700-BPDC-TPDC	4.8	2.0	85.1	8.71	6.44	8.71	3122.9	0.602	0.800
LIFM-90	4.6	2.0	84.2	7.97	6.96	7.97	2933.4	0.576	0.737
BUT-67	4.7	2.1	75.7	7.96	6.29	7.90	1708.7	0.461	0.501
PU-1	5.1	1.6	83.4	10.92	6.03	10.92	2683.6	0.543	0.753
BUT-11	4.6	1.7	82.9	10.25	4.93	10.25	2026.8	0.558	0.616
PCN-700-NDC-BDDC	3.9	1.7	83.2	8.45	7.68	8.45	2768.5	0.577	0.736
LIFM-78	3.9	1.5	85.1	7.02	6.43	7.00	2307.9	0.555	0.613
LIFM-76	3.8	1.5	85.9	6.94	6.36	6.94	2317.5	0.543	0.599
LIFM-83	3.8	1.5	86.3	7.05	6.33	7.05	2385.2	0.548	0.609
LIFM-77	3.8	1.5	86.1	6.99	6.42	6.99	2353.3	0.546	0.602
LIFM-80	3.9	1.4	85.7	7.25	6.45	7.03	2405.6	0.566	0.628
LIFM-79	3.9	1.4	85.7	7.29	6.45	7.08	2329.4	0.559	0.621
LIFM-84	3.8	1.4	85.8	7.19	6.45	7.01	2385.5	0.555	0.613
LIFM-75	3.8	1.4	85.7	7.18	6.49	7.13	2346.0	0.553	0.610
LIFM-73	3.9	1.4	85.9	7.33	6.59	7.13	2337.0	0.557	0.610
LIFM-74	3.8	1.4	85.4	7.08	6.44	7.08	2366.8	0.554	0.611
BUT-66	6.2	1.3	54.0	6.98	6.18	6.98	1311.7	0.406	0.387
PCN-700-BPDC	4.0	1.3	86.1	12.88	12.47	12.88	3030.2	0.663	0.987
BUT-10	3.6	1.4	83.6	9.55	4.98	9.55	2452.5	0.581	0.679
PCN-700-NDC-TPDC	3.6	1.4	84.1	11.96	6.95	8.29	2971.5	0.613	0.818
Zr-MTBC	3.5	1.3	87.9	14.54	8.01	13.52	3733.6	0.671	1.154
NNU-28	3.9	1.4	80.6	16.54	5.19	16.14	2481.7	0.543	0.746
LIFM-86	3.6	1.3	86.4	7.16	6.63	7.16	2345.4	0.552	0.597
LIFM-85	3.5	1.4	85.7	7.14	6.50	7.14	2288.7	0.541	0.591
PCN-700-DOBPDC	3.6	1.3	83.4	11.13	10.18	11.13	2399.5	0.577	0.723
DUT-98-op	4.0	1.2	84.9	12.44	9.15	12.44	1812.7	0.574	0.677
MOF-806	3.6	1.3	87.2	12.79	5.94	12.79	2578.5	0.619	0.790
PCN-702	3.0	1.5	85.9	8.76	7.54	8.20	3213.6	0.612	0.813
LIFM-71	3.4	1.3	85.1	6.94	6.35	6.94	2135.9	0.527	0.556
LIFM-72	3.3	1.3	86.2	7.01	6.43	7.01	2190.0	0.527	0.560
PCN-700-BDDC	3.2	1.4	86.6	8.46	8.06	8.46	2895.8	0.597	0.780
PCN-133	4.2	1.2	79.5	8.94	7.55	8.94	3224.2	0.663	0.962
LIFM-82	3.0	1.4	86.5	7.21	6.50	7.21	2366.9	0.548	0.605
LIFM-94	2.8	1.5	83.0	8.29	7.39	8.29	2190.9	0.507	0.608

Structure	S_{CF_4/CH_4}	ΔN_{CF_4} (mol/kg)	R_{CF_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
PCN-56	3.4	1.2	87.1	16.66	7.14	16.66	4230.5	0.707	1.393
UiO-67-Me	3.3	1.3	83.4	12.18	5.84	12.18	2473.3	0.583	0.746
UiO-68-alkyne	3.4	1.1	86.4	16.62	7.30	16.61	3951.0	0.687	1.298
ZrDMTD	3.4	1.0	87.2	16.67	6.69	16.67	3892.2	0.707	1.292
PCN-58	3.4	1.1	85.5	12.65	5.89	12.65	3535.7	0.627	1.047
UiO-NDI	3.5	1.1	83.7	20.99	8.59	20.99	4142.9	0.718	1.560
PCN-700-NDC	3.4	1.1	84.2	13.81	13.06	13.80	2901.4	0.654	0.935
NPF-300-5	3.3	1.0	87.4	15.52	8.29	15.52	3822.5	0.720	1.318
Zr-BTDC	3.8	0.9	84.1	10.84	5.95	10.84	2136.0	0.575	0.626
NPF-300-2	3.2	1.1	87.5	16.83	11.51	16.82	3913.5	0.725	1.373
UiO-BPYDC	3.4	1.0	88.4	12.44	6.53	12.44	2763.0	0.646	0.867
UiO-67Me	3.2	1.0	86.6	10.49	5.24	10.49	2768.2	0.594	0.791
UiO-67	3.1	1.0	87.8	12.83	5.96	12.83	2966.8	0.638	0.883
MOF-535	3.0	1.0	89.0	16.67	5.57	16.67	3557.2	0.712	1.277
PCN-700-BDC-BDDC	2.5	1.3	81.9	8.84	7.52	8.84	2353.2	0.542	0.642
PCN-700-MA	3.3	1.0	83.5	13.64	12.88	13.63	2705.8	0.639	0.875
LIFM-92	2.4	1.3	82.6	7.97	6.97	7.97	2761.6	0.550	0.689
UiO-67-NH2	3.1	1.0	86.7	11.52	5.33	11.52	2792.0	0.610	0.811
LIFM-70	2.6	1.2	85.0	6.96	6.41	6.96	2078.0	0.523	0.550
PCN-703	2.9	1.2	81.3	10.69	8.20	8.61	2555.0	0.585	0.733
UiO-67-BN	3.2	0.9	87.2	11.04	5.27	11.02	1805.6	0.491	0.536
Zr-cca	3.3	1.0	83.7	9.93	5.34	9.89	2445.7	0.590	0.677
UiO-68-NH2	3.0	0.9	88.0	17.62	8.85	17.62	4269.9	0.737	1.508
PCN-701	3.3	1.0	81.3	13.91	13.24	13.83	2612.8	0.637	0.859
NU-801	3.1	0.8	89.2	12.04	6.91	11.85	3415.2	0.679	1.031
NPF-300-6	3.1	0.9	87.6	15.39	10.53	15.39	3904.8	0.751	1.490
NPF-300-8	2.8	1.0	87.3	15.60	10.64	15.52	4018.3	0.741	1.437
LIFM-31	3.4	0.8	83.4	13.99	13.15	13.99	2160.1	0.613	0.723
UiO-68-OH	3.0	0.9	88.0	16.62	7.35	16.62	4192.9	0.737	1.447
UiO-68-ol	2.9	0.9	87.3	16.27	7.81	16.27	4091.0	0.713	1.366
UiO-67-Cl	3.1	0.8	87.1	12.55	6.16	12.55	2601.7	0.608	0.769
PIZOF-2	3.9	0.6	83.9	17.81	10.25	17.81	2064.1	0.551	0.826
CPM-99H2	2.7	0.9	87.9	22.40	8.37	21.74	4694.8	0.785	1.979
UiO-68-C=O	2.8	0.8	88.2	16.88	8.72	16.87	4092.5	0.742	1.474
Zr6-SDC-Br2	3.0	0.7	88.1	14.65	6.50	14.65	2928.2	0.653	0.835
BINAP-MOF	2.6	0.9	88.2	17.60	6.98	17.60	5595.6	0.717	1.757
Zr6-Cl2AzoBDC	2.9	0.7	87.9	14.24	8.54	14.24	2815.0	0.671	0.984

Structure	S_{CF_4/CH_4}	ΔN_{CF_4} (mol/kg)	R_{CF_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
LIFM-32	2.8	0.8	87.5	13.62	12.39	13.35	2187.9	0.598	0.722
LMOF-1	2.5	0.8	89.3	20.49	8.47	20.49	4720.1	0.780	1.911
UBMOF-8	2.8	0.8	88.7	14.91	8.62	14.91	3686.2	0.717	1.306
UiO-68	2.7	0.8	88.2	17.07	9.31	17.07	4068.9	0.753	1.594
Zr-L6	3.3	0.6	84.6	17.29	9.16	17.29	2093.0	0.567	0.869
Zr6-EDB-Br2	2.9	0.7	87.8	14.82	6.48	14.82	2945.5	0.656	0.833
3D-MOF-D	2.7	0.7	88.5	12.16	9.29	12.15	4143.4	0.728	1.444
PCN-160-imine	2.7	0.7	89.1	14.53	8.28	14.53	3631.1	0.714	1.269
Zr6-AzoBDC	2.7	0.7	89.6	14.40	8.33	14.40	3540.6	0.708	1.215
Zr-L7	3.3	0.5	85.8	18.06	11.02	18.06	1993.9	0.597	0.899
Zrptba	2.5	0.7	89.3	18.73	7.06	18.73	4142.0	0.763	1.643
NU-1101	2.1	0.9	89.3	18.00	7.57	18.00	4783.3	0.740	1.652
Zr-L2	3.0	0.6	86.9	14.84	11.01	14.83	2381.5	0.588	0.946
Zr-TDC	3.2	0.8	74.9	9.81	5.22	9.79	1620.6	0.530	0.488
MOF-1004	2.5	0.7	88.9	28.83	13.66	28.83	4310.1	0.788	2.067
ZrOMTP	2.7	0.6	89.2	18.72	7.16	18.72	3037.2	0.703	1.204
UBMOF-9	2.3	0.6	89.3	15.05	7.26	15.03	3576.3	0.681	1.154
Zrbtba	2.4	0.6	89.0	18.72	7.30	18.72	4466.0	0.770	1.747
BUT-30	2.4	0.6	88.9	15.63	8.89	15.63	3850.3	0.728	1.375
BPHV-MOF	2.4	0.6	89.0	14.39	9.02	14.39	4552.2	0.773	1.724
LIFM-29	2.7	0.6	83.4	11.59	10.02	11.59	1839.9	0.543	0.564
TPHN-MOF	2.4	0.6	88.6	18.31	9.73	18.31	5064.5	0.799	2.194
Zr-L4	2.9	0.4	87.1	19.05	12.79	19.04	1958.5	0.613	0.963
Zr-L1	2.8	0.5	86.9	19.02	13.46	19.02	2114.8	0.627	1.057
Zr-L3	2.9	0.4	87.3	18.79	12.69	18.79	1983.2	0.607	0.954
PIZOF-1	2.8	0.5	87.3	18.21	10.94	18.21	2144.5	0.606	0.994
Zr-L5	3.0	0.4	86.6	19.03	12.74	19.03	1819.4	0.600	0.880
UiO-67-Br2	2.8	0.4	87.4	10.44	5.25	10.44	1796.1	0.538	0.515
bpyv-MOF	2.2	0.5	89.7	13.71	9.57	13.71	4521.2	0.765	1.652
LIFM-30	2.6	0.4	87.8	11.68	9.75	11.68	1901.9	0.529	0.570
NPF-200	2.1	0.5	89.0	18.35	10.46	18.35	4868.6	0.770	1.975
NU-1103	2.0	0.6	89.1	23.91	11.21	23.91	5639.0	0.840	2.890
NU-1104	2.0	0.6	89.2	25.53	10.66	25.53	5542.1	0.843	2.956
PCN-111	2.1	0.5	89.5	18.84	10.94	18.84	4503.6	0.790	1.966
PCN-704	2.0	0.8	77.0	10.70	8.30	8.73	2432.5	0.577	0.713
LIFM-33	1.9	0.6	87.7	12.56	9.79	12.53	1639.8	0.514	0.561
NU-800	2.1	0.5	89.9	13.68	6.84	13.68	4426.3	0.746	1.295
PCN-230	1.8	0.6	88.7	29.36	14.88	29.36	6807.5	0.877	4.644
nitro-MOF	1.9	0.5	88.7	23.79	13.37	23.75	6054.4	0.865	3.632
Zr-L1-Br4	1.6	0.4	87.8	12.33	9.75	12.33	1635.8	0.519	0.518

Structure	S_{CF_4/CH_4}	ΔN_{CF_4} (mol/kg)	R_{CF_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
MOF-805	1.4	0.7	76.5	9.23	4.80	9.23	1677.5	0.507	0.489
PCN-57	0.8	0.4	89.9	17.81	5.52	17.76	3864.2	0.670	1.243
JLU-Liu35	1.2	0.3	89.1	12.74	7.47	12.73	3186.2	0.616	0.910

GCD: Global Cavity Diameter, PLD: Pore Limiting Diameter, LCD: Largest Cavity Diameter, SA: Surface Area, V_f: Void Fraction, V_p: Pore Volume

Table S2. Separation performance metrics and structural features of the ranked Zr-MOFs for the separation of CH_4/H_2 gas mixture.

Structure	S_{CH_4/H_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
MOF-812	61.6	3.0	70.7	5.80	3.97	5.79	939.8	0.345	0.294
BUT-67	36.7	4.1	82.7	7.96	6.29	7.90	1708.7	0.461	0.501
BUT-66	46.2	3.4	74.7	6.98	6.18	6.98	1311.7	0.406	0.387
Zr-DTDC	44.0	3.1	75.1	8.42	4.02	8.42	1140.1	0.449	0.382
MOF-805	30.7	3.5	82.0	9.23	4.80	9.23	1677.5	0.507	0.489
PCN-700-BDC-BDDC	24.7	3.7	82.2	8.84	7.52	8.84	2353.2	0.542	0.642
LIFM-92	23.0	3.8	83.0	7.97	6.97	7.97	2761.6	0.550	0.689
LIFM-90	21.3	3.8	84.2	7.97	6.96	7.97	2933.4	0.576	0.737
PCN-700-BPDC-TPDC	19.7	3.8	85.1	8.71	6.44	8.71	3122.9	0.602	0.800
PCN-702	19.4	3.8	85.2	8.76	7.54	8.20	3213.6	0.612	0.813
Zr-AbBA	14.8	4.1	84.8	17.87	4.48	17.87	3109.8	0.639	1.094
MOF-525	15.3	3.9	87.3	16.27	4.27	16.27	2586.2	0.641	0.923
PCN-700-NDC-BDDC	20.6	3.7	83.9	8.45	7.68	8.45	2768.5	0.577	0.736
LIFM-94	25.2	3.5	80.7	8.29	7.39	8.29	2190.9	0.507	0.608
DUT-52	23.8	3.3	84.3	9.23	4.42	9.23	2002.4	0.526	0.557
LIFM-82	22.6	3.3	84.2	7.21	6.50	7.21	2366.9	0.548	0.605
PCN-704	20.0	3.4	83.3	10.70	8.30	8.73	2432.5	0.577	0.713
BUT-10	18.7	3.4	84.9	9.55	4.98	9.55	2452.5	0.581	0.679
PCN-700-NDC-TPDC	17.5	3.5	85.2	11.96	6.95	8.29	2971.5	0.613	0.818
PCN-703	18.8	3.4	84.3	10.69	8.20	8.61	2555.0	0.585	0.733
LIFM-78	21.5	3.2	84.1	7.02	6.43	7.00	2307.9	0.555	0.613
Zr-TDC	23.7	3.0	85.4	9.81	5.22	9.79	1620.6	0.530	0.488
LIFM-74	20.9	3.1	84.9	7.08	6.44	7.08	2366.8	0.554	0.611
LIFM-70	23.6	3.0	83.1	6.96	6.41	6.96	2078.0	0.523	0.550
LIFM-83	20.9	3.1	84.7	7.05	6.33	7.05	2385.2	0.548	0.609
LIFM-85	21.6	3.1	84.2	7.14	6.50	7.14	2288.7	0.541	0.591
UiO-67-Me	17.3	3.3	85.5	12.18	5.84	12.18	2473.3	0.583	0.746
LIFM-79	20.3	3.1	84.9	7.29	6.45	7.08	2329.4	0.559	0.621
LIFM-76	21.2	3.1	84.2	6.94	6.36	6.94	2317.5	0.543	0.599
BUT-11	20.2	3.2	83.6	10.25	4.93	10.25	2026.8	0.558	0.616
LIFM-80	19.9	3.1	85.1	7.25	6.45	7.03	2405.6	0.566	0.628
LIFM-75	20.2	3.1	84.7	7.18	6.49	7.13	2346.0	0.553	0.610
LIFM-77	20.8	3.1	84.3	6.99	6.42	6.99	2353.3	0.546	0.602
LIFM-84	20.4	3.1	84.4	7.19	6.45	7.01	2385.5	0.555	0.613
LIFM-71	22.4	2.9	83.1	6.94	6.35	6.94	2135.9	0.527	0.556

Structure	S_{CH_4/H_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
Zr-MTBC	10.9	3.5	87.9	14.54	8.01	13.52	3733.6	0.671	1.154
LIFM-86	20.6	3.0	84.8	7.16	6.63	7.16	2345.4	0.552	0.597
NNU-28	16.8	3.3	83.9	16.54	5.19	16.14	2481.7	0.543	0.746
PCN-700-DOBPDC	18.2	3.1	84.2	11.13	10.18	11.13	2399.5	0.577	0.723
LIFM-72	21.4	2.9	84.1	7.01	6.43	7.01	2190.0	0.527	0.560
PCN-57	11.4	3.5	85.4	17.81	5.52	17.76	3864.2	0.670	1.243
LIFM-73	19.6	3.0	85.0	7.33	6.59	7.13	2337.0	0.557	0.610
PU-1	16.9	3.1	85.2	10.92	6.03	10.92	2683.6	0.543	0.753
PCN-700-BDDC	16.9	3.2	83.4	8.46	8.06	8.46	2895.8	0.597	0.780
UiO-67-BN	19.4	2.7	88.0	11.04	5.27	11.02	1805.6	0.491	0.536
PCN-700-NDC	13.7	3.1	86.9	13.81	13.06	13.80	2901.4	0.654	0.935
NU-1101	8.4	3.4	87.7	18.00	7.57	18.00	4783.3	0.740	1.652
Zr-cca	16.1	2.9	87.5	9.93	5.34	9.89	2445.7	0.590	0.677
MOF-806	14.3	3.0	86.4	12.79	5.94	12.79	2578.5	0.619	0.790
UiO-67Me	13.6	2.9	87.2	10.49	5.24	10.49	2768.2	0.594	0.791
PCN-700-MA	13.2	2.8	86.8	13.64	12.88	13.63	2705.8	0.639	0.875
UiO-67	11.9	2.9	87.8	12.83	5.96	12.83	2966.8	0.638	0.883
PCN-701	13.7	2.9	85.7	13.91	13.24	13.83	2612.8	0.637	0.859
BINAP-MOF	7.0	3.1	88.5	17.60	6.98	17.60	5595.6	0.717	1.757
PCN-133	12.2	2.9	85.1	8.94	7.55	8.94	3224.2	0.663	0.962
PCN-700-BPDC	11.8	2.9	86.2	12.88	12.47	12.88	3030.2	0.663	0.987
NPF-300-8	8.7	3.1	86.5	15.60	10.64	15.52	4018.3	0.741	1.437
UiO-67-NH2	12.6	2.8	87.1	11.52	5.33	11.52	2792.0	0.610	0.811
PCN-56	8.7	3.0	86.6	16.66	7.14	16.66	4230.5	0.707	1.393
LMOF-1	6.3	3.0	88.6	20.49	8.47	20.49	4720.1	0.780	1.911
MOF-535	8.5	2.9	88.4	16.67	5.57	16.67	3557.2	0.712	1.277
NPF-300-2	8.6	2.9	87.0	16.83	11.51	16.82	3913.5	0.725	1.373
NPF-300-5	8.6	2.9	87.3	15.52	8.29	15.52	3822.5	0.720	1.318
DUT-98-op	14.8	2.6	85.1	12.44	9.15	12.44	1812.7	0.574	0.677
HHU-1	22.7	2.0	85.9	8.90	4.43	8.90	1107.9	0.512	0.356
CPM-99H2	6.1	2.9	88.3	22.40	8.37	21.74	4694.8	0.785	1.979
UiO-67-Cl	12.1	2.6	88.0	12.55	6.16	12.55	2601.7	0.608	0.769
UiO-BPYDC	11.1	2.5	88.1	12.44	6.53	12.44	2763.0	0.646	0.867
UiO-68-alkyne	8.8	2.8	85.6	16.62	7.30	16.61	3951.0	0.687	1.298
UiO-68-ol	8.2	2.8	86.7	16.27	7.81	16.27	4091.0	0.713	1.366
PCN-58	10.6	2.7	84.6	12.65	5.89	12.65	3535.7	0.627	1.047
ZrDMTD	8.4	2.7	86.6	16.67	6.69	16.67	3892.2	0.707	1.292

Structure	S_{CH_4/H_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
NU-801	9.4	2.6	88.8	12.04	6.91	11.85	3415.2	0.679	1.031
UiO-68	6.8	2.7	88.3	17.07	9.31	17.07	4068.9	0.753	1.594
LIFM-33	15.6	2.3	85.1	12.56	9.79	12.53	1639.8	0.514	0.561
UiO-68-NH2	7.2	2.7	87.4	17.62	8.85	17.62	4269.9	0.737	1.508
Zrptba	6.4	2.7	88.8	18.73	7.06	18.73	4142.0	0.763	1.643
UiO-68-OH	7.4	2.7	87.6	16.62	7.35	16.62	4192.9	0.737	1.447
NPF-300-6	7.2	2.6	87.7	15.39	10.53	15.39	3904.8	0.751	1.490
PCN-230	3.0	2.9	88.8	29.36	14.88	29.36	6807.5	0.877	4.644
Zr-BTDC	13.4	2.3	85.7	10.84	5.95	10.84	2136.0	0.575	0.626
UBMOF-9	8.3	2.5	88.5	15.05	7.26	15.03	3576.3	0.681	1.154
UiO-NDI	7.7	2.8	84.2	20.99	8.59	20.99	4142.9	0.718	1.560
LIFM-31	12.9	2.3	85.9	13.99	13.15	13.99	2160.1	0.613	0.723
UBMOF-8	7.6	2.5	88.0	14.91	8.62	14.91	3686.2	0.717	1.306
NU-1103	4.0	2.7	89.1	23.91	11.21	23.91	5639.0	0.840	2.890
UiO-68-C=O	6.9	2.5	87.7	16.88	8.72	16.87	4092.5	0.742	1.474
Zrbtba	5.8	2.5	88.6	18.72	7.30	18.72	4466.0	0.770	1.747
LIFM-29	14.7	2.1	85.6	11.59	10.02	11.59	1839.9	0.543	0.564
MOF-1004	5.4	2.6	88.0	28.83	13.66	28.83	4310.1	0.788	2.067
LIFM-32	12.2	2.2	85.6	13.62	12.39	13.35	2187.9	0.598	0.722
NU-1104	3.9	2.6	88.8	25.53	10.66	25.53	5542.1	0.843	2.956
BPHV-MOF	5.7	2.4	89.1	14.39	9.02	14.39	4552.2	0.773	1.724
3D-MOF-D	6.5	2.4	88.6	12.16	9.29	12.15	4143.4	0.728	1.444
NPF-200	5.0	2.5	88.9	18.35	10.46	18.35	4868.6	0.770	1.975
PCN-160-imine	7.3	2.4	88.0	14.53	8.28	14.53	3631.1	0.714	1.269
TPHN-MOF	4.9	2.5	88.3	18.31	9.73	18.31	5064.5	0.799	2.194
Zr6-AzoBDC	7.2	2.2	88.3	14.40	8.33	14.40	3540.6	0.708	1.215
Zr6-Cl2AzoBDC	8.7	2.2	86.9	14.24	8.54	14.24	2815.0	0.671	0.984
bpyv-MOF	5.5	2.3	89.2	13.71	9.57	13.71	4521.2	0.765	1.652
BUT-30	6.6	2.2	87.9	15.63	8.89	15.63	3850.3	0.728	1.375
UiO-66-PDC	20.7	1.8	77.5	8.44	4.30	8.43	1128.6	0.446	0.359
UiO-66	22.1	1.8	74.4	8.56	4.10	8.56	1054.0	0.438	0.358
nitro-MOF	3.1	2.4	89.0	23.79	13.37	23.75	6054.4	0.865	3.632
Zr-L1-Br4	14.3	1.8	84.8	12.33	9.75	12.33	1635.8	0.519	0.518
ZrOMTP	6.5	2.1	89.7	18.72	7.16	18.72	3037.2	0.703	1.204
NU-800	6.4	2.1	89.5	13.68	6.84	13.68	4426.3	0.746	1.295
Zr6-SDC-Br2	9.6	2.0	86.5	14.65	6.50	14.65	2928.2	0.653	0.835
JLU-Liu35	8.3	2.0	87.2	12.74	7.47	12.73	3186.2	0.616	0.910
Zr6-EDB-Br2	9.4	1.9	85.9	14.82	6.48	14.82	2945.5	0.656	0.833

Structure	S_{CH_4/H_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
PCN-111	4.6	2.1	88.2	18.84	10.94	18.84	4503.6	0.790	1.966
Zr-L6	8.3	1.8	86.8	17.29	9.16	17.29	2093.0	0.567	0.869
Zr-L2	7.0	1.8	87.1	14.84	11.01	14.83	2381.5	0.588	0.946
LIFM-30	10.0	1.5	87.9	11.68	9.75	11.68	1901.9	0.529	0.570
PCN-59	13.5	1.9	74.0	14.50	4.28	14.50	2243.6	0.469	0.652
Zr-L1	6.4	1.6	87.5	19.02	13.46	19.02	2114.8	0.627	1.057
PIZOF-1	6.6	1.6	87.6	18.21	10.94	18.21	2144.5	0.606	0.994
Zr-L7	7.0	1.5	86.8	18.06	11.02	18.06	1993.9	0.597	0.899
PIZOF-2	8.0	1.5	85.2	17.81	10.25	17.81	2064.1	0.551	0.826
UiO-67-Br2	8.1	1.3	87.7	10.44	5.25	10.44	1796.1	0.538	0.515
Zr-L4	6.1	1.4	87.4	19.05	12.79	19.04	1958.5	0.613	0.963
Zr-L3	6.2	1.4	87.1	18.79	12.69	18.79	1983.2	0.607	0.954
Zr-L5	6.0	1.3	86.8	19.03	12.74	19.03	1819.4	0.600	0.880
UiO-66-OH	11.8	1.2	75.6	7.65	3.87	7.65	872.9	0.393	0.303
UiO-66-F	11.1	1.1	77.5	7.67	3.92	7.67	892.8	0.398	0.306
Zr6-fBPDC	6.0	0.8	88.7	13.38	3.87	13.38	1490.6	0.515	0.509
UiO-66-NH2	11.3	1.1	72.9	7.64	3.80	7.64	828.2	0.365	0.285

GCD: Global Cavity Diameter, PLD: Pore Limiting Diameter, LCD: Largest Cavity Diameter, SA: Surface Area, V_f: Void Fraction, V_p: Pore Volume

Table S3. Separation performance metrics and structural features of the ranked Zr-MOFs (determined with PACMOF charges) for the separation of CH_4/N_2 gas mixture.

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
BUT-67	4.5	3.6	81.1	7.96	6.29	7.90	1708.7	0.461	0.501
Zr-AbBA	3.4	3.9	84.0	17.87	4.48	17.87	3109.8	0.639	1.094
PCN-702	3.8	3.5	84.5	8.76	7.54	8.20	3213.6	0.612	0.813
MOF-812	6.3	2.6	68.9	5.80	3.97	5.79	939.8	0.345	0.294
PCN-700-BDC-BDDC	4.2	3.3	81.0	8.84	7.52	8.84	2353.2	0.542	0.642
MOF-525	3.2	3.6	86.8	16.27	4.27	16.27	2586.2	0.641	0.923
PCN-700-BPDC-TPDC	3.7	3.5	84.1	8.71	6.44	8.71	3122.9	0.602	0.800
LIFM-90	3.8	3.4	82.9	7.97	6.96	7.97	2933.4	0.576	0.737
PCN-700-NDC-BDDC	3.8	3.4	83.1	8.45	7.68	8.45	2768.5	0.577	0.736
LIFM-92	3.8	3.4	81.6	7.97	6.97	7.97	2761.6	0.550	0.689
BUT-66	5.1	2.9	72.8	6.98	6.18	6.98	1311.7	0.406	0.387
Zr-DTDC	5.2	2.8	73.7	8.42	4.02	8.42	1140.1	0.449	0.382
DUT-52	4.0	3.0	83.2	9.23	4.42	9.23	2002.4	0.526	0.557
PCN-704	3.8	3.2	82.7	10.70	8.30	8.73	2432.5	0.577	0.713
LIFM-82	4.0	3.0	83.0	7.21	6.50	7.21	2366.9	0.548	0.605
PCN-703	3.7	3.2	83.5	10.69	8.20	8.61	2555.0	0.585	0.733
PCN-700-NDC-TPDC	3.5	3.2	84.1	11.96	6.95	8.29	2971.5	0.613	0.818
MOF-805	4.0	3.1	80.5	9.23	4.80	9.23	1677.5	0.507	0.489
PCN-57	3.1	3.4	85.1	17.81	5.52	17.76	3864.2	0.670	1.243
LIFM-78	3.9	2.9	83.4	7.02	6.43	7.00	2307.9	0.555	0.613
UiO-67-Me	3.5	3.1	84.6	12.18	5.84	12.18	2473.3	0.583	0.746
Zr-MTBC	2.8	3.3	87.7	14.54	8.01	13.52	3733.6	0.671	1.154
LIFM-70	4.1	2.8	81.9	6.96	6.41	6.96	2078.0	0.523	0.550
LIFM-83	3.8	2.8	83.4	7.05	6.33	7.05	2385.2	0.548	0.609
LIFM-79	3.8	2.9	83.8	7.29	6.45	7.08	2329.4	0.559	0.621
LIFM-94	3.7	3.1	79.2	8.29	7.39	8.29	2190.9	0.507	0.608
NNU-28	3.5	3.0	83.1	16.54	5.19	16.14	2481.7	0.543	0.746
PCN-700-BDDC	3.5	3.0	83.0	8.46	8.06	8.46	2895.8	0.597	0.780
PCN-700-DOBPDC	3.7	2.9	83.5	11.13	10.18	11.13	2399.5	0.577	0.723
LIFM-74	3.7	2.8	83.5	7.08	6.44	7.08	2366.8	0.554	0.611
Zr-TDC	3.9	2.7	84.3	9.81	5.22	9.79	1620.6	0.530	0.488
LIFM-75	3.7	2.8	83.9	7.18	6.49	7.13	2346.0	0.553	0.610
LIFM-80	3.7	2.8	84.2	7.25	6.45	7.03	2405.6	0.566	0.628
LIFM-77	3.8	2.8	83.3	6.99	6.42	6.99	2353.3	0.546	0.602
LIFM-84	3.7	2.8	83.7	7.19	6.45	7.01	2385.5	0.555	0.613

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
LIFM-76	3.8	2.8	82.8	6.94	6.36	6.94	2317.5	0.543	0.599
LIFM-71	4.0	2.7	82.4	6.94	6.35	6.94	2135.9	0.527	0.556
LIFM-85	3.7	2.8	82.9	7.14	6.50	7.14	2288.7	0.541	0.591
LIFM-86	3.8	2.7	83.5	7.16	6.63	7.16	2345.4	0.552	0.597
LIFM-72	3.9	2.7	83.0	7.01	6.43	7.01	2190.0	0.527	0.560
PU-1	3.4	2.8	84.2	10.92	6.03	10.92	2683.6	0.543	0.753
LIFM-73	3.6	2.7	83.5	7.33	6.59	7.13	2337.0	0.557	0.610
PCN-700-NDC	3.2	2.8	85.9	13.81	13.06	13.80	2901.4	0.654	0.935
BUT-11	3.4	2.8	82.2	10.25	4.93	10.25	2026.8	0.558	0.616
NU-1101	2.5	3.2	87.0	18.00	7.57	18.00	4783.3	0.740	1.652
BUT-10	2.9	3.1	83.6	9.55	4.98	9.55	2452.5	0.581	0.679
Zr-cca	3.3	2.6	86.6	9.93	5.34	9.89	2445.7	0.590	0.677
UiO-67-BN	3.5	2.5	86.8	11.04	5.27	11.02	1805.6	0.491	0.536
UiO-67Me	3.2	2.7	86.3	10.49	5.24	10.49	2768.2	0.594	0.791
PCN-701	3.2	2.7	85.4	13.91	13.24	13.83	2612.8	0.637	0.859
PCN-700-MA	3.2	2.7	86.1	13.64	12.88	13.63	2705.8	0.639	0.875
MOF-806	3.0	2.8	85.7	12.79	5.94	12.79	2578.5	0.619	0.790
BINAP-MOF	2.3	3.0	88.0	17.60	6.98	17.60	5595.6	0.717	1.757
UiO-67	2.9	2.7	87.2	12.83	5.96	12.83	2966.8	0.638	0.883
UiO-67-NH2	3.0	2.6	86.9	11.52	5.33	11.52	2792.0	0.610	0.811
NPF-300-8	2.6	2.9	86.1	15.60	10.64	15.52	4018.3	0.741	1.437
PCN-700-BPDC	3.0	2.7	85.6	12.88	12.47	12.88	3030.2	0.663	0.987
PCN-133	2.9	2.8	84.8	8.94	7.55	8.94	3224.2	0.663	0.962
PCN-56	2.6	2.9	85.9	16.66	7.14	16.66	4230.5	0.707	1.393
NPF-300-2	2.5	2.8	86.5	16.83	11.51	16.82	3913.5	0.725	1.373
NPF-300-5	2.6	2.8	87.2	15.52	8.29	15.52	3822.5	0.720	1.318
MOF-535	2.5	2.8	88.0	16.67	5.57	16.67	3557.2	0.712	1.277
LMOF-1	2.2	2.9	88.3	20.49	8.47	20.49	4720.1	0.780	1.911
UiO-67-Cl	2.9	2.4	87.7	12.55	6.16	12.55	2601.7	0.608	0.769
UiO-68-alkyne	2.6	2.7	85.4	16.62	7.30	16.61	3951.0	0.687	1.298
CPM-99H2	2.1	2.8	87.9	22.40	8.37	21.74	4694.8	0.785	1.979
DUT-98-op	3.2	2.4	84.2	12.44	9.15	12.44	1812.7	0.574	0.677
UiO-68-ol	2.5	2.6	86.4	16.27	7.81	16.27	4091.0	0.713	1.366
LIFM-33	3.5	2.1	84.5	12.56	9.79	12.53	1639.8	0.514	0.561
NU-801	2.6	2.5	88.4	12.04	6.91	11.85	3415.2	0.679	1.031
UiO-68	2.3	2.6	87.9	17.07	9.31	17.07	4068.9	0.753	1.594
UBMOF-9	2.5	2.5	88.3	15.05	7.26	15.03	3576.3	0.681	1.154
ZrDMTD	2.5	2.6	86.1	16.67	6.69	16.67	3892.2	0.707	1.292
UiO-68-NH2	2.4	2.6	86.9	17.62	8.85	17.62	4269.9	0.737	1.508
Zrptba	2.2	2.6	88.5	18.73	7.06	18.73	4142.0	0.763	1.643

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
LIFM-31	3.2	2.1	85.5	13.99	13.15	13.99	2160.1	0.613	0.723
UiO-NDI	2.5	2.6	84.2	20.99	8.59	20.99	4142.9	0.718	1.560
UiO-BPYDC	2.6	2.4	87.2	12.44	6.53	12.44	2763.0	0.646	0.867
UiO-68-OH	2.4	2.5	87.1	16.62	7.35	16.62	4192.9	0.737	1.447
Zr-BTDC	3.1	2.1	85.2	10.84	5.95	10.84	2136.0	0.575	0.626
NPF-300-6	2.4	2.5	87.0	15.39	10.53	15.39	3904.8	0.751	1.490
PCN-230	1.7	2.9	88.4	29.36	14.88	29.36	6807.5	0.877	4.644
HHU-1	3.7	1.8	84.8	8.90	4.43	8.90	1107.9	0.512	0.356
PCN-58	2.5	2.5	83.9	12.65	5.89	12.65	3535.7	0.627	1.047
Zrbtba	2.2	2.5	88.7	18.72	7.30	18.72	4466.0	0.770	1.747
UBMOF-8	2.4	2.4	87.7	14.91	8.62	14.91	3686.2	0.717	1.306
MOF-1004	2.2	2.5	87.8	28.83	13.66	28.83	4310.1	0.788	2.067
LIFM-32	3.0	2.1	85.2	13.62	12.39	13.35	2187.9	0.598	0.722
LIFM-29	3.3	1.9	85.2	11.59	10.02	11.59	1839.9	0.543	0.564
3D-MOF-D	2.2	2.3	88.5	12.16	9.29	12.15	4143.4	0.728	1.444
BPHV-MOF	2.1	2.4	88.9	14.39	9.02	14.39	4552.2	0.773	1.724
NU-1104	1.8	2.5	88.6	25.53	10.66	25.53	5542.1	0.843	2.956
NU-1103	1.8	2.6	88.5	23.91	11.21	23.91	5639.0	0.840	2.890
PCN-160-imine	2.4	2.3	87.6	14.53	8.28	14.53	3631.1	0.714	1.269
UiO-68-C=O	2.2	2.4	87.2	16.88	8.72	16.87	4092.5	0.742	1.474
NPF-200	2.0	2.4	88.7	18.35	10.46	18.35	4868.6	0.770	1.975
TPHN-MOF	2.0	2.4	88.0	18.31	9.73	18.31	5064.5	0.799	2.194
BUT-30	2.3	2.1	87.9	15.63	8.89	15.63	3850.3	0.728	1.375
bpyv-MOF	2.1	2.2	89.1	13.71	9.57	13.71	4521.2	0.765	1.652
Zr-L1-Br4	3.3	1.7	84.0	12.33	9.75	12.33	1635.8	0.519	0.518
ZrOMTP	2.2	2.1	89.6	18.72	7.16	18.72	3037.2	0.703	1.204
Zr6-Cl2AzoBDC	2.4	2.1	86.5	14.24	8.54	14.24	2815.0	0.671	0.984
NU-800	2.2	2.1	89.3	13.68	6.84	13.68	4426.3	0.746	1.295
Zr6-SDC-Br2	2.7	1.9	85.6	14.65	6.50	14.65	2928.2	0.653	0.835
nitro-MOF	1.7	2.4	88.7	23.79	13.37	23.75	6054.4	0.865	3.632
Zr6-AzoBDC	2.1	2.1	87.6	14.40	8.33	14.40	3540.6	0.708	1.215
Zr6-EDB-Br2	2.7	1.8	85.7	14.82	6.48	14.82	2945.5	0.656	0.833
UiO-66	3.9	1.6	72.8	8.56	4.10	8.56	1054.0	0.438	0.358
PCN-111	2.0	2.0	87.9	18.84	10.94	18.84	4503.6	0.790	1.966
JLU-Liu35	2.3	1.9	86.8	12.74	7.47	12.73	3186.2	0.616	0.910
Zr-L2	2.5	1.7	86.7	14.84	11.01	14.83	2381.5	0.588	0.946
UiO-66-PDC	3.5	1.6	75.9	8.44	4.30	8.43	1128.6	0.446	0.359
Zr-L6	2.5	1.7	86.1	17.29	9.16	17.29	2093.0	0.567	0.869
LIFM-30	2.8	1.4	87.4	11.68	9.75	11.68	1901.9	0.529	0.570
UiO-67-Br2	2.9	1.2	87.3	10.44	5.25	10.44	1796.1	0.538	0.515

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
PIZOF-2	2.6	1.5	85.5	17.81	10.25	17.81	2064.1	0.551	0.826
Zr-L1	2.2	1.5	87.2	19.02	13.46	19.02	2114.8	0.627	1.057
PIZOF-1	2.3	1.5	87.1	18.21	10.94	18.21	2144.5	0.606	0.994
Zr-L7	2.3	1.5	86.2	18.06	11.02	18.06	1993.9	0.597	0.899
UiO-66-NH2	4.0	1.0	71.9	7.64	3.80	7.64	828.2	0.365	0.285
Zr-L4	2.3	1.4	87.0	19.05	12.79	19.04	1958.5	0.613	0.963
Zr-L3	2.2	1.3	87.0	18.79	12.69	18.79	1983.2	0.607	0.954
UiO-66-OH	3.5	1.0	73.6	7.65	3.87	7.65	872.9	0.393	0.303
Zr-L5	2.1	1.2	86.5	19.03	12.74	19.03	1819.4	0.600	0.880
Zr6-fBPDC	2.2	0.8	88.4	13.38	3.87	13.38	1490.6	0.515	0.509
PCN-59	1.5	1.4	71.2	14.50	4.28	14.50	2243.6	0.469	0.652
UiO-66-F	1.7	1.0	76.2	7.67	3.92	7.67	892.8	0.398	0.306

GCD: Global Cavity Diameter, PLD: Pore Limiting Diameter, LCD: Largest Cavity Diameter, SA: Surface Area, V_f: Void Fraction, V_p: Pore Volume

Table S4. Separation performance metrics and structural features of the ranked Zr-MOFs (determined with EQeq charges) for the separation of CH_4/N_2 gas mixture.

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
BUT-67	4.7	3.6	81.1	7.96	6.29	7.90	1708.7	0.461	0.501
MOF-812	6.6	2.7	68.9	5.80	3.97	5.79	939.8	0.345	0.294
Zr-AbBA	3.4	3.8	83.9	17.87	4.48	17.87	3109.8	0.639	1.094
PCN-700-BPDC-TPDC	3.7	3.5	84.3	8.71	6.44	8.71	3122.9	0.602	0.800
MOF-525	3.2	3.6	86.6	16.27	4.27	16.27	2586.2	0.641	0.923
LIFM-90	3.8	3.4	83.0	7.97	6.96	7.97	2933.4	0.576	0.737
MOF-805	4.4	3.1	80.7	9.23	4.80	9.23	1677.5	0.507	0.489
PCN-702	3.6	3.5	83.9	8.76	7.54	8.20	3213.6	0.612	0.813
LIFM-92	3.9	3.4	81.4	7.97	6.97	7.97	2761.6	0.550	0.689
BUT-66	5.2	2.9	73.1	6.98	6.18	6.98	1311.7	0.406	0.387
PCN-700-BDC-BDDC	4.0	3.3	80.6	8.84	7.52	8.84	2353.2	0.542	0.642
PCN-700-NDC-BDDC	3.7	3.3	82.9	8.45	7.68	8.45	2768.5	0.577	0.736
LIFM-94	4.2	3.1	79.4	8.29	7.39	8.29	2190.9	0.507	0.608
Zr-DTDC	5.2	2.8	73.6	8.42	4.02	8.42	1140.1	0.449	0.382
PCN-703	3.7	3.2	83.5	10.69	8.20	8.61	2555.0	0.585	0.733
PCN-700-NDC-TPDC	3.5	3.2	84.1	11.96	6.95	8.29	2971.5	0.613	0.818
PCN-704	3.8	3.2	82.6	10.70	8.30	8.73	2432.5	0.577	0.713
DUT-52	3.9	3.0	83.1	9.23	4.42	9.23	2002.4	0.526	0.557
PCN-57	3.1	3.3	84.4	17.81	5.52	17.76	3864.2	0.670	1.243
Zr-MTBC	2.8	3.3	87.5	14.54	8.01	13.52	3733.6	0.671	1.154
UiO-67-Me	3.5	3.1	84.8	12.18	5.84	12.18	2473.3	0.583	0.746
BUT-10	3.5	3.1	83.7	9.55	4.98	9.55	2452.5	0.581	0.679
NNU-28	3.5	3.0	83.2	16.54	5.19	16.14	2481.7	0.543	0.746
PCN-700-BDDC	3.5	3.0	82.9	8.46	8.06	8.46	2895.8	0.597	0.780
PCN-700-DOBPDC	3.7	2.9	83.2	11.13	10.18	11.13	2399.5	0.577	0.723
LIFM-82	3.5	3.0	83.0	7.21	6.50	7.21	2366.9	0.548	0.605
BUT-11	3.7	2.9	82.3	10.25	4.93	10.25	2026.8	0.558	0.616
Zr-TDC	3.8	2.6	84.1	9.81	5.22	9.79	1620.6	0.530	0.488
NU-1101	2.6	3.2	87.0	18.00	7.57	18.00	4783.3	0.740	1.652
LIFM-78	3.5	2.9	83.2	7.02	6.43	7.00	2307.9	0.555	0.613
PU-1	3.4	2.8	84.0	10.92	6.03	10.92	2683.6	0.543	0.753
PCN-700-NDC	3.2	2.8	85.8	13.81	13.06	13.80	2901.4	0.654	0.935
LIFM-79	3.4	2.8	83.9	7.29	6.45	7.08	2329.4	0.559	0.621
LIFM-74	3.4	2.8	83.6	7.08	6.44	7.08	2366.8	0.554	0.611
LIFM-83	3.4	2.8	83.3	7.05	6.33	7.05	2385.2	0.548	0.609

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
LIFM-80	3.3	2.8	84.1	7.25	6.45	7.03	2405.6	0.566	0.628
LIFM-85	3.4	2.8	82.8	7.14	6.50	7.14	2288.7	0.541	0.591
LIFM-84	3.3	2.8	83.6	7.19	6.45	7.01	2385.5	0.555	0.613
LIFM-75	3.3	2.8	83.6	7.18	6.49	7.13	2346.0	0.553	0.610
LIFM-70	3.5	2.7	81.8	6.96	6.41	6.96	2078.0	0.523	0.550
Zr-cca	3.3	2.7	86.8	9.93	5.34	9.89	2445.7	0.590	0.677
MOF-806	3.1	2.8	85.8	12.79	5.94	12.79	2578.5	0.619	0.790
LIFM-77	3.4	2.8	83.1	6.99	6.42	6.99	2353.3	0.546	0.602
LIFM-76	3.4	2.8	82.8	6.94	6.36	6.94	2317.5	0.543	0.599
UiO-67Me	3.1	2.7	86.4	10.49	5.24	10.49	2768.2	0.594	0.791
PCN-701	3.2	2.7	85.2	13.91	13.24	13.83	2612.8	0.637	0.859
BINAP-MOF	2.4	3.0	88.1	17.60	6.98	17.60	5595.6	0.717	1.757
UiO-67-BN	3.5	2.5	86.9	11.04	5.27	11.02	1805.6	0.491	0.536
LIFM-86	3.3	2.7	83.6	7.16	6.63	7.16	2345.4	0.552	0.597
LIFM-71	3.4	2.7	82.3	6.94	6.35	6.94	2135.9	0.527	0.556
PCN-700-MA	3.2	2.6	85.9	13.64	12.88	13.63	2705.8	0.639	0.875
PCN-133	3.0	2.8	85.0	8.94	7.55	8.94	3224.2	0.663	0.962
LIFM-72	3.4	2.6	82.8	7.01	6.43	7.01	2190.0	0.527	0.560
UiO-67	2.9	2.7	87.2	12.83	5.96	12.83	2966.8	0.638	0.883
LIFM-73	3.2	2.7	83.5	7.33	6.59	7.13	2337.0	0.557	0.610
PCN-56	2.7	2.9	86.2	16.66	7.14	16.66	4230.5	0.707	1.393
NPF-300-8	2.6	2.9	86.0	15.60	10.64	15.52	4018.3	0.741	1.437
PCN-700-BPDC	3.0	2.7	85.9	12.88	12.47	12.88	3030.2	0.663	0.987
UiO-67-NH2	3.0	2.6	86.7	11.52	5.33	11.52	2792.0	0.610	0.811
NPF-300-2	2.6	2.8	86.6	16.83	11.51	16.82	3913.5	0.725	1.373
MOF-535	2.5	2.8	88.0	16.67	5.57	16.67	3557.2	0.712	1.277
LMOF-1	2.2	2.9	88.4	20.49	8.47	20.49	4720.1	0.780	1.911
NPF-300-5	2.6	2.7	86.9	15.52	8.29	15.52	3822.5	0.720	1.318
CPM-99H2	2.2	2.9	88.2	22.40	8.37	21.74	4694.8	0.785	1.979
UiO-68-alkyne	2.6	2.7	85.5	16.62	7.30	16.61	3951.0	0.687	1.298
PCN-58	3.0	2.5	84.0	12.65	5.89	12.65	3535.7	0.627	1.047
UiO-67-Cl	2.9	2.4	87.7	12.55	6.16	12.55	2601.7	0.608	0.769
DUT-98-op	3.2	2.3	83.9	12.44	9.15	12.44	1812.7	0.574	0.677
UiO-68-ol	2.5	2.6	86.1	16.27	7.81	16.27	4091.0	0.713	1.366
ZrDMTD	2.6	2.6	86.0	16.67	6.69	16.67	3892.2	0.707	1.292
UiO-BPYDC	2.8	2.4	87.4	12.44	6.53	12.44	2763.0	0.646	0.867
NU-801	2.6	2.5	88.4	12.04	6.91	11.85	3415.2	0.679	1.031
UiO-68	2.3	2.6	87.7	17.07	9.31	17.07	4068.9	0.753	1.594
UiO-NDI	2.6	2.6	84.2	20.99	8.59	20.99	4142.9	0.718	1.560
UBMOF-9	2.5	2.4	88.1	15.05	7.26	15.03	3576.3	0.681	1.154

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
UiO-68-NH2	2.4	2.6	86.9	17.62	8.85	17.62	4269.9	0.737	1.508
Zrptba	2.2	2.6	88.5	18.73	7.06	18.73	4142.0	0.763	1.643
UiO-68-OH	2.4	2.5	87.1	16.62	7.35	16.62	4192.9	0.737	1.447
PCN-230	1.7	2.9	88.4	29.36	14.88	29.36	6807.5	0.877	4.644
NPF-300-6	2.4	2.5	86.9	15.39	10.53	15.39	3904.8	0.751	1.490
Zr-BTDC	3.1	2.1	85.2	10.84	5.95	10.84	2136.0	0.575	0.626
UBMOF-8	2.4	2.4	87.8	14.91	8.62	14.91	3686.2	0.717	1.306
MOF-1004	2.2	2.5	87.8	28.83	13.66	28.83	4310.1	0.788	2.067
Zrbtba	2.1	2.5	88.7	18.72	7.30	18.72	4466.0	0.770	1.747
UiO-68-C=O	2.3	2.4	87.1	16.88	8.72	16.87	4092.5	0.742	1.474
LIFM-33	3.0	2.1	84.5	12.56	9.79	12.53	1639.8	0.514	0.561
PCN-160-imine	2.4	2.3	87.7	14.53	8.28	14.53	3631.1	0.714	1.269
NU-1103	1.9	2.6	88.6	23.91	11.21	23.91	5639.0	0.840	2.890
BPHV-MOF	2.1	2.4	89.0	14.39	9.02	14.39	4552.2	0.773	1.724
3D-MOF-D	2.2	2.3	88.4	12.16	9.29	12.15	4143.4	0.728	1.444
NU-1104	1.8	2.5	88.7	25.53	10.66	25.53	5542.1	0.843	2.956
HHU-1	3.4	1.8	85.0	8.90	4.43	8.90	1107.9	0.512	0.356
NPF-200	2.0	2.4	88.7	18.35	10.46	18.35	4868.6	0.770	1.975
TPHN-MOF	2.1	2.4	87.9	18.31	9.73	18.31	5064.5	0.799	2.194
LIFM-31	2.7	2.1	85.4	13.99	13.15	13.99	2160.1	0.613	0.723
Zr6-AzoBDC	2.4	2.1	87.9	14.40	8.33	14.40	3540.6	0.708	1.215
BUT-30	2.3	2.2	88.1	15.63	8.89	15.63	3850.3	0.728	1.375
Zr6-Cl2AzoBDC	2.6	2.1	86.6	14.24	8.54	14.24	2815.0	0.671	0.984
bpyv-MOF	2.1	2.2	89.1	13.71	9.57	13.71	4521.2	0.765	1.652
LIFM-29	2.9	1.9	84.8	11.59	10.02	11.59	1839.9	0.543	0.564
LIFM-32	2.6	2.0	84.8	13.62	12.39	13.35	2187.9	0.598	0.722
NU-800	2.2	2.1	89.4	13.68	6.84	13.68	4426.3	0.746	1.295
ZrOMTP	2.2	2.1	89.5	18.72	7.16	18.72	3037.2	0.703	1.204
Zr-L1-Br4	3.2	1.7	84.3	12.33	9.75	12.33	1635.8	0.519	0.518
JLU-Liu35	2.5	1.9	87.1	12.74	7.47	12.73	3186.2	0.616	0.910
nitro-MOF	1.7	2.4	88.7	23.79	13.37	23.75	6054.4	0.865	3.632
Zr6-SDC-Br2	2.7	1.9	85.5	14.65	6.50	14.65	2928.2	0.653	0.835
PCN-59	3.8	1.7	73.4	14.50	4.28	14.50	2243.6	0.469	0.652
Zr6-EDB-Br2	2.7	1.8	85.4	14.82	6.48	14.82	2945.5	0.656	0.833
PCN-111	2.0	2.1	88.1	18.84	10.94	18.84	4503.6	0.790	1.966
UiO-66	3.8	1.6	73.0	8.56	4.10	8.56	1054.0	0.438	0.358
UiO-66-PDC	3.7	1.6	75.9	8.44	4.30	8.43	1128.6	0.446	0.359
Zr-L6	2.5	1.7	86.3	17.29	9.16	17.29	2093.0	0.567	0.869
Zr-L2	2.5	1.7	86.7	14.84	11.01	14.83	2381.5	0.588	0.946
UiO-67-Br2	2.9	1.2	87.3	10.44	5.25	10.44	1796.1	0.538	0.515

Structure	S_{CH_4/N_2}	ΔN_{CH_4} (mol/kg)	R_{CH_4} (%)	GCD (Å)	PLD (Å)	LCD (Å)	SA (m^2/g)	V_f	V_p (cm^3/g)
Zr-L1	2.3	1.6	87.4	19.02	13.46	19.02	2114.8	0.627	1.057
PIZOF-2	2.6	1.5	85.2	17.81	10.25	17.81	2064.1	0.551	0.826
PIZOF-1	2.3	1.5	87.0	18.21	10.94	18.21	2144.5	0.606	0.994
Zr-L7	2.4	1.5	86.2	18.06	11.02	18.06	1993.9	0.597	0.899
LIFM-30	2.3	1.4	87.2	11.68	9.75	11.68	1901.9	0.529	0.570
UiO-66-OH	3.8	1.0	74.0	7.65	3.87	7.65	872.9	0.393	0.303
UiO-66-NH2	4.0	1.0	71.5	7.64	3.80	7.64	828.2	0.365	0.285
Zr-L4	2.2	1.4	87.0	19.05	12.79	19.04	1958.5	0.613	0.963
Zr-L3	2.2	1.3	87.0	18.79	12.69	18.79	1983.2	0.607	0.954
Zr-L5	2.1	1.2	86.6	19.03	12.74	19.03	1819.4	0.600	0.880
Zr6-fBPDC	1.9	0.8	88.2	13.38	3.87	13.38	1490.6	0.515	0.509
UiO-66-F	1.6	1.0	75.8	7.67	3.92	7.67	892.8	0.398	0.306

GCD: Global Cavity Diameter, PLD: Pore Limiting Diameter, LCD: Largest Cavity Diameter, SA: Surface Area, V_f: Void Fraction, V_p: Pore Volume