

Supplementary Information

Computational Screening of Metal-Organic Frameworks for Biogas Purification

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Table S1. Selectivity data for 40 MOFs used in the third stage of the screening.

MOF	$S_{\text{CO}_2/\text{CH}_4}$	$S_{\text{N}_2/\text{CH}_4}$	$S_{\text{H}_2\text{S}/\text{CH}_4}$	$S_{\text{NH}_3/\text{CH}_4}$
ACUTOI_clean	3.3E+01	1.2E-01	8.0E+02	3.0E+03
ARUYES_clean	4.6E+01	1.7E-01	7.6E+02	4.2E+03
CADQOP_clean	1.2E+01	2.2E-01	5.5E+01	1.2E+03
COYTEQ_clean	2.1E+02	3.4E-01	1.5E+02	1.0E+04
COYTIU_clean	3.3E+02	4.0E-01	1.6E+02	1.7E+04
DAPXID_ion_b	1.4E+01	4.1E-01	5.8E+01	2.4E+03
EGELUY01_manual	6.9E+01	1.9E-01	1.1E+03	9.6E+03
EJEGOQ_clean	1.1E+01	4.0E-01	7.1E+01	6.6E+03
ELIJOZ_clean	4.4E+01	1.5E-01	9.6E+01	3.8E+03
EVURAP_clean	4.6E+01	1.3E-01	1.0E+02	4.6E+03
FAFDEX_clean	2.3E+01	2.0E-01	1.7E+03	2.4E+04
FATKUI_clean	7.5E+01	2.7E-01	1.9E+02	1.1E+04
GAMTEU_clean	1.9E+01	1.5E-01	1.3E+02	2.3E+03
GIQXEK_clean	1.8E+01	2.2E-01	4.8E+01	2.2E+03
GIQYEL_clean	1.7E+01	2.2E-01	4.5E+01	2.0E+03
GUPJEG01_clean	3.2E+02	1.3E+00	2.3E+01	8.1E+01
HEDBEZ_clean	1.4E+01	1.9E-01	6.6E+01	2.6E+03
HUCBAJ_charged	1.2E+01	1.1E-01	1.7E+02	1.2E+03
HUZSUR_clean	1.1E+01	2.9E-01	4.5E+01	1.0E+03
HUZSUR01_clean	1.4E+01	2.9E-01	4.5E+01	9.9E+02
IRISAD01_charged	1.2E+02	1.0E+00	2.7E+01	4.8E+01
JIVHIG_clean	1.0E+01	1.4E-01	4.6E+01	9.1E+02
JOSNAG_clean	1.8E+02	5.6E-01	3.2E+01	1.8E+04
JOSNAG01_clean	1.5E+02	5.6E-01	3.0E+01	1.4E+04
KIPJIE_clean	2.0E+01	2.5E-01	7.3E+01	8.1E+02
LOJFOF_clean	1.4E+01	1.4E-01	4.4E+01	6.1E+02
MEJZIM_clean	2.6E+01	1.6E-01	3.1E+01	6.0E+02
MITISIS_charged	6.0E+00	2.7E-01	3.7E+01	6.2E+02
NEXXEV_clean	2.2E+01	2.9E-01	5.2E+01	1.4E+03
NISBEX_clean	2.0E+01	2.1E-01	4.1E+01	1.9E+03
PEJMOI_clean	1.6E+01	2.7E-01	2.0E+01	2.0E+03
QONQEQ_manual	6.0E+01	1.8E-01	9.2E+02	8.2E+03
QUSCAJ_clean	3.6E+01	1.6E-01	5.7E+02	9.9E+03
SAKNOJ_clean	4.1E+00	2.8E-01	1.7E+01	1.3E+02
VODSEM_clean	2.4E+01	2.7E-01	2.0E+02	1.4E+04
WASTUG_clean	2.4E+01	4.3E-01	7.0E+01	5.4E+03
XICNOO01_clean	1.0E+01	3.6E-01	6.5E+01	3.3E+03
XOTXAG_clean	8.9E+01	2.5E-01	2.9E+02	1.5E+04
ZIMJOW_clean	2.2E+01	2.1E-01	7.0E+01	2.9E+03
ZUQVOW_charged	5.3E+01	4.1E-01	1.3E+02	8.3E+03

$S_{1/2}$ = Selectivity of species 1 over species 2

Table S2. Working capacities for 40 MOFs used in the third stage of the screening.

MOF	ΔQ_{CO_2} (mol/kg)	ΔQ_{N_2} (mol/kg)	$\Delta Q_{\text{H}_2\text{S}}$ (mol/kg)	ΔQ_{NH_3} (mol/kg)
ACUTOI_clean	2.8E-01	3.1E-05	9.8E-02	2.0E-01
ARUYES_clean	3.5E-01	2.0E-04	3.6E-01	7.2E-01
CADQOP_clean	2.7E+00	2.8E-03	2.8E-01	1.1E+00
COYTEQ_clean	5.4E-01	5.3E-05	1.2E-02	8.2E-03
COYTIU_clean	3.1E-01	5.7E-05	8.7E-03	2.6E-01
DAPXID_ion_b	1.7E+00	3.4E-03	1.6E-01	1.5E+00
EGELUY01_manual	6.8E-01	1.9E-04	3.1E-01	1.3E+00
EJEGOQ_clean	1.4E-01	4.3E-04	2.4E-02	2.6E-01
ELIJOZ_clean	6.5E-01	1.0E-04	3.4E-02	1.3E-01
EVURAP_clean	3.0E-01	4.2E-05	3.0E-02	1.9E-01
FAFDEX_clean	5.1E-02	3.7E-05	1.7E-01	7.2E-01
FATKUI_clean	5.1E-01	1.8E-04	4.8E-02	2.8E-01
GAMTEU_clean	8.0E-01	3.5E-04	9.5E-02	6.8E-02
GIQXEK_clean	1.4E+00	1.2E-03	9.3E-02	9.6E-02
GIQYEL_clean	1.5E+00	1.2E-03	9.7E-02	1.7E+00
GUPJEG01_clean	1.0E+00	2.9E-04	1.8E-03	6.5E-03
HEDBEZ_clean	7.5E-01	6.0E-04	7.6E-02	1.9E-01
HUCBAJ_charged	1.3E+00	6.9E-04	1.3E-01	6.0E-01
HUZZUR_clean	1.7E+00	3.4E-03	1.6E-01	8.2E-01
HUZZUR01_clean	2.3E+00	4.1E-03	2.0E-01	8.6E-01
IRISAD01_charged	1.8E+00	1.0E-03	9.6E-03	1.7E-02
JIVHIG_clean	1.1E+00	9.5E-04	1.3E-01	8.3E-01
JOSNAG_clean	1.0E+00	1.9E-04	4.1E-03	4.1E-01
JOSNAG01_clean	1.0E+00	2.2E-04	4.5E-03	2.2E-01
KIPJIE_clean	1.2E+00	1.1E-03	1.2E-01	1.7E-01
LOJFOF_clean	1.3E+00	1.1E-03	1.4E-01	3.4E-01
MEJZIM_clean	7.7E-01	3.8E-04	2.8E-02	1.1E-01
MITSES_charged	1.6E+00	4.7E-03	2.1E-01	1.0E+00
NEXXEV_clean	2.9E+00	4.8E-03	2.1E-01	9.4E-01
NISBEX_clean	8.5E-01	5.7E-04	3.9E-02	5.3E-01
PEJMOI_clean	4.3E-01	1.1E-03	2.8E-02	0.0E+00
QONQEQ_manual	5.3E-01	4.4E-05	3.0E-01	1.9E+00
QUSCAJ_clean	2.9E-02	2.0E-04	2.4E-01	1.6E+00
SAKNOJ_clean	1.8E+00	8.0E-03	1.7E-01	3.5E-01
VODSEM_clean	4.2E-01	4.3E-04	1.1E-01	9.4E-01
WASTUG_clean	9.1E-01	1.3E-03	6.7E-02	1.1E+00
XICNOO01_clean	1.2E+00	2.9E-03	1.0E-01	1.3E+00
XOTXAG_clean	2.1E-01	1.1E-04	4.5E-02	4.9E-01
ZIMJOW_clean	6.6E-01	3.9E-04	4.5E-02	3.0E-01
ZUQVOW_charged	2.5E+00	1.2E-03	1.2E-01	2.5E+00

ΔQ_1 = Working capacity of species 1

Table S3. Regenerability of 40 MOFs used in the third stage of the screening.

MOF	R _{CO₂}	R _{N₂}	R _{H₂S}	R _{NH₃}
ACUTOI_clean	2.5E+01	1.2E+01	1.7E+01	8.7E+00
ARUYES_clean	1.5E+01	3.5E+01	4.3E+01	1.6E+01
CADQOP_clean	8.3E+01	7.2E+01	8.4E+01	1.5E+01
COYTEQ_clean	2.7E+01	2.5E+01	3.8E+01	3.8E-01
COYTIU_clean	1.5E+01	3.6E+01	4.2E+01	1.1E+01
DAPXID_ion_b	8.7E+01	8.7E+01	8.7E+01	1.9E+01
EGELUY01_manual	1.8E+01	2.8E+01	2.2E+01	1.1E+01
EJEGOQ_clean	7.1E+01	8.5E+01	8.3E+01	9.6E+00
ELIJOZ_clean	2.7E+01	1.8E+01	2.9E+01	2.8E+00
EVURAP_clean	1.5E+01	1.1E+01	3.0E+01	4.2E+00
FAFDEX_clean	1.9E+01	2.5E+01	3.8E+01	1.2E+01
FATKUI_clean	3.9E+01	5.7E+01	6.5E+01	6.4E+00
GAMTEU_clean	4.2E+01	3.5E+01	3.3E+01	1.3E+00
GIQXEK_clean	7.2E+01	7.3E+01	7.9E+01	1.8E+00
GIQYEL_clean	8.2E+01	7.7E+01	8.9E+01	3.5E+01
GUPJEG01_clean	7.5E+01	7.8E+01	8.3E+01	8.4E+01
HEDBEZ_clean	6.4E+01	5.7E+01	6.2E+01	3.9E+00
HUCBAJ_charged	4.3E+01	3.9E+01	1.4E+01	9.5E+00
HUZSUR_clean	7.4E+01	8.4E+01	7.6E+01	1.7E+01
HUZSUR01_clean	6.2E+01	8.3E+01	7.7E+01	1.5E+01
IRISAD01_charged	8.4E+01	8.4E+01	9.0E+01	9.0E+01
JIVHIG_clean	6.0E+01	5.6E+01	7.0E+01	2.2E+01
JOSNAG_clean	6.7E+01	6.2E+01	6.8E+01	1.2E+01
JOSNAG01_clean	6.6E+01	5.9E+01	6.9E+01	7.0E+00
KIPJIE_clean	6.8E+01	7.8E+01	8.7E+01	1.1E+01
LOJFOF_clean	4.4E+01	5.4E+01	6.7E+01	1.2E+01
MEJZIM_clean	5.8E+01	6.9E+01	7.8E+01	1.5E+01
MIT SIS_charged	8.7E+01	8.7E+01	8.4E+01	2.5E+01
NEXXEV_clean	4.3E+01	8.1E+01	5.9E+01	1.0E+01
NISBEX_clean	7.7E+01	7.5E+01	7.7E+01	2.2E+01
PEJMOI_clean	3.7E+01	8.2E+01	8.5E+01	0.0E+00
QONQEQ_manual	1.4E+01	5.9E+00	2.4E+01	1.7E+01
QUSCAJ_clean	2.0E+00	4.6E+01	4.7E+01	1.8E+01
SAKNOJ_clean	8.8E+01	8.7E+01	9.0E+01	2.4E+01
VODSEM_clean	5.6E+01	7.6E+01	8.3E+01	9.7E+00
WASTUG_clean	7.3E+01	8.6E+01	8.1E+01	1.7E+01
XICNOO01_clean	8.4E+01	8.7E+01	5.1E+01	1.3E+01
XOTXAG_clean	1.2E+01	3.4E+01	3.7E+01	7.6E+00
ZIMJOW_clean	7.3E+01	6.7E+01	7.0E+01	1.1E+01
ZUQVOW_charged	7.5E+01	7.2E+01	6.5E+01	2.2E+01

R₁ = Regenerability of species 1

Table S4. Pore characteristics of 40 MOFs used in the third stage of the screening.

MOF	GCD(Å)	PLD (Å)	LCD (Å)	SA(m ² /g)	Vf	V _p (cm ³ /g)
ACUTOI_clean	5.19	4.54	5.19	548.8	0.245	0.143
ARUYES_clean	5.38	4.58	5.37	1074.4	0.383	0.259
CADQOP_clean	6.72	4.82	6.72	2124.9	0.583	0.532
COYTEQ_clean	3.84	3.38	3.84	570.3	0.261	0.146
COYTIU_clean	3.82	3.33	3.81	544.0	0.263	0.146
DAPXID_ion_b	14.13	12.09	14.13	2445.6	0.620	0.810
EGELUY01_manual	7.46	7.06	7.46	1936.5	0.511	0.539
EJEGOQ_clean	13.13	3.18	13.13	496.5	0.436	0.146
ELIJOZ_clean	5.03	3.85	5.03	937.5	0.345	0.233
EVURAP_clean	4.92	4.01	4.91	866.5	0.333	0.221
FAFDEX_clean	4.85	4.05	4.85	709.9	0.271	0.192
FATKUI_clean	4.72	3.91	4.72	737.5	0.302	0.171
GAMTEU_clean	4.97	3.20	4.97	838.9	0.375	0.263
GIQXEK_clean	5.02	3.94	5.02	1151.8	0.454	0.266
GIQYEL_clean	5.05	3.96	5.05	1181.9	0.459	0.271
GUPJEG01_clean	3.68	3.36	3.68	284.4	0.181	0.116
HEDBEZ_clean	5.55	3.63	5.47	779.8	0.397	0.192
HUCBAJ_charged	5.86	3.90	5.86	1462.4	0.396	0.330
HUZSUR_clean	9.15	7.41	9.12	1933.3	0.473	0.531
HUZSUR01_clean	9.88	8.67	9.87	2132.0	0.510	0.605
IRISAD01_charged	3.59	3.40	3.59	495.9	0.403	0.190
JIVHIG_clean	5.86	3.79	5.86	1070.3	0.260	0.261
JOSNAG_clean	4.32	3.48	4.27	783.6	0.308	0.206
JOSNAG01_clean	4.34	3.49	4.33	824.8	0.316	0.212
KIPJIE_clean	6.99	5.51	6.98	696.8	0.283	0.171
LOJFOF_clean	5.77	5.03	5.76	1082.3	0.295	0.254
MEJZIM_clean	5.33	3.56	5.23	485.1	0.225	0.133
MIT SIS_charged	7.97	6.52	7.97	1812.4	0.529	0.497
NEXXEV_clean	10.14	9.60	10.14	2498.5	0.564	0.804
NISBEX_clean	4.32	3.42	4.32	643.2	0.255	0.177
PEJMOI_clean	7.77	4.72	7.53	774.7	0.340	0.190
QONQEQ_manual	7.41	7.01	7.40	1923.8	0.508	0.538
QUSCAJ_clean	5.41	3.75	5.41	1351.0	0.361	0.308
SAKNOJ_clean	15.48	8.59	15.48	2159.6	0.622	0.752
VODSEM_clean	5.27	4.81	5.27	531.4	0.276	0.160
WASTUG_clean	10.47	7.26	10.01	1318.8	0.597	0.374
XICNOO01_clean	19.50	6.85	19.47	2184.5	0.694	0.763
XOTXAG_clean	4.59	3.72	4.55	1093.7	0.322	0.221
ZIMJOW_clean	4.93	3.18	4.93	666.2	0.279	0.164
ZUQVOW_charged	5.73	3.64	5.73	3307.8	0.617	0.665

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

Table S5. MOFs ranked by the product of the selectivities for CO₂, H₂S, and NH₃ over CH₄.

MOF	Ranking
FAFDEX_clean	1
COYTIU_clean	2
EGELUY01_manual	3
QONQEQ_manual	4
XOTXAG_clean	5
COYTEQ_clean	6
QUSCAJ_clean	7
FATKUI_clean	8
ARUYES_clean	9
JOSNAG_clean	10
ACUTOI_clean	11
VODSEM_clean	12
JOSNAG01_clean	13
ZUQVOW_charged	14
EVURAP_clean	15
ELIJOS_clean	16
WASTUG_clean	17
GAMTEU_clean	18
EJEGOQ_clean	19
ZIMJOW_clean	20
HUCBAJ_charged	21
HEDBEZ_clean	22
XICNOO01_clean	23
GIQXEK_clean	24
DAPXID_ion_b	25
NISBEX_clean	26
NEXXEV_clean	27
GIQYEL_clean	28
KIPJIE_clean	29
CADQOP_clean	30
PEJMOI_clean	31
HUZZSUR01_clean	32
GUPJEG01_clean	33
HUZZSUR_clean	34
MEJZIM_clean	35
JIVHIG_clean	36
LOJFOF_clean	37
IRISAD01_charged	38
MITSIS_charged	39
SAKNOJ_clean	40

Table S6. MOFs ranked by the weighted sum of working capacities.

MOF	Ranking
NEXXEV_clean	1
CADQOP_clean	2
ZUQVOW_charged	3
HUZZSUR01_clean	4
SAKNOJ_clean	5
DAPXID_ion_b	6
HUZZSUR_clean	7
IRISAD01_charged	8
MITSIS_charged	9
GIQYEL_clean	10
GIQXEK_clean	11
LOJFOF_clean	12
HUCBAJ_charged	13
XICNOO01_clean	14
JIVHIG_clean	15
KIPJIE_clean	16
JOSNAG_clean	17
GUPJEG01_clean	18
JOSNAG01_clean	19
WASTUG_clean	20
NISBEX_clean	21
EGELUY01_manual	22
GAMTEU_clean	23
MEJZIM_clean	24
HEDBEZ_clean	25
QONQEQ_manual	26
ZIMJOW_clean	27
ELIJOS_clean	28
FATKUI_clean	29
COYTEQ_clean	30
VODSEM_clean	31
ARUYES_clean	32
PEJMOI_clean	33
COYTIU_clean	34
EVURAP_clean	35
ACUTOI_clean	36
XOTXAG_clean	37
QUSCAJ_clean	38
EJEGOO_clean	39
FAFDEX_clean	40

Table S7. MOFs ranked by the regenerability criterion.

MOF	Ranking
SAKNOJ_clean	1
IRISAD01_charged	2
GIQYEL_clean	3
MITSIS_charged	4
DAPXID_ion_b	5
GUPJEG01_clean	6
NISBEX_clean	7
CADQOP_clean	8
WASTUG_clean	9
HUZZSUR_clean	10
ZUQVOW_charged	11
KIPJIE_clean	12
JIVHIG_clean	13
XICNOO01_clean	14
MEJZIM_clean	15
HUZZSUR01_clean	16
EJEGOOQ_clean	17
ZIMJOW_clean	18
JOSNAG_clean	19
VODSEM_clean	20
GIQXEK_clean	21
LOJFOF_clean	22
JOSNAG01_clean	23
PEJMOI_clean	24
NEXXEV_clean	25
QUSCAJ_clean	26
ARUYES_clean	27
HEDBEZ_clean	28
FAFDEX_clean	29
FATKUI_clean	30
QONQEQ_manual	31
COYTIU_clean	32
HUCBAJ_charged	33
EGELUY01_manual	34
GAMTEU_clean	35
ACUTOI_clean	36
COYTEQ_clean	37
ELIJOS_clean	38
XOTXAG_clean	39
EVURAP_clean	40

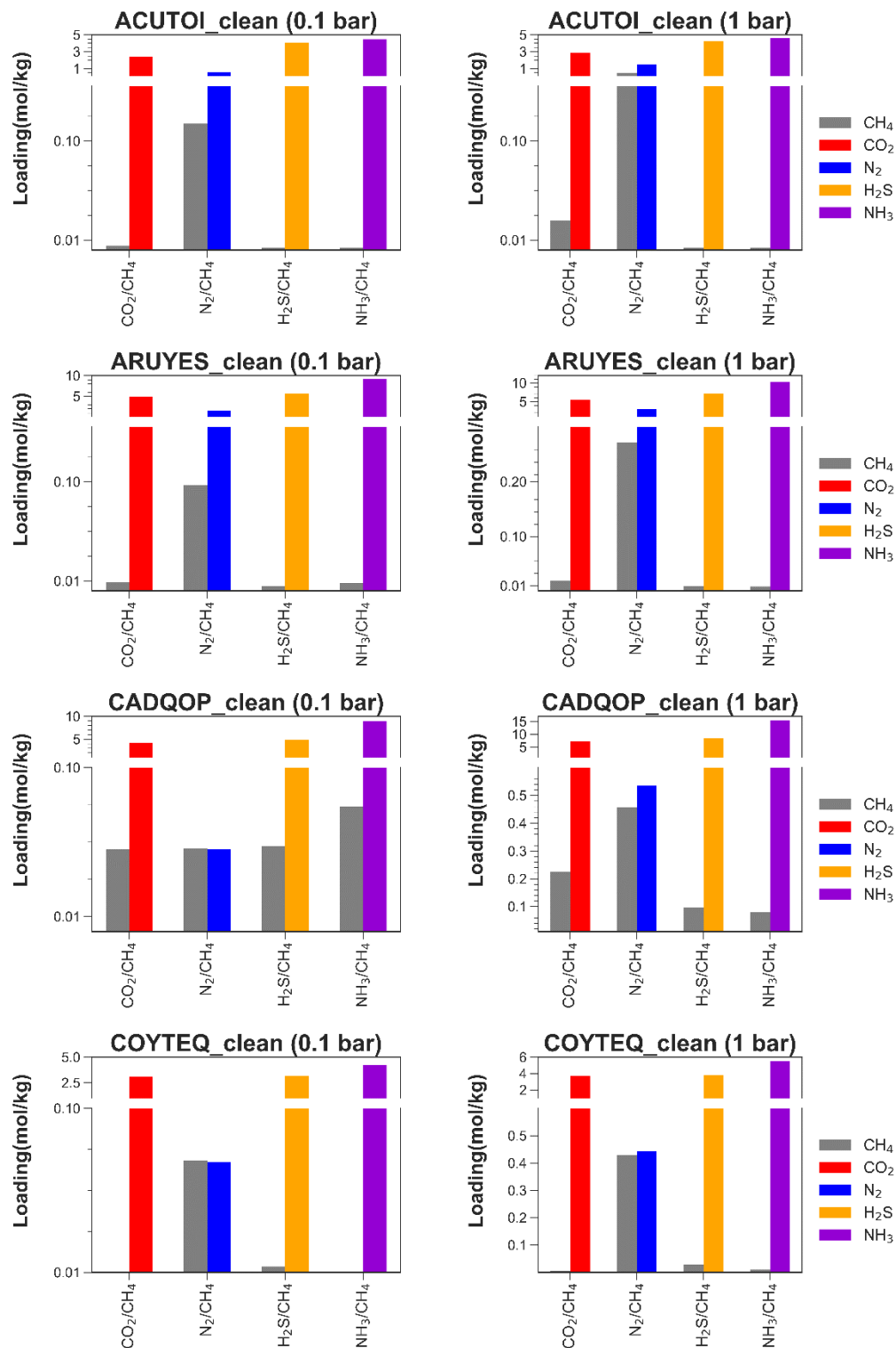


Figure S1. Binary GCMC results for several selected CoRE MOFs.

