

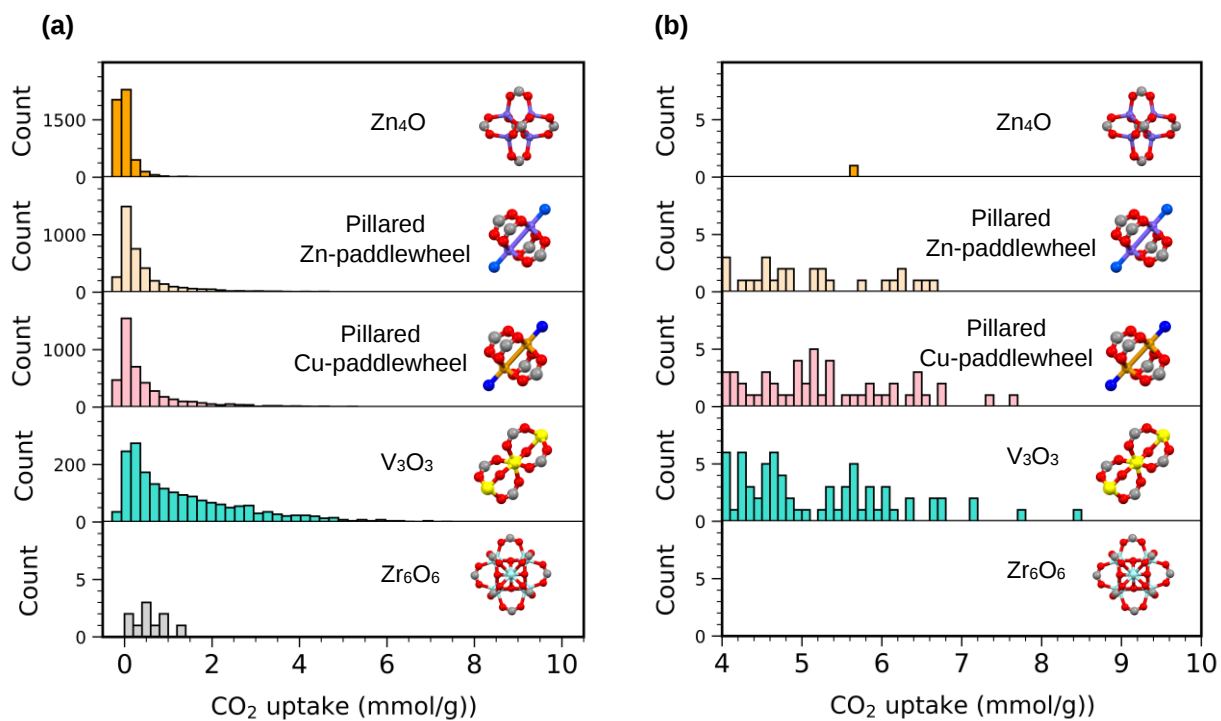
Supplementary information

Integrating stability metrics with high-throughput computational screening of metal–organic frameworks for CO₂ capture

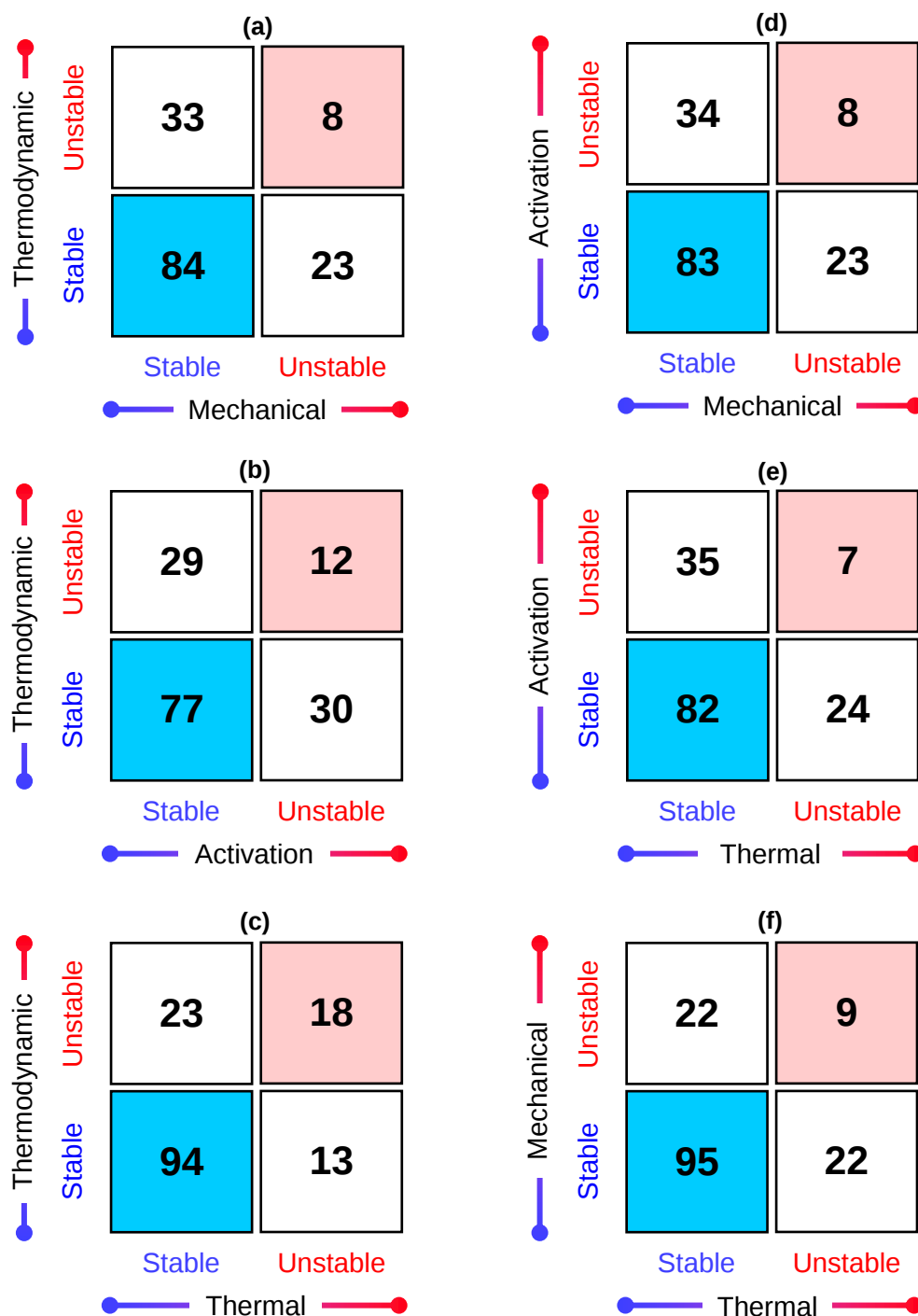
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Supplementary Fig. 1 Count of hMOFs for each metal node type *versus* CO₂ uptake. (a) DB-5 subset (15,219 hMOFs) (b) 148 top-performing hMOFs.



Supplementary Fig. 2 Correlations among stability metrics. (a) thermodynamic stability *versus* mechanical stability, (b) thermodynamic stability *versus* activation stability, (c) thermodynamic stability *versus* thermal stability, (d) activation stability *versus* mechanical stability, (e) activation stability *versus* thermal stability, and (f) mechanical stability *versus* thermal stability. The number indicates the count of hMOFs in each stability measure. The total number in each plot (a) to (f) is 148.

Supplementary Table 1. 51 top-performing stable hMOFs.

ARC-MOF Name	Separation Performance*		Mechanical Stability			Thermodynamic Stability		Activation Stability	Thermal Stability
	CO ₂ uptake (mmol/g)	CO ₂ /N ₂ selectivity	K _H (GPa)	G _H (GPa)	E _H (GPa)	F (kJ/mol)	Δ _{LM} F (kJ/mol)	Score (0.0 → 1.0)	T _d (°C)
DB5-hypotheticalMOF_6003053_0_0_3_16_16_7	7.17	302	16.37	7.77	19.61	20.30	1.52	0.67	427
DB5-hypotheticalMOF_29878_0_0_2_24_2_10	6.72	323	19.58	9.63	24.21	15.27	-1.38	0.94	307
DB5-hypotheticalMOF_1003061_0_0_3_22_10_10	6.64	341	13.43	9.05	21.30	18.97	0.15	0.67	387
DB5-hypotheticalMOF_1002893_0_0_3_22_9_5	6.61	311	18.90	10.78	26.42	21.45	2.58	0.76	305
DB5-hypotheticalMOF_24443_0_0_1_5_9_7	6.52	224	19.45	9.03	22.90	16.46	0.44	0.64	310
DB5-hypotheticalMOF_1003085_0_0_3_22_11_10	6.37	280	14.47	9.34	22.86	18.73	-0.10	0.50	406
DB5-hypotheticalMOF_17181_0_0_1_7_9_10	6.30	317	18.26	8.60	21.95	18.76	3.23	0.60	346
DB5-hypotheticalMOF_24824_0_0_1_5_11_5	6.13	235	14.24	9.10	22.44	18.43	2.55	0.69	301
DB5-hypotheticalMOF_36337_1_0_2_16_2_10	6.08	246	25.01	10.13	25.57	17.05	2.37	0.70	309
DB5-hypotheticalMOF_6004424_0_0_3_27_1_12	6.07	346	23.23	12.08	30.18	16.50	-2.27	0.74	411
DB5-hypotheticalMOF_1002847_0_0_3_16_24_12	6.06	251	13.00	7.28	18.26	15.88	-2.83	0.83	392
DB5-hypotheticalMOF_1001507_0_0_3_11_24_12	5.96	263	13.13	9.12	21.94	15.96	-2.81	0.69	452
DB5-hypotheticalMOF_36346_0_0_2_16_2_12	5.88	339	28.34	11.91	30.04	16.51	0.05	0.92	335
DB5-hypotheticalMOF_25095_0_0_1_14_2_12	5.79	276	12.95	7.47	18.46	13.78	-2.69	0.73	375
DB5-hypotheticalMOF_1003070_0_0_3_22_10_6	5.69	271	15.59	9.16	22.27	20.36	1.47	0.52	356
DB5-hypotheticalMOF_12119_0_0_0_5_1_12	5.62	288	10.34	4.83	12.46	16.34	-0.57	0.70	396
DB5-hypotheticalMOF_6004013_0_0_3_23_5_10	5.52	242	13.28	8.74	21.34	18.54	-0.24	0.63	447
DB5-hypotheticalMOF_6003813_0_0_3_23_7_12	5.48	275	19.97	10.14	25.14	19.67	0.91	0.51	480
DB5-hypotheticalMOF_1003134_0_0_3_22_5_7	5.38	326	22.60	13.27	32.86	21.80	3.03	0.69	388
DB5-hypotheticalMOF_1002857_0_0_3_16_11_12	5.30	243	20.60	10.75	26.70	16.79	-1.98	0.83	380
DB5-hypotheticalMOF_29125_0_0_2_25_7_12	5.24	228	10.35	6.04	14.98	20.95	2.65	0.74	364
DB5-hypotheticalMOF_23758_0_0_1_6_9_9	5.24	266	19.68	8.90	22.71	14.90	-0.73	0.69	323
DB5-hypotheticalMOF_34386_0_0_2_6_2_12	5.06	245	34.65	13.44	34.22	16.05	2.85	0.73	305
DB5-hypotheticalMOF_36097_0_0_2_16_9_12	4.99	209	24.10	9.43	24.09	16.79	-1.09	0.74	376
DB5-hypotheticalMOF_33328_0_0_2_13_9_12	4.95	207	19.17	9.18	23.14	16.70	-0.47	0.66	328
DB5-hypotheticalMOF_24239_0_0_1_6_10_12	4.90	261	14.62	7.90	19.66	15.82	0.21	0.79	390
DB5-hypotheticalMOF_19779_0_0_1_4_2_5	4.81	330	23.44	12.52	31.32	12.73	-3.96	0.83	341
DB5-hypotheticalMOF_6000648_0_0_3_12_22_5	4.78	222	13.69	8.25	20.59	20.96	2.05	0.74	320
DB5-hypotheticalMOF_36707_0_0_2_16_1_14	4.75	392	25.35	13.88	34.64	17.71	1.98	0.89	352
DB5-hypotheticalMOF_1002639_0_0_3_5_21_14	4.72	238	14.56	8.20	20.65	18.00	-0.87	0.59	389
DB5-hypotheticalMOF_1002648_0_0_3_5_25_7	4.71	226	12.77	8.19	20.24	18.88	0.10	0.72	441
DB5-hypotheticalMOF_1003115_0_0_3_22_13_12	4.68	283	14.46	8.00	20.25	18.53	-0.20	0.76	378
DB5-hypotheticalMOF_6004505_1_0_3_27_0_0	4.64	207	24.35	15.38	37.41	18.46	-0.56	0.66	395
DB5-hypotheticalMOF_1002666_0_0_3_5_24_10	4.63	232	16.92	9.86	24.12	18.19	-0.59	0.71	428
DB5-hypotheticalMOF_6002593_0_0_3_20_5_7	4.58	327	21.36	11.63	28.91	21.79	3.03	0.69	362
DB5-hypotheticalMOF_1003086_0_0_3_22_11_14	4.57	206	18.28	9.24	23.02	19.74	0.87	0.60	437
DB5-hypotheticalMOF_23903_0_0_1_6_2_12	4.56	215	25.43	8.76	22.15	14.01	-2.09	0.82	379
DB5-hypotheticalMOF_6000647_0_0_3_12_22_10	4.52	240	13.70	8.24	20.49	18.66	-0.19	0.71	388
DB5-hypotheticalMOF_6004567_0_0_3_27_5_10	4.45	229	21.12	10.98	27.62	18.30	-0.46	0.87	419
DB5-hypotheticalMOF_6004510_0_0_3_27_0_4	4.33	231	25.32	15.88	38.50	17.92	-1.05	0.72	388
DB5-hypotheticalMOF_20634_0_0_1_10_9_14	4.33	229	11.32	7.36	18.09	14.81	-1.07	0.88	388
DB5-hypotheticalMOF_34381_0_0_2_6_2_10	4.30	201	34.61	13.73	34.86	16.46	3.80	0.70	302
DB5-hypotheticalMOF_1002637_0_0_3_5_21_10	4.30	230	22.97	8.90	22.25	16.56	-2.23	0.78	406
DB5-hypotheticalMOF_1000859_0_0_3_1_17_6	4.27	202	11.97	13.71	29.16	18.89	-0.12	0.52	356
DB5-hypotheticalMOF_1002736_0_0_3_5_11_7	4.26	266	26.34	17.53	42.90	21.11	2.24	0.88	374
DB5-hypotheticalMOF_23760_0_0_1_6_9_11	4.24	233	21.55	9.05	22.98	12.41	-3.28	0.85	378
DB5-hypotheticalMOF_1002775_0_0_3_5_13_4	4.24	240	35.00	14.76	37.64	19.43	0.54	0.84	391
DB5-hypotheticalMOF_1001363_0_0_3_11_17_12	4.07	285	29.60	14.22	36.04	17.27	-1.47	0.79	401
DB5-hypotheticalMOF_6002506_0_0_3_20_1_8	4.05	213	17.79	11.93	28.69	19.31	0.40	0.70	325
DB5-hypotheticalMOF_5041966_0_0_1_8_5_0	4.03	219	25.39	10.63	27.32	17.65	1.96	0.81	386
DB5-hypotheticalMOF_1000880_0_0_3_1_26_10	4.03	291	26.93	15.51	38.43	17.62	-1.14	0.75	441

* CO₂ uptake and CO₂/N₂ selectivity at 298 K and 0.9 bar for a mixture of CO₂/N₂ (17%/83%) from the ARC-MOF database.

Supplementary Table 2. Building blocks of 51 top-performing stable hMOFs.

ARC-MOF Name	Metal Node	Primary Linker	Secondary Linker	Functional Group
DB5-hypotheticalMOF_6003053_0_0_3_16_16_7				$R-$
DB5-hypotheticalMOF_29878_0_0_2_24_2_10				$R-$
DB5-hypotheticalMOF_1003061_0_0_3_22_10_10				$R-$
DB5-hypotheticalMOF_1002893_0_0_3_22_9_5				$R-NH_2$
DB5-hypotheticalMOF_24443_0_0_1_5_9_7				$R-$
DB5-hypotheticalMOF_1003085_0_0_3_22_11_10				$R-$
DB5-hypotheticalMOF_17181_0_0_1_7_9_10				$R-$
DB5-hypotheticalMOF_24824_0_0_1_5_11_5				$R-NH_2$
DB5-hypotheticalMOF_36337_1_0_2_16_2_10				$R-$
DB5-hypotheticalMOF_6004424_0_0_3_27_1_12				$R-$
DB5-hypotheticalMOF_1002847_0_0_3_16_24_12				$R-$
DB5-hypotheticalMOF_1001507_0_0_3_11_24_12				$R-$
DB5-hypotheticalMOF_36346_0_0_2_16_2_12				$R-$
DB5-hypotheticalMOF_25095_0_0_1_14_2_12				$R-$
DB5-hypotheticalMOF_1003070_0_0_3_22_10_6				$R-N$
DB5-hypotheticalMOF_12119_0_0_0_5_1_12				$R-$
DB5-hypotheticalMOF_6004013_0_0_3_23_5_10				$R-$
DB5-hypotheticalMOF_6003813_0_0_3_23_7_12				$R-$

DB5-hypotheticalMOF_1003134_0_0_3_22_5_7				
DB5-hypotheticalMOF_1002857_0_0_3_16_11_12				
DB5-hypotheticalMOF_29125_0_0_2_25_7_12				
DB5-hypotheticalMOF_23758_0_0_1_6_9_9				
DB5-hypotheticalMOF_34386_0_0_2_6_2_12				
DB5-hypotheticalMOF_36097_0_0_2_16_9_12				
DB5-hypotheticalMOF_33328_0_0_2_13_9_12				
DB5-hypotheticalMOF_24239_0_0_1_6_10_12				
DB5-hypotheticalMOF_19779_0_0_1_4_2_5				
DB5-hypotheticalMOF_6000648_0_0_3_12_22_5				
DB5-hypotheticalMOF_36707_0_0_2_16_1_14				
DB5-hypotheticalMOF_1002639_0_0_3_5_21_14				
DB5-hypotheticalMOF_1002648_0_0_3_5_25_7				
DB5-hypotheticalMOF_1003115_0_0_3_22_13_12				
DB5-hypotheticalMOF_6004505_1_0_3_27_0_0				
DB5-hypotheticalMOF_1002666_0_0_3_5_24_10				
DB5-hypotheticalMOF_6002593_0_0_3_20_5_7				
DB5-hypotheticalMOF_1003086_0_0_3_22_11_14				
DB5-hypotheticalMOF_23903_0_0_1_6_2_12				

DB5-hypotheticalMOF_6000647_0_0_3_12_22_10				
DB5-hypotheticalMOF_6004567_0_0_3_27_5_10				
DB5-hypotheticalMOF_6004510_0_0_3_27_0_4				
DB5-hypotheticalMOF_20634_0_0_1_10_9_14				
DB5-hypotheticalMOF_34381_0_0_2_6_2_10				
DB5-hypotheticalMOF_1002637_0_0_3_5_21_10				
DB5-hypotheticalMOF_1000859_0_0_3_1_17_6				
DB5-hypotheticalMOF_1002736_0_0_3_5_11_7				
DB5-hypotheticalMOF_23760_0_0_1_6_9_11				
DB5-hypotheticalMOF_1002775_0_0_3_5_13_4				
DB5-hypotheticalMOF_1001363_0_0_3_11_17_12				
DB5-hypotheticalMOF_6002506_0_0_3_20_1_8				
DB5-hypotheticalMOF_5041966_0_0_1_8_5_0				
DB5-hypotheticalMOF_1000880_0_0_3_1_26_10				

A: extension point