Supporting Information:

Predictive framework for shape selective separations in three-dimensional zeolites and metal-organic frameworks

Eric L. First, Chrysanthos E. Gounaris, and Christodoulos A. Floudas*

Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544

E-mail: floudas@titan.princeton.edu

Element data table

The van der Waals radii in Table S1 are from the Cambridge Structural Database (ref. 21 in main text) and the Lennard-Jones coefficients from the Universal Force Field (UFF) (ref. 22 in main text). The Lennard-Jones parameters, ε_i and ε_j, used in Models 1 and 2 are related to the data tabulated in Table S1 by $\varepsilon = (\text{L-J coeff.})R/2$, where R is the gas constant. The division by 2 avoids double-counting in summations over single atoms instead of interacting pairs.

*To whom correspondence should be addressed

Table S1: Elemental radii and Lennard-Jones coefficients

Atomic No.	Element	Radius (Å)	Coeff. (K)	Atomic No.	Element	Radius (Å)	Coeff. (K)
1	H	1.09	22.14	53	I	1.98	170.59
2	He	1.40	28.18	54	Xe	2.16	167.07
3	Li	1.82	12.58	55	Cs	2.00	22.64
4	Be	2.00	42.77	56	Ba	2.00	183.17
5	B	2.00	90.58	57	La	2.00	8.55
6	C	1.70	52.84	58	Ce	2.00	6.54
7	N	1.55	34.72	59	Pr	2.00	5.03
8	O	1.52	30.19	60	Nd	2.00	5.03
9	F	1.47	25.16	61	Pm	2.00	4.53
10	Ne	1.54	21.14	62	Sm	2.00	4.03
11	Na	2.27	15.10	63	Eu	2.00	4.03
12	Mg	1.73	55.86	64	Gd	2.00	4.53
13	Al	2.00	254.12	65	Tb	2.00	3.52
14	Si	2.10	202.29	66	Dy	2.00	3.52
15	P	1.80	153.48	67	Ho	2.00	3.52
16	S	1.80	137.88	68	Er	2.00	3.52
17	Cl	1.75	114.23	69	Tm	2.00	3.02
18	Ar	1.88	93.10	70	Yb	2.00	114.73
19	K	2.75	17.61	71	Lu	2.00	20.63
20	Ca	2.00	119.77	72	Hf	2.00	36.23
21	Sc	2.00	9.56	73	Ta	2.00	40.76
22	Ti	2.00	8.55	74	W	2.00	33.72
23	V	2.00	8.05	75	Re	2.00	33.21
24	Cr	2.00	7.55	76	Os	2.00	18.62
25	Mn	2.00	6.54	77	Ir	2.00	36.73
26	Fe	2.00	6.54	78	Pt	1.72	40.26
27	Co	2.00	7.05	79	Au	1.66	19.63
28	Ni	1.63	7.55	80	Hg	1.55	193.74
29	Cu	1.40	2.52	81	Tl	1.96	342.19
30	Zn	1.39	62.40	82	Pb	2.02	333.63
31	Ga	1.87	208.83	83	Bi	2.00	260.67
32	Ge	2.00	190.72	84	Po	2.00	163.55
33	As	1.85	155.49	85	At	2.00	142.91
34	Se	1.90	146.44	86	Rn	2.00	124.80
35	Br	1.85	126.31	87	Fr	2.00	25.16
36	Kr	2.02	110.71	88	Ra	2.00	203.30
37	Rb	2.00	20.13	89	Ac	2.00	16.61
38	Sr	2.00	118.26	90	Th	2.00	13.08
39	Y	2.00	36.23	91	Pa	2.00	11.07
40	Zr	2.00	34.72	92	U	1.86	11.07
41	Nb	2.00	29.69	93	Np	2.00	9.56
42	Mo	2.00	28.18	94	Pu	2.00	8.05
43	Tc	2.00	24.15	95	Am	2.00	7.05
44	Ru	2.00	28.18	96	Cm	2.00	6.54
45	Rh	2.00	26.67	97	Bk	2.00	6.54
46	Pd	1.63	24.15	98	Cf	2.00	6.54
47	Ag	1.72	18.12	99	Es	2.00	6.04
48	Cd	1.58	114.73	100	Fm	2.00	6.04
49	In	1.93	301.43	101	Md	2.00	5.54
50	Sn	2.17	285.32	102	No	2.00	5.54
51	Sb	2.00	225.94	103	Lr	2.00	5.54
52	Te	2.06	200.28				

Lists of structures studied

Table S2: Zeolites

ABW	ACO	AEI	AEL	AEN	AET	AFG	AFI	AFN	AFO	AFR	AFS
AFT	AFX	AFY	AHT	ANA	APC	APD	AST	ATN	ATO	ATS	ATT
ATV	AWO	AWW	BCT	BEA	BEC	BIK	BOF	BOG	BPH	BRE	CAN
CAS	CDO	CFI	CGF	CGS	CHA	CHI	CLO	CON	DAC	DDR	DFO
DFT	DOH	DON	EAB	EDI	EMT	EON	EPI	ERI	ESV	ETR	EUO
EZT	FAR	FAU	FER	FRA	GIS	GIU	GME	GON	GOO	HEU	IFR
IHW	IMF	IRR	ISV	ITE	ITH	ITR	ITW	IWR	IWS	IWV	IWW
JBW	JRY	JST	KFI	LAU	LEV	LIO	LIT	LOS	LOV	LTA	LTF
LTJ	LTL	LTN	MAR	MAZ	MEI	MEL	MEP	MER	MFI	MFS	MON
MOR	MOZ	MRE	MSE	MSO	MTF	MTN	MTT	MTW	MVY	MWW	NAB
NAT	NES	NON	NPO	NPT	NSI	OBW	OFF	OSI	OSO	OWE	PAR
PAU	PHI	PON	PUN	RHO	RON	RRO	RSN	RTE	RTH	RUT	RWR
RWY	SAF	SAO	SAS	SAT	SAV	SBE	SBN	SBS	SBT	SFE	SFF
SFG	SFH	SFN	SFO	SFS	SFV	SGT	SIV	SOD	SOF	SOS	SSF
SSY	STF	STI	STO	STT	STW	SVR	SZR	TER	THO	TOL	TON
TSC	TUN	UEI	UFI	UOS	USI	UTL	UWY	VET	VFI	VNI	VSV
WEI	WEN	YUG	ZON								

Table S3: MOFs: Crystallography Open Database

1501629	4101542	4103047	4103048	4103258	4103388	4103390	4103958	4104729
4104808	4104809	4104810	4105434	4105439	4105440	4300890	4300942	4300944
4301222	4301256	4301605	4302828	4303157	4303505	4305834	4307220	4307524
4307525	4308377	4308378	4308624	4310108	4313271	4313272	4313273	4313274
4313605	4315410	4315411	4316572	4317142	4317144	4317145	4317344	4324115
7004449	7007422	7017273	7100446	7101040	7101309	7101569	7102883	7103324
7103562	7103584	7104519	7104520	7104521	7104522	7104523	7104643	7104703
7106327	7106328	7106329	7106356	7106537	7106538	7106539	7106600	7106601
7106667	7106668	7106669	7106796	7106797	7106798	7106799	7106984	7106988
7107024	7200803	7200804	7205296	7205297	7205298	7205299	7205300	7205301
7205970								

Table S4: MOFs: Cambridge Structural Database

AENCSE10	AFEHUO	AFIXAO	AFIXES	BACMOH	BACMOH10	BAHGUN
BIMDEF	BIMDIL	CIDNIM	CUIMDZ01	DEFKUU	DEHFUR	DOQRUW
EDIKEH	ENCDBZ01	ENCUCC10	ETCUCY10	FALLOT	GORQAF	GUJVAI
HEGCEB	HIXDOH01	HODWUS	HUJVOX	HUKRIO	HUYKIV	HUYKUH
IDIWIB	IDIWOH	JARMEU	JARMEU10	JEJFAF	JOKXAI	JOKXAI10
JOKXEM	JOKXEM10	JOKXOW	JOKXOW10	JOKXUC	JOKXUC10	JOKYAJ
JOKYAJ10	JOKYEN	JOKYEN10	JOKYIR	JOKYIR10	JOKYOX	JOKYOX10
JOSNAG	KECRAL	KECRAL10	KECRAL12	KEGZOL	KEGZOL01	KEXFIC
KEXFIC10	KUSZED	LAMFEK	LAMFIO	LAMFOU	LAMGUB	LAMHAI
LATCEO	LATCIS	LEJBUX	LITHUR	LORNEL	LUYNAU	MAXFIA
MIHBAG	MIMVEJ	MINVUA	MINVUA01	MODPOK	NICZAA01	NIGHOA
NINHOH	NUJCEA	NUJCIE	NUMMOX	OGOJOJ	PIZJEN	PUTYAE
PUTYEI	PUWCEP	PUWCUF	QALWUV	QAMXIL	QAYTOZ	QEFNAQ
QIJLAW	QOJKAB	QOJTUE	QOJVAM	QOPHEI	RAFRUL	RASGAT
REGJIW	REVSOA	RIDKOE	RONZID	SAJRAW10	SUDBOI	TENQOS
TILVOZ	TILVUF	TILWAM	TILWEQ	UGUQOC	UGUTOF	UGUXAV
UHAXUW	VABMER	VOCQAF	WABVIF	WABVOL	WABWAY	WILRIS
WIWQOI	WIWQUO	XANXUF	XAYMUF	XECJAQ	XOTHAP	YARYEV
YEFNIG	YEFPAA	YEFPUU	YUTGEZ	ZIWTII	ZUTBAR	ZUVTEP
ZUYWAR						

Table S5: Zeolitic imidazolate frameworks

ZIF-1	ZIF-2	ZIF-3	ZIF-4	ZIF-5	ZIF-6	ZIF-7	ZIF-8	ZIF-9	ZIF-10	ZIF-11
ZIF-12	ZIF-14	ZIF-60	ZIF-62	ZIF-64	ZIF-68	ZIF-69	ZIF-70	ZIF-72	ZIF-73	ZIF-74
ZIF-75	ZIF-77									

Table S6: MOFs: MOFomics user submissions

DUT-10(Zn)	DUT-12	DUT-23(Cu)	Eu(BTC)	F-MOF-11	F-MOF-8	GWMOF-6	MIL-120(Ga)
MIL-124	MOF-5	MOF-604	MOF-646	MOF-69c	MOF-72	MOF-80	WALCIX
Zn(bpb)							

Table S7: Hypothetical MOFs

961	967	982	1036	1298	2688	2752	4406	4920	4923	4926	4929
4932	4935	4938	4940	4943	4946	4949	4952	4955	4958	4961	4964
4966	4969	4972	4975	4977	4980	4983	4987	4990	4993	4999	5002
5007	5010	5013	5016	5019	5023	5026	5032	5035	5038	5041	5044
5047	5050	5053	5056	5059	5061	5063	5067	5072	5076	5079	5082
5360	5438	5441	5444	5447	5449	5451	5453	5455	5458	5461	5463
5465	5468	5471	5473	5475	5477	5483	5491	5500	5502	5516	5518
5521	5526	5529	5533	5536	5541	5865	5868	5872	5875	5878	5893
5898	5901	5905	5908	5914	5931	5939	5942	5946	5949	5956	5963
5966	5970	5972	5976	5980	5983	5985	5990	5996	6000	6004	6396
6399	6402	6411	6428	6430	6433	6979	6982	6985	6988	6991	6994
6997	7000	7005	7008	7011	7013	7018	7026	7033	7040	7054	7063
7066	7071	7076	7081	7084	7087	7090	7093	7096	7101	7104	7108
7551	7556	7558	7560	7562	7564	7566	7573	7585	7899	7913	7932
8078	8086	8088	8089	8119	8134	8137	8140	8143	8146	8150	8154
8157	8159	8163	8166	8169	8172	8174	8177	8180	8182	8185	8189
8192	8195	8199	8202	8205	8208	8212	8215	8218	8221	8224	8227
8230	8232	8234	8237	8240	8242	8245	8249	8253	8257	8260	8263
8266	8269	8271	8274	8277	8280	8283	8287	8289	8292	8295	8298
8301	8350	8525	8527	8529	8532	8535	8537	8540	8542	8545	8548
8550	8553	8556	8560	8562	8565	8568	8570	8573	8580	8583	8586
8589	8591	8593	8595	8600	8605	8607	8608	8609	8610	8612	8619
8620	8628	8629	8630	8631	8632	8634	8636	8637	8638	8640	8646
8653	8686	8688	8690	8691	8693	8695	8698	8700	8702	8709	8718
8721	8730	8749	9162	9216	9679	9766	9985	9996	9999	10041	10500
10537	10914	12098	12134	12888	12925	13268	13302	13326	14255	17376	17408
17423	17553	17561	17571	17581	17592	17595	17604	17610	17989	17991	17994
18000	18008	18012	18019	18021	18024	18026	18029	18030	18033	18034	18040
18047	18054	18057	18058	18061	18062	18068	18072	18075	18078	18081	18086
18088	18090	18092	18094	18095	18098	18104	18105	18107	18108	18112	18646
19775	19783	19787	19797	19803	19911	19913	19915	19917	19919	19922	19925
19926	19927	19929	19952	19955	19956	20032	20085	20124	20127	20130	20133
20136	20139	20141	20144	20146	20149	20151	20153	20156	20158	20161	20166
20169	20172	20175	20178	20181	20183	20184	20185	20188	20190	20192	20194
20197	20199	20200	20204	20208	20211	20214	20216	20217	20219	20221	20224
20226	20228	20230	20231	20234	20237	20239	20241	20244	20247	20250	20252
20255	20258	20260	20276	20282	20285	20491	20493	20494	20496	20499	20501
20503	20505	20507	20508	20510	20512	20514	20516	20518	20520	20524	20525
20526	20529	20530	20532	20540	20542	20544	20545	20547	20549	20553	20555
20557	20559	20561	20563	20567	20569	20574	20577	20818	20820	20822	20825
20827	20829	20833	20835	20838	20841	20843	20844	20847	20849	20851	20853
20855	20857	20859	20862	20868	20870	20872	20875	20877	20879	20881	20883
20890	20892	20896	20899	20901	20903	20904	20906	20908	20911	20915	20917
20922	20926	20928	20929	20931	20932	21198	21199	21200	21202	21206	21207
21208	21209	21210	21212	21214	21216	21219	21220	21221	21222	21223	21224
21225	21227	21237	21238	21241	21245	21247	21249	21251	21252	21253	21256
21257	21258	21272	21274	21276	21278	21281	21283	21291	21293	21295	21297
21299	21303	21603	21606	21609	21612	21615	21618	21621	21623	21625	21628
21630	21632	21635	21638	21640	21643	21645	21648	21650	21652	21655	21657
21658	21661	21662	21665	21666	21669	21671	21674	21676	21678	21680	21681

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Table S7: Hypothetical MOFs – Continued

21684	21687	21691	21694	21696	21699	21701	21702	21703	21704	21707	21708
21709	21710	21713	21718	22009	22013	22015	22017	22019	22021	22022	22024
22025	22027	22029	22031	22032	22034	22036	22038	22039	22042	22052	22057
22062	22064	22066	22068	22070	22073	22074	22075	22076	22087	22089	22091
22093	22095	22097	22099	22103	22104	22106	22113	22115	22165	22166	22168
22170	22172	22174	22176	22178	22180	22182	22184	22186	22188	22190	22191
22193	22225	22243	22248	22253	22256	22381	22383	22385	22387	22389	22391
22394	22396	22398	22400	22402	22405	22407	22409	22412	22414	22416	22418
22420	22422	22424	22426	22428	22430	22432	22434	22436	22438	22440	22442
22445	22447	22449	22452	22454	22456	22458	22460	22463	22465	22467	22469
22471	22473	22475	22477	22479	22482	22484	22486	22488	22490	22492	22494
22643	22645	22646	22649	22651	22653	22654	22655	22656	22657	22659	22663
22665	22666	22667	22669	22671	22672	22673	22674	22679	22680	22682	22683
22685	22687	22688	22690	22699	22704	22705	22707	22711	22716	22727	22733
22734	22735	22737	22738	22741	22743	22746	22749	22750	22752	22753	22754
22755	22756	22757	22758	22760	22761	22762	22765	22770	22773	22774	22777
22778	22779	22780	22781	22782	22783	22784	22785	23054	23059	23064	23071
23074	23077	23083	23115	23118	23417	23418	23419	23420	23422	23423	23426
23427	23429	23431	23432	23880	23881	23882	23883	23885	23886	23888	23891
23892	23894	23895	23896	23899	23908	23910	23911	23916	23917	23920	23922
23924	23929	23934	24167	24168	24170	24174	24175	24176	24177	24178	24179
24181	24182	24183	24205	24539	24755	24758	24808	25078	25350	25397	25401
25818	25833	26229	26241	26780	26788	27055	27056	27924	27928	27940	27944
27962	27972	27984	27986	27992	28015	28024	28136	28150	28183	28198	28554
28556	28558	28561	28563	28565	28567	28569	28571	28574	28576	28580	28583
28586	28594	28595	28604	28608	28611	28614	28617	28624	28630	28631	28633
28635	28637	28639	28642	28649	29201	29857	29912	30477	30479	30481	30482
30484	30485	30488	30490	30491	30492	30518	30526	30528	30667	30681	30684
30686	30688	30691	30693	30695	30697	30700	30703	30705	30707	30709	30711
30713	30715	30717	30719	30722	30724	30726	30728	30729	30732	30733	30737
30738	30742	30744	30747	30749	30751	30752	30755	30760	30762	30765	30766
30768	30771	30772	30775	30776	30778	30779	30780	30783	30785	30786	30790
30792	30794	30796	30799	30800	30803	30811	30859	30863	30959	31045	31047
31049	31051	31052	31054	31055	31057	31059	31060	31062	31064	31066	31068
31069	31070	31072	31074	31075	31076	31078	31090	31091	31092	31094	31095
31096	31098	31101	31102	31104	31106	31108	31110	31112	31116	31120	31122
31364	31366	31368	31370	31372	31374	31378	31381	31383	31385	31387	31389
31391	31393	31395	31397	31399	31404	31406	31407	31408	31410	31415	31418
31420	31424	31426	31428	31429	31432	31434	31436	31437	31438	31440	31442
31444	31449	31450	31452	31453	31456	31459	31461	31462	31463	31723	31725
31726	31728	31729	31730	31732	31733	31734	31735	31736	31737	31739	31741
31744	31746	31758	31759	31760	31762	31768	31769	31771	31772	31773	31774
31775	31776	31777	31778	31792	31794	31798	31800	31802	31804	31808	31810
31814	31816	32113	32116	32120	32122	32124	32126	32128	32129	32132	32134
32137	32139	32141	32144	32145	32147	32149	32151	32154	32156	32157	32160
32162	32168	32170	32172	32174	32176	32179	32180	32183	32186	32187	32189
32192	32194	32196	32197	32200	32201	32202	32203	32205	32206	32209	32210
32211	32215	32217	32220	32222	32330	32500	32503	32505	32507	32508	32510
32512	32513	32515	32517	32519	32521	32522	32523	32524	32526	32529	32530
32532	32533	32544	32545	32550	32555	32557	32558	32560	32561	32562	32563

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Table S7: Hypothetical MOFs – Continued

32564	32565	32575	32579	32581	32582	32584	32586	32588	32590	32592	32594
32596	32600	32601	32602	32606	32652	32654	32656	32659	32661	32663	32665
32667	32669	32671	32672	32674	32676	32677	32679	32681	32735	32737	32738
32739	32740	32742	32744	32881	32883	32885	32887	32889	32891	32893	32895
32897	32899	32901	32903	32905	32907	32909	32911	32913	32915	32917	32920
32922	32924	32926	32928	32930	32932	32935	32937	32939	32941	32943	32945
32947	32949	32951	32953	32955	32957	32959	32962	32964	32966	32968	32970
32972	32974	32976	32979	32982	32984	33150	33152	33153	33155	33157	33158
33160	33161	33163	33165	33166	33168	33169	33176	33180	33182	33184	33187
33188	33190	33191	33192	33198	33199	33201	33202	33203	33211	33216	33217
33225	33229	33230	33232	33233	33234	33238	33247	33248	33250	33251	33252
33254	33255	33256	33257	33258	33259	33261	33262	33269	33270	33272	33273
33275	33276	33277	33278	33280	33540	33550	33551	33559	33576	33604	33608
33615	33619	33905	33907	33908	33910	33911	33912	33915	33916	33917	33918
33919	33920	33949	33952	33958	34364	34365	34367	34368	34370	34371	34373
34374	34375	34378	34388	34392	34394	34395	34399	34400	34401	34402	34403
34404	34406	34639	34641	34643	34646	34647	34648	34649	34650	34651	34652
34653	34663	34669	34670	34671	35242	35570	35836	35852	35854	35856	35864
36343	36349	36712	37266	37463	37466	37476	37478				

Portal activation energies and pore limiting diameters

Table S8: Top 10 zeolites for each separation (PLD in Å, energies in J/mol)

CO_2/N_2				
	PLD	Sel.	CO_2	N_2
MAR	3.0	0.44	2070	325
ANA	3.0	0.44	2017	308
TOL	2.6	0.41	1836	293
NON	2.9	0.40	3383	1027
LOS	3.1	0.38	1251	45
MVY	3.1	0.34	1030	0
FAR	2.7	0.34	1210	124
AFG	2.7	0.31	5864	2275
MSO	2.6	0.28	6287	2518
SGT	2.7	0.27	6647	2666

CO_2/CH_4				
	PLD	Sel.	CO_2	CH_4
DOH	3.3	0.83	311	7450
GIU	2.9	0.78	523	9021
SOD	3.2	0.75	669	10814
FRA	3.3	0.74	118	3884
FAR	2.7	0.60	1210	11263
LOS	3.1	0.60	1251	15441
MVY	3.1	0.53	1030	5026
TOL	2.6	0.45	1836	8685
ANA	3.0	0.44	2017	14805
AHT	3.4	0.40	9	1300

CO_2/H_2				
	PLD	Sel.	CO_2	H_2
RUT	2.2	1.00	18890	0
LIT	2.4	0.99	12561	0
MEP	2.3	0.99	12272	0
LTN	2.4	0.99	11664	0
LIO	2.5	0.99	11663	0
MTN	2.5	0.98	10326	0
AST	2.5	0.98	9909	0
SGT	2.7	0.93	6647	0
MSO	2.6	0.92	6287	0
AFG	2.7	0.90	5864	0

O_2/N_2				
	PLD	Sel.	O_2	N_2
AFG	2.7	0.14	1551	2275
SGT	2.7	0.13	1857	2666
NON	2.9	0.13	581	1027
MSO	2.6	0.13	1771	2518
AST	2.5	0.10	3332	4499
MTN	2.5	0.09	3528	4735
MAR	3.0	0.08	104	325
ANA	3.0	0.08	94	308
TOL	2.6	0.08	87	293
MEP	2.3	0.08	4336	5757

Propane/propylene				
	PLD	Sel.	Propane	Propylene
JBW	3.8	0.92	12040	181
IHW	4.0	0.91	6251	23
SAT	3.6	0.84	4517	0
BIK	3.6	0.79	13779	585
AFN	3.7	0.67	5750	643
ESV	3.7	0.67	9957	928
CDO	3.9	0.67	2742	0
NAB	3.2	0.64	2514	0
ITW	3.4	0.62	10801	1141
CGF	3.5	0.55	15981	1505

Ethane/ethylene				
	PLD	Sel.	Ethane	Ethylene
CAS	3.5	0.80	5992	293
BRE	3.5	0.79	3836	0
LOV	3.4	0.71	4403	318
EAB	3.4	0.68	2841	0
AHT	3.4	0.67	2795	17
BCT	3.2	0.66	5770	700
CGF	3.5	0.54	1936	0
VNI	3.2	0.54	1912	0
NSI	3.4	0.51	1796	0
MVY	3.1	0.46	9671	1819

Styrene/ethylbenzene				
	PLD	Sel.	Styrene	Ethylbenz.
HEU	4.3	1.00	0	13277
WEI	3.9	0.89	301	28572
PAR	2.7	0.88	0	5381
CGS	4.3	0.45	1929	11840
LAU	2.8	0.22	1589	2959
MFI	5.0	0.21	0	599
OBW	5.3	0.21	82	700
SVR	4.5	0.14	4540	10089
DAC	4.8	0.14	0	387
PON	3.9	0.07	6436	13940

Xylenes					
	PLD	Sel.	M-xyl.	O-xyl.	P-xyl.
OBW	5.3	0.96	8540	7925	0
MEL	5.7	0.95	6888	8113	0
MWW	5.2	0.92	5789	7405	0
MTT	5.7	0.92	6838	5914	0
OWE	4.4	0.87	4879	5341	0
FER	5.3	0.81	4071	4259	0
SZR	5.3	0.80	4130	3826	0
IMF	5.9	0.78	3469	4283	0
TON	5.7	0.72	3610	2868	0
LAU	2.8	0.71	10830	13400	831

Table S9: Top 10 MOFs for each separation (PLD in Å, energies in J/mol)

CO_2/N_2				
	PLD	Sel.	CO_2	N_2
H-31733	2.2	0.40	2128	470
H-20085	3.0	0.40	1600	198
H-8640	2.9	0.40	2089	467
H-24755	2.5	0.39	2719	810
H-22671	2.8	0.39	2523	719
H-33915	2.7	0.39	1906	402
H-22653	2.8	0.38	3136	1005
HUKRIO	3.1	0.38	1406	125
BIMDEF	2.5	0.38	1586	242
HIXDOH01	2.8	0.37	4091	1447

CO_2/CH_4				
	PLD	Sel.	CO_2	CH_4
H-31090	2.7	0.77	455	6872
ZIF-12	3.2	0.69	463	4839
H-31091	3.1	0.68	364	4185
ZIF-11	3.3	0.67	187	3409
H-31075	3.3	0.67	155	3264
H-28183	3.3	0.61	0	2360
H-31095	3.1	0.60	216	2887
HUKRIO	3.1	0.57	1406	17546
H-20574	2.9	0.55	461	3192
QOPHEI	2.6	0.55	1355	8562

CO_2/H_2				
	PLD	Sel.	CO_2	H_2
XECJAQ	2.2	1.00	25162	0
H-23429	2.2	1.00	22770	0
C-4308624	2.3	1.00	19190	0
ZIF-7	2.4	1.00	18314	0
H-7932	2.3	1.00	17865	0
HODWUS	2.4	1.00	17246	0
DOQRUW	2.4	1.00	16368	0
H-33192	2.2	1.00	15992	0
H-8089	2.4	1.00	14804	0
ZIF-9	2.4	1.00	14648	0

O_2/N_2				
	PLD	Sel.	O_2	N_2
H-20520	2.2	0.14	1094	1715
HIXDOH01	2.8	0.14	899	1447
H-7562	2.6	0.13	1210	1781
BACMOH10	2.6	0.12	1422	2021
H-8568	2.5	0.12	2278	3166
H-22643	2.7	0.12	1365	1945
H-22659	2.7	0.12	1365	1945
H-22653	2.8	0.12	594	1005
H-22699	2.7	0.12	1543	2167
H-31055	2.5	0.12	1223	1763

Propane/propylene				
	PLD	Sel.	Propane	Propylene
H-30749	3.5	0.99	14515	21
H-30785	3.4	0.98	9861	0
H-30794	3.6	0.98	9407	0
H-30778	3.7	0.96	21785	95
H-21207	3.6	0.96	9785	56
H-30717	4.1	0.95	7516	0
H-31407	3.9	0.92	6327	0
H-5518	3.8	0.92	6246	0
H-32907	4.2	0.85	4683	0
H-32935	4.2	0.85	4683	0

Ethane/ethylene				
	PLD	Sel.	Ethane	Ethylene
REGJIW	2.9	0.93	6702	0
H-32575	3.6	0.93	6669	0
H-33150	3.6	0.93	6669	0
H-31723	3.6	0.93	6667	0
H-31064	3.6	0.93	6665	0
H-31076	3.6	0.93	6665	0
H-22075	3.5	0.88	6617	135
H-31746	3.0	0.84	4634	20
H-20518	3.4	0.83	4367	0
ENCUCC10	3.4	0.79	4092	41

Styrene/ethylbenzene				
	PLD	Sel.	Styrene	Ethylbenz.
H-22188	3.9	1.00	0	20297
H-32211	3.9	1.00	0	19443
H-32176	4.0	1.00	0	19232
H-32147	4.0	1.00	0	17562
H-21707	3.5	1.00	0	17499
H-32149	3.8	1.00	0	17355
H-31397	3.9	1.00	0	16554
H-32156	3.7	1.00	0	15357
H-32168	3.9	1.00	0	13809
H-32194	4.0	0.99	0	12933

Xylenes					
	PLD	Sel.	M-xyl.	O-xyl.	P-xyl.
H-28604	4.2	0.98	8102	28604	0
H-28637	4.2	0.98	8101	28637	0
H-18081	4.8	0.98	8101	18081	0
H-18068	4.8	0.98	8101	18068	0
H-18058	4.8	0.98	8101	18058	0
H-18054	4.8	0.98	8101	18054	0
H-18047	4.8	0.98	8101	18047	0
H-18030	4.8	0.98	8101	18030	0
H-28633	4.2	0.98	8104	11737	0
H-18078	4.8	0.98	10192	8504	0

COD structures are labeled as C-(number), and hypothetical MOFs are labeled as H-(number).