Supporting Information

High-Efficiency Prediction of Water Adsorption Performance of Porous Adsorbents by Lattice Grand Canonical Monte Carlo Molecular Simulation

Zhilu Liu [a], Wei Li [b] and Song Li [a,*]

[a] School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan 430074, China.

[b] Energy & Electricity Research Center, Jinan University, Zhuhai, 519070, China.

* Corresponding author email: songli@hust.edu.cn.

S1. MOFs used in this work

The process for selecting MOFs used in LGCMC is shown in Figure S1a. Taking 392 MOFs with experimental water adsorption isotherms in our updated EWAID database [1-2] as a starting point, among which 191 MOFs with the corresponding crystal structures were collected from CCDC database [3] or RASPA package [4]. Then, these crystal structures were examined one by one: (1) unreasonable structures (e.g., atoms overlap or missing) were deleted, (2) solvent molecules and free ions in structures were removed, (3) geometric optimization with forcite methods in Material Studio were executed for all structures, thus 150 MOFs remained. The measured structural properties in experiments including accessible surface area (S_a), available pore volume (V_a) and pore diameter (D_p) of MOFs were collected from their reported literature, and theoretical features were computed by Zeo++0.3 [5] (in Table S1 and Figure S1b-d). We found that the difference between the structural properties of experimental samples and perfect crystals existed ascribing the defects, unremoved solvent or free ions in experimental samples. It cannot expect molecular simulations to accurately predict the experimental uptake for any adsorbates in those adsorbents with unmatched structural properties of the provided crystal structures. [6] Therefore, according to the standard that all three structural properties of the ratio measured/computed in the 80% to 120% range, 6 MOFs with consistent measured and computed structural properties were eventually adopted.

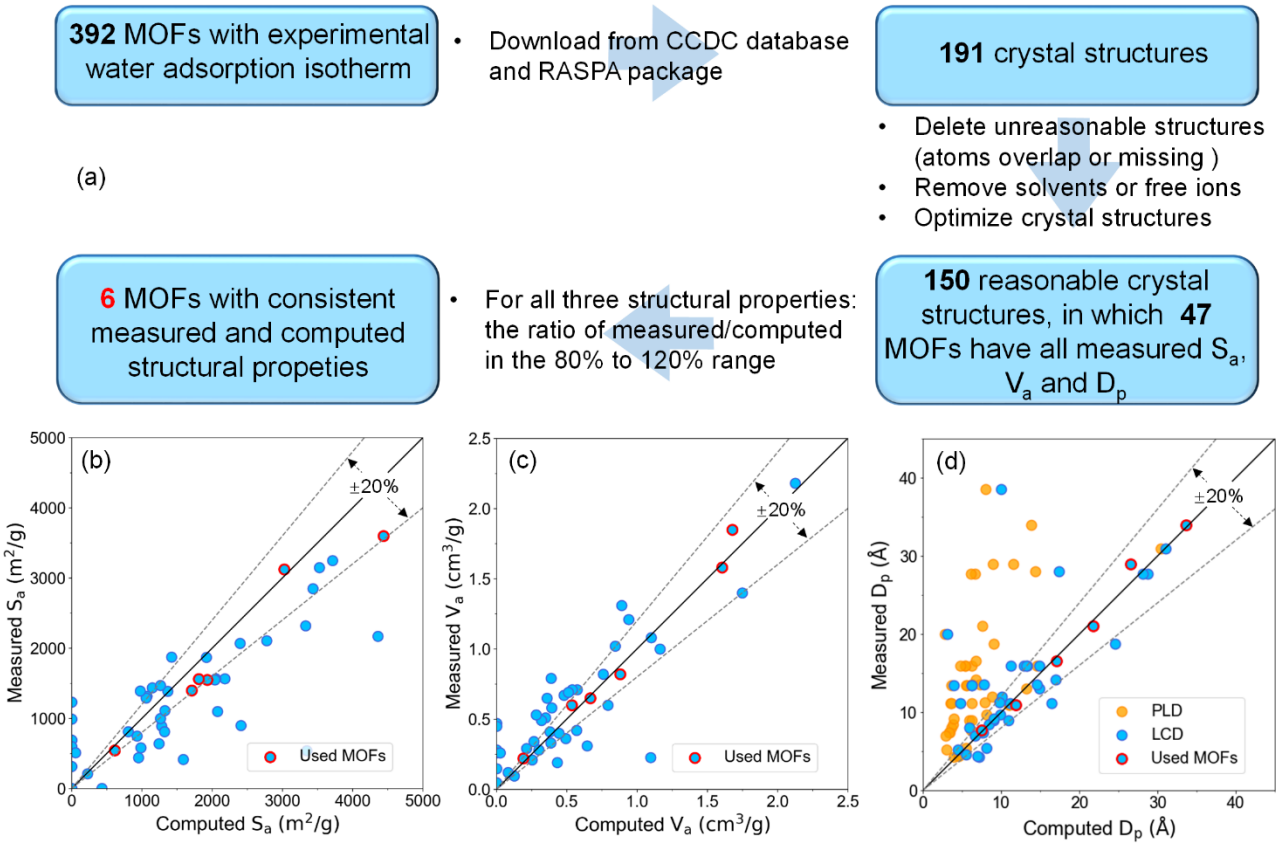

Figure S1. (a) The process for selecting MOFs with consistent experimental and simulated structural features. Comparative distribution of experimental and simulated structural features of 47 MOFs, (b) accessible surface area (S_a), (c) available pore volume (V_a) and (d) pore diameter (D_p), where experimental features collected from literature and simulated features calculated by Zeo++0.3. Calculated PLD and LCD represented pore limited diameter and largest cavity diameter. Especially, 6 MOFs used in LGCMC further (i.e., all three structural properties of the ratio measured/computed in the 80% to 120% range) were highlighted.

Table S1. Source of experimental and crystal structures, and structural properties of MOFs used in this work

No.	Adsorbent	Ref. of MOFs (DOI)	Source of crystal file	Sort of crystal file	Mea. S_a (m^2/g)	Note	Mea. V_a (cm^3/g)	Note	Mea. D_p (Å)	Note	Com. S_a (m^2/g)	Com. V_a (cm^3/g)	Com. LCD (Å)	Com. PLD (Å)
1	([Ni(L6)2]4H2O)n	10.1016/j.micromeso.2013.01.020	from CCDC,FEVDIV,903258	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	4.33	2.00
2	(H2dab)[Zn2(ox)3]	10.1021/Ja203291n	from CCDC,KALGOV,866153	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	889.2	0.306	5.40	4.25
3	[{Zn(L)(H2O)2}(NO3)2*2H2O]n	10.1002/anie.201206724	from CCDC,GEVSAD,883147	Clean cif: remove solvent, save bound water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	4.11	2.61
4	[Cd(L'1)(Cl)](H2O)	10.1021/cg3008443	from CCDC,HEBJUV,851353	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.38	2.53
5	[Cd(L'2)(Cl)](H2O)	10.1021/cg3008443	from CCDC,HEBKEG,851355	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	652.1	0.195	5.34	4.54
6	[Cd(L'2)2(Br)2](H2O)3	10.1021/cg3008443	from CCDC,HEBKIK,851356	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.31	1.88
7	[Cd(L'3)(Cl)](H2O)2	10.1021/cg3008443	from CCDC,HEBKOQ,851357	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.08	1.76
8	[Cd(mpto)2.CH3CH2OH]n	10.1007/s40242-015-5051-0	from CCDC,EKIGIQ,974839	Clean cif: remove solvent	25.8	s1	n.d.	n.d.	n.d.	n.d.	0.0	0.000	4.29	2.64
9	[Co(L)(PIN)]dioxane	10.1039/C2CE26533H	from CCDC,REHTUV,893711	False cif: unmodifiy excressive atom	244	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
10	[Co2(BDC)2(BPNO)]*H2BDC*2MeOH	10.1002/ejic.201200851	from CCDC,ADAXEK,851173	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	5.8	d2	752.3	0.230	5.81	4.05
11	[Co3(ndc)-(HCOO)3(mu3-OH)(H2O)]n	10.1002/chem.201103687	from CCDC,CANYIB,850046	True cif: save bound water	1386	s1	0.58	v1	13.6	d2	1364.9	0.392	7.80	7.26
12	[Co4L3(u3-OH)(H2O)3](SO4)0.5	10.1039/C5DT02651B	from CCDC,WUZBUQ,1411211	True cif	n.d.	n.d.	n.d.	n.d.	18	d1	581.6	0.222	11.25	10.84
13	[Cu(INA)2(NH3)2(H2O)2]	10.1016/j.jssc.2015.02.014	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
14	[Cu(INA)2]	10.1016/j.jssc.2015.02.014	n.d.	n.d.	164.4	s1	n.d.	n.d.	4.99	d2	n.d.	n.d.	n.d.	n.d.
15	[Cu(INAIP)]*2H2O	10.1039/C0cc04689b	from CCDC,UNABUH01,787727	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	2.69	1.07
16	[Cu2(H2btp)(H2O)2(12-bis(4-pyridl)ethylene)]	10.1039/c5dt01137j	from CCDC,VUMBOW,1053216	Clean cif: remove solvent	2.8	s1	0.095	v1	13.4	d2	430.2	0.126	6.19	5.46
17	[Cu2(H2btp)(H2O)2(13-bis(4-pyridl)propane)]	10.1039/c5dt01137j	n.d.	n.d.	3	s1	0.083	v1	14	d2	n.d.	n.d.	n.d.	n.d.
18	[Cu2(H2btp)(H2O)2(bipyridine)]	10.1039/c5dt01137j	from CCDC,VUMBIQ,1053215	Clean cif: remove solvent	1.1	s1	0.047	v1	11.2	d2	0.0	0.000	4.81	3.49
19	[Cu2(pzdc)2(pyz)]*2H2O}	10.1016/j.jcis.2007.05.090	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	6	d2	n.d.	n.d.	n.d.	n.d.
20	[La3L4(H2O)6]-Cl	10.1039/C5DT02651B	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	19	d1	n.d.	n.d.	n.d.	n.d.
21	[Mn(mpto)2.CH3CH2OH]2	10.1007/s40242-015-5051-0	from CCDC,EKIGOW,974840	Clean cif: remove solvent	86.2	s1	n.d.	n.d.	n.d.	n.d.	0.0	0.000	4.15	2.51
22	[Ni(dipn)]2[Ni(dipn)(H2O)][Fe(CN)6]2.2H2O	10.1021/Ja069166b	from CCDC,HIFTUM,645084	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	602.3	0.177	5.81	4.30
23	[Ni(pca)(bdc)0.5(H2O)2]	10.1021/Ic301481p	from CCDC,MAYFOJ,870177	True cif: save bound water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	2.02	0.77
24	[Ni8(L5)6]	10.1002/anie.201303484	n.d.	n.d.	2215	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
25	[Ni8(L5-CF3)6]	10.1002/anie.201303484	n.d.	n.d.	1985	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

26	[Ni8(L5-CH3)6]	10.1039/C3cs60475f	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
27	[PbL2]*2DMF*6H2O	10.1039/C2dt30935a	from CCDC,TEYCAD,854707	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	13	d3	1045.2	0.346	10.04	9.18
28	[PbL2]*DMF*2H2O	10.1039/C2dt30935a	from CCDC,TEYBUW,854708	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	13	d3	631.6	0.177	8.08	5.62
29	[Zn(NO2-BDC)(dmbpy).5](C2H6O)(H2O)	10.1021/acs.inorgchem.5b00335	from CCDC,CUQDUP,1026965	False cif: unmodifiy excressive atom	925	s1	n.d.	n.d.	9	d2	n.d.	n.d.	n.d.	n.d.
30	[Zn2(ip)2(bpy)2]*DMF}n	10.1039/B703502k	from CCDC,HILXAC,639850	Clean cif: modify excressive atom	300	s1	n.d.	n.d.	6	d2	0.0	0.000	3.03	1.95
31	[Zn3(TCPB)2*2H2O]*2H2O*4DMF	10.1002/asia.201200601	from CCDC,GICNIR,879381	Clean cif: remove solvent	573	s1	n.d.	n.d.	4.3	d2	983.4	0.263	4.65	4.27
32	[Zn4O(mipcapz)3]n on [Zn4O(dmcapz)3]n	10.1002/adfm.201302854	n.d.	n.d.	640	s1	0.279	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
33	{(H2PIP)0.5[VO(CEP)]*H2O}	10.1021/Ic200463k	from CCDC,EZOXEX,851054	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.94	2.25
34	{[Cu(azpy)(glut)](H2O)2}	10.1021/Cg2004672	from CCDC,UZUNEJ,844078	True cif	131	s2	n.d.	n.d.	7.8	d3	737.2	0.238	7.30	6.59
35	{[Cu2(4-pmpmd)2(CH3OH)4(opd)2]*2H2O}	10.1021/Cg3017563	from CCDC,TEWGEJ01,858869	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	6.48	d3	0.0	0.000	4.56	2.94
36	{[Cu2(pzdc)2(bpy)]*4H2O}	10.1016/j.jcis.2007.05.090	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	9	d2	n.d.	n.d.	n.d.	n.d.
37	{[Cu4(OH)2(tci)2-(bpy)2]·11H2O}	10.1039/c5dt00762c	from CCDC,KUDWAJ1042056	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	12.54	d1	1865.6	0.488	7.17	6.54
38	{[Dy(ox)(Bpybc)(H2O)]*OH*13H2O}n	10.1039/C3cc38260e	from CCDC,REWSUJ,910631	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	8.4	d3	743.2	0.211	5.81	5.34
39	{[Ni(bpe)2(N(CN)2)](N(CN)2)}n	10.1038/Nmat1827	from CCDC,PEYSIW,615995	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	6.78	d3	0.0	0.000	4.46	3.64
40	{[Zn-(C10H2O8)0.5(C10S2N2H8)]*5H2O]}n	10.1021/Ic402095u	from CCDC,PITRIV,976591	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	12.7	d3	0.0	0.000	4.42	3.00
41	{[Zn(oxo-pba)2(bpy)]4H2O}n	10.1039/c5ra14267a	from CCDC,FUMZIY,987770	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	6.2	d3	258.5	0.071	4.89	4.07
42	{[Zn2(bpdc)2(azpy)]*2H2O*2DMF}n	10.1021/Ic500234r	from CCDC,KOGSIK,1011817	Clean cif: modify excressive atom	235	s1	n.d.	n.d.	8.2	d3	2739.8	0.829	9.77	6.71
43	{[Zn2(bpdc)2(azpy)]*2H2O*2DMF}n Nanoscale	10.1021/Ic500234r	n.d.	n.d.	385	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
44	{[Zn3(bpdc)3(azpy)]*4H2O*2DEF}n	10.1021/Ic500234r	from CCDC,KOGSOQ,1011818	True cif	200	s1	n.d.	n.d.	11.9	d2	927.8	0.263	6.71	5.36
45	{[Zn4O(bfbpdc)3-(bpy)0.5(H2O)]*(3DMF)(H2O)}n	10.1021/ic302645rb	n.d.	n.d.	1450	s1	0.59	v1	10.76	d3	n.d.	n.d.	n.d.	n.d.
46	{[ZnL(HCO2)(H2O)]*DMF}	10.1039/C3dt51123e	from CCDC,PIHQUU,906705	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	537.9	0.175	4.55	3.93
47	1 C76H116N14O42Zn3	10.1071/Ch12270	from CCDC,GERNOI,808121	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	7.15	3.38
48	13R(Co)	10.1021/jacs.8b07290	from CCDC,NIRCID,1508857	Clean cif: remove solvent	293	s1	n.d.	n.d.	8	d3	1073.0	0.293	6.89	4.05
49	1-LiCl	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

50	23R(Co)	10.1021/jacs.8b07290	from CCDC,NIRCOJ,1508858	False cif: unmodifiy excressive atom	267	s1	n.d.	n.d.	8	d3	n.d.	n.d.	n.d.	n.d.
51	2D [Cu(bpy)2(OTf)2]n	10.1021/Ja201170c	from CCDC,UXUNUX,842275	Clean cif: remove solvent	740	s1	0.295	v1	n.d.	n.d.	3208.8	0.682	6.33	5.30
52	33R(Co)	10.1021/jacs.8b07290	from CCDC,NIRCUP,1508859	Clean cif: remove solvent	241	s1	n.d.	n.d.	8	d3	994.4	0.281	7.17	4.04
53	3S(Co)	10.1021/jacs.8b07290	from CCDC,NIRCAV,1508855	False cif: unmodifiy excressive atom	281	s1	n.d.	n.d.	8	d3	n.d.	n.d.	n.d.	n.d.
54	43R(Co)	10.1021/jacs.8b07290	from CCDC,NIRCEZ,1508856	Clean cif: remove solvent	203	s1	n.d.	n.d.	8	d3	0.0	0.000	5.72	2.08
55	Al(OH)-(1,4-NDC)	10.1021/ja802589u	from CCDC,WOJJOV,710000	Clean cif: remove solvent	546	s2	0.22	v1	7.7	d3	614.1	0.190	7.48	6.12
56	AlaZnBr	10.1039/C3CC41842A	from CCDC,BEPNUH,918490	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	12.5	d3	1002.7	0.316	9.23	9.08
57	AlaZnCl	10.1039/C3CC41842A	from CCDC,BEPPAP,918489	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	12.5	d3	1179.7	0.364	9.10	8.96
58	AlaZnOAc	10.1039/C3CE41083H	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
59	ALFFIVE-1-Ni	10.1126/science.aam8310	from CCDC,DAXNEY,1538215	False cif: unmodifiy excressive atom	258	s1	0.1	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
60	Aluminum fumarate	10.1021/acs.iecr.5b03509	form RASPA	True cif	971	s1	0.85	v1	n.d.	n.d.	1315.6	0.415	5.84	5.38
61	Basolite^TM F300(Fe)	10.1177/0954406212456469	n.d.	n.d.	1600	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
62	BIT-66(V)	10.1002/anie.201914762	n.d.	n.d.	1417	s1	0.87	v1	25.8	d2	n.d.	n.d.	n.d.	n.d.
63	BIT-72(Al)	10.1021/acsami.7b17026	n.d.	n.d.	1618	s1	0.59	v1	6.2	d2	n.d.	n.d.	n.d.	n.d.
64	BIT-73(Al)	10.1021/acsami.7b17026	n.d.	n.d.	1511	s1	0.56	v1	6.6	d2	n.d.	n.d.	n.d.	n.d.
65	BIT-74(Al)	10.1021/acsami.7b17026	n.d.	n.d.	1394	s1	0.51	v1	5.7	d2	n.d.	n.d.	n.d.	n.d.
66	Blucher-101408	10.1039/C3cs60475f	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
67	Bu-FeCr	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
68	BUT-155(Cu)	10.1021/acsami.7b07920	from CCDC,SENSAI,1544772	Clean cif: modify excressive atom	2070	s1	0.82	v1	16	d3	2395.4	0.759	11.24	6.25
69	BUT-46A(Zr)	10.1021/acsami.8b09333	from CCDC,VIKRIT,1821894	True cif	1550	s1	0.69	v1	16	d2	2036.8	0.511	13.18	4.82
70	BUT-46B(Zr)	10.1021/acsami.8b09333	from CCDC,VIKSAM,1821990	False cif: unmodifiy excressive atom	1403	s1	0.65	v1	16	d2	n.d.	n.d.	n.d.	n.d.
71	BUT-46F(Zr)	10.1021/acsami.8b09333	from CCDC,VIKRUF,1821896	True cif	1563	s1	0.71	v1	16	d2	2050.2	0.539	12.91	5.36
72	BUT-46W(Zr)	10.1021/acsami.8b09333	from CCDC,VIKROZ,1821895	True cif	1565	s1	0.71	v1	16	d2	2178.4	0.574	13.34	5.35
73	C10H4O12Eu2	10.1039/C0cc00148a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	5	d2	n.d.	n.d.	n.d.	n.d.
74	C115.5H202N14O43Zn4	10.1039/C0cc02496a	from CCDC,WAGYUA,780176	True cif	n.d.	n.d.	n.d.	n.d.	13	d3	4548.1	1.675	16.87	10.73
75	C11H15BrN2O4Zn	10.1021/Ja2078637	from CCDC,IBIDAA,831059	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	822.6	0.297	10.18	10.06
76	C11H15ClN2O4Zn	10.1021/Ja2078637	from CCDC,IBICUT,831058	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	928.3	0.339	10.18	10.00
77	C12H17ClN2O3Cd	10.1021/Cg3008443	from CCDC,HEBJUV,851353	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	9.8	d3	0.0	0.000	3.38	2.53
78	C15H27N2O10Dy	10.1021/Cg800204q	from CCDC,COWMAD,624390	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.0	0.000	2.52	0.97
79	C15H27N2O10Er	10.1021/Cg800205q	from CCDC,COWMOR,624393	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.0	0.000	2.49	0.92
80	C15H27N2O10Ho	10.1021/Cg800206q	from CCDC,COWMIL,624392	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.0	0.000	2.51	0.92
81	C15H27N2O10Tb	10.1021/Cg800207q	from CCDC,COWMEH,624391	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.0	0.000	2.54	0.97
82	C15H27N2O10Tm	10.1021/Cg800208q	from CCDC,COWMUX,624394	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.0	0.000	2.46	0.96

83	C18H21Br2N4O9Cd2	10.1021/Cg3008443	from CCDC,HEBKIK,851356	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	12	d3	0.0	0.000	3.31	1.88
84	C24H40N2O16Cl2Cd3	10.1016/j.inoche.2006.02.029	from CCDC,PEHQID,281927	Clean cif: remove Cl-	n.d.	n.d.	0.07	v1	8.4	d3	0.0	0.000	5.14	3.60
85	C26H24Br2Cu2N8O3	10.1039/C2ra21865h	from CCDC,REGVEG,704681	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	4.43	1.44
86	C28H24CoN10	10.1039/C1ce05847a	from CCDC,FALSAO,834081	Clean cif: remove solvent	137	s1	n.d.	n.d.	6	d2	574.1	0.170	5.50	4.58
87	C32H24Cu3N6O12	10.1002/chem.200802730	from CCDC,GUXKAM,704817	True cif	445	s1	n.d.	n.d.	9.8	d3	595.2	0.143	4.98	4.01
88	C32H46N4O8Zn	10.1039/C2jm15604k	from CCDC,FECZIY,870505	False cif: unmodifiy excressive atom	n.d.	n.d.	n.d.	n.d.	7.21	d2	n.d.	n.d.	n.d.	n.d.
89	C4H8HoKO12 Dehydrated	10.1021/Cm9014749	from CCDC,AQOVIM,829511	False cif: lake of H atom	69.1	s2	0.1042	v1	3.6	d3	n.d.	n.d.	n.d.	n.d.
90	C55H52Fe4N20O18	10.1016/j.ica.2012.02.002	from CCDC,YAQVAP,704682	Clean cif: remove solvent, save bound water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.94	1.88
91	C62H44N2O8Zn2	10.1021/ic200937u	from CCDC,UDANAQ,804771	False cif: unmodifiy excressive atom	960	s1	0.43	v1	10.5	d2	n.d.	n.d.	n.d.	n.d.
92	C62H50Cd3K2N2O26	10.1039/C3ce26788a	from CCDC,PILJAX,916312	Clean cif: remove solvent	8.27	s1	n.d.	n.d.	12.7	d2	1371.2	0.375	5.83	5.02
93	C9H11ClN2O4Cd	10.1021/Cg3008443	from CCDC,HEBKEG,851355	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	652.3	0.195	5.34	4.54
94	CALF-25	10.1021/Ja306812r	from CCDC,YEYBOV,944654	True cif	385	s1	n.d.	n.d.	4.6	d2	270.3	0.073	4.80	4.18
95	CAU-1(Al)-(OH)2	10.1039/C4CE01073F	n.d.	n.d.	n.d.	n.d.	0.5	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
96	CAU-1(Al)-NH2	10.1039/C2CE06620C	n.d.	n.d.	1530	s1	0.64	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
97	CAU-1(Al)-NHCH3	10.1039/C2CE06620C	n.d.	n.d.	1340	s1	0.53	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
98	CAU-1(Al)-NHCOCH3	10.1039/C2CE06620C	n.d.	n.d.	680	s1	0.3	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
99	CAU-10-CH3	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
100	CAU-10-H	10.1039/C4cs00078a	from RASPA	True cif	600	s1	0.26	v1	7	d2	0.0	0.000	6.64	2.91
101	CAU-10-NH2	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
102	CAU-10-NO2	10.1039/C4cs00078a	n.d.	n.d.	440	s1	0.18	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
103	CAU-10-OCH3	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
104	CAU-10-OH	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
105	CAU-10-pydc	10.1002/adma.201502418	n.d.	n.d.	926	s1	0.43	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
106	CAU-13	10.1021/Ic500288w	from CCDC,JIZWAS,980340	True cif	380	s1	0.15	v1	n.d.	n.d.	440.0	0.192	4.85	4.07
107	CAU-1-NH2	10.1039/C2ce06620c	n.d.	n.d.	1530	s1	0.64	v2	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
108	CAU-1-NHCH3	10.1039/C2ce06620c	n.d.	n.d.	1340	s1	0.53	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
109	CAU-1-NHCOCH3	10.1039/C2ce06620c	n.d.	n.d.	680	s1	0.3	v2	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
110	CAU-23	10.1038/s41467-019-10960-0	from CCDC,ZOVHUQ,1878820	Clean cif: remove solvent	1250	s1	n.d.	n.d.	7.6	d1	1505.7	0.419	7.22	6.14
111	CAU-3(Al)	10.1039/C2DT12005D	from CCDC,CAXTAY,799243	False cif: lake of H atom	1550	s1	0.64	v1	27	d3	n.d.	n.d.	n.d.	n.d.
112	CAU-3(Al)-NH2	10.1039/C2DT12005D	from CCDC,CAXTEC,799244	False cif: lake of H atom	1250	s1	0.53	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
113	CAU-6(Al)	10.1039/C2CC34909D	from CCDC,TABLAN,2042447	False cif: lake of H atom	620	s1	0.25	v1	10	d3	n.d.	n.d.	n.d.	n.d.
114	CAU-8(Al)	10.5517/ccz5qc6	from CCDC,ZESZEE,899228	True cif	n.d.	n.d.	0.25	v1	n.d.	n.d.	1208.1	0.326	7.01	5.36
115	Cd (II)-MOF [Cd(L)(DMF)]	10.1039/C4dt00230j	from CCDC,KETHEY02,971223	False cif: unmodifiy excressive atom	231.31	s1	n.d.	n.d.	6	d2	n.d.	n.d.	n.d.	n.d.
116	Cd(BTTB)	10.1039/C4TA01372G	from CCDC,GOSDEZ,986372	True cif	415	s1	0.19	v1	5.41	d1	1587.0	0.433	8.09	5.51

117	Cd2(sdb)2(pcih)2	10.1021/acs.inorgchem.8b00078	from CCDC,JESTEJ,1480164	True cif	n.d.	n.d.	0.22	v1	4.4	d2	498.3	0.140	4.75	4.36
118	Cd3L2	10.1021/cg301559s	from CCDC,SEQSAK,855034	Clean cif: remove solvent	417	s1	n.d.	n.d.	8	d3	519.0	0.166	4.77	4.15
119	CID-3	10.1039/C0cc00027b	from CCDC,LUYHOD,745860	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	8.1	d2	0.0	0.000	4.64	3.48
120	Co(BTTB)(AZPY)	10.1039/C4TA01372G	from CCDC,GOSFAX,986376	False cif: unmodifiy excressive atom	805	s1	0.39	v1	4.94	d1	n.d.	n.d.	n.d.	n.d.
121	Co(BTTB)(BPY)	10.1039/C4TA01372G	from CCDC,GOSDOJ,968375	False cif: unmodifiy excressive atom	843	s1	0.4	v1	4.06	d1	n.d.	n.d.	n.d.	n.d.
122	Co(BTTB)(DMBPY)	10.1021/la503269f	from CCDC,ONULOA,992483	True cif	809	s1	0.29	v1	4.41	d1	805.6	0.213	6.96	4.53
123	Co2Cl2(BTDD)	10.1021/acscentsci.7b00186	n.d.	n.d.	1912	s1	n.d.	n.d.	22	d1	n.d.	n.d.	n.d.	n.d.
124	Co2Cl2BBTA	10.1021/jacs.8b09655	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	13	d3	n.d.	n.d.	n.d.	n.d.
125	Cobalt Triazolyl Phosphonate MOF	10.1039/c5dt02651b	from CCDC,WUZBUQ,1411211	True cif	n.d.	n.d.	n.d.	n.d.	13	d2	581.6	0.222	11.25	10.84
126	Cobalt Triazolyl Phosphonate MOF (95%RH)	10.1039/c5dt02651b	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	13	d2	n.d.	n.d.	n.d.	n.d.
127	Cobalt Triazolyl Phosphonate MOF (Activated at 403K)	10.1039/c5dt02651b	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	13	d2	n.d.	n.d.	n.d.	n.d.
128	Co-CUK-1	10.5517/ccdc.csd.cc25synl	from CCDC,VECTEG,2019980	True cif	510	s1	0.26	v1	13.4	d1	52.5	0.025	3.93	3.65
129	Co-MOF-74(M)	10.5517/ccdc.csd.cc2459tg	from CCDC,AJECIE,1971315	Clean cif: remove solvent	1314	s1	0.51	v1	12	d2	1069.5	0.350	10.06	8.88
130	Co-MOF-74(S)	10.1016/j.cattod.2011.08.019	n.d.	n.d.	1327	s1	0.52	v1	12	d2	n.d.	n.d.	n.d.	n.d.
131	CoNIm	10.1039/C2CC36651G	from CCDC,REGXOS,886561	True cif	1858	s2	n.d.	n.d.	22	d3	1549.9	0.573	19.51	7.12
132	CPO-27-Ni	10.1039/C2dt31112g	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	11	d2	n.d.	n.d.	n.d.	n.d.
133	Cr3(BTC)2	10.1039/C7DT02957H	n.d.	n.d.	1330	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
134	Cr-MIL(101)	10.1039/C4cs00078a	from RASPA	True cif	3124	s1	1.58	v1	34	d2	3025.9	1.605	33.66	13.86
135	Cr-MIL-101-NO2	10.1039/C4cs00078a	n.d.	n.d.	2146	s1	1.19	v1	34	d2	n.d.	n.d.	n.d.	n.d.
136	Cr-soc-MOF-1	10.1016/j.chempr.2017.11.005	from CCDC,QEPQIO,1542714	False cif: unmodifiy excressive atom	4549	s1	2.1	v1	17	d3	n.d.	n.d.	n.d.	n.d.
137	Cu(mtpm)Cl2	10.1021/ja306401j	from CCDC,EDAPIK,886221	Clean cif: remove Cl-	n.d.	n.d.	n.d.	n.d.	8	d3	2923.8	0.844	8.35	7.82
138	Cu2(dmcapz)2	10.1002/chem.201201820	from CCDC,ZECKID,882685	Clean cif: remove solvent	539	s1	0.227	v1	9.7	d3	3345.6	1.096	9.83	8.07
139	Cu2(pzdc)2bpe	10.1016/j.jcis.2007.05.090	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
140	Cu2Cl2BBTA	10.1021/jacs.8b09655	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	13	d3	n.d.	n.d.	n.d.	n.d.
141	Cu6(Trz)10(H2O)4[H2SiW12O40]·8H2O	10.1002/chem.201501515	from CCDC,DUGGOD,1058210	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	5.65	d1	0.0	0.000	6.06	2.89
142	CuBTC	10.1002/bkcs.10087	from RASPA	True cif	1507	s1	n.d.	n.d.	n.d.	n.d.	2201.7	0.697	13.20	6.66
143	CuEBTC	10.1021/cg300518k	from CCDC,LAZXOB,896250	Clean cif: remove solvent	1434	s1	0.65	v1	9	d3	1145.9	0.359	9.06	5.90
144	CuMBTC	10.1021/cg300518k	from CCDC,LAZXIV,896249	True cif	1471	s1	0.79	v1	9	d3	1261.6	0.389	10.91	6.28
145	Cu-MOF	10.1021/la803818p	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
146	Cu-Tria	10.1021/acssuschemeng.0c08256	n.d.	n.d.	188	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
147	DETA-MIL-101	10.1039/C2ce06608d	n.d.	n.d.	1560	s1	1.1	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

148	DMOF	10.1021/Ie202325p	n.d.	n.d.	1960	s1	0.58	v1	7.5	d3	n.d.	n.d.	n.d.	n.d.
149	DMOF(Zn)-A	10.1021/La304151r	n.d.	n.d.	760	s1	0.33	v1	4.8	d1	n.d.	n.d.	n.d.	n.d.
150	DMOF(Zn)-Br	10.1021/La304151r	n.d.	n.d.	1315	s1	0.53	v1	5	d1	n.d.	n.d.	n.d.	n.d.
151	DMOF(Zn)-N	10.1021/La304151r	n.d.	n.d.	1420	s1	0.57	v1	5.7	d1	n.d.	n.d.	n.d.	n.d.
152	DMOF(Zn)-NH3	10.1021/Ie202326p	n.d.	n.d.	2010	s1	0.58	v1	7.5	d3	n.d.	n.d.	n.d.	n.d.
153	DMOF-Cl2	10.1021/La304151r	n.d.	n.d.	1175	s1	0.45	v1	3.8	d2	n.d.	n.d.	n.d.	n.d.
154	DMOF-NO2	10.1021/La304151r	n.d.	n.d.	1310	s1	0.53	v1	6.2	d2	n.d.	n.d.	n.d.	n.d.
155	DMOF-OH	10.1021/La304151r	n.d.	n.d.	1130	s1	0.54	v1	7.5	d2	n.d.	n.d.	n.d.	n.d.
156	DMOF-TM(Co)	10.1021/la503269f	n.d.	n.d.	1052	s1	0.49	v1	3.5	d1	n.d.	n.d.	n.d.	n.d.
157	DMOF-TM(Cu)	10.1021/la503269f	n.d.	n.d.	1041	s1	0.46	v1	3.5	d1	n.d.	n.d.	n.d.	n.d.
158	DMOF-TM(Ni)	10.1021/la503269f	n.d.	n.d.	1095	s1	0.48	v1	3.5	d1	n.d.	n.d.	n.d.	n.d.
159	DMOF-TM1(Zn)	10.1021/la304204k	n.d.	n.d.	1210	s1	0.53	v1	7.5	d3	n.d.	n.d.	n.d.	n.d.
160	DMOF-TM2(Zn)	10.1021/la304204k	n.d.	n.d.	1050	s1	0.51	v1	3.5	d3	n.d.	n.d.	n.d.	n.d.
161	DUT-10(Zn)	10.1002/ejic.201000415	from CCDC,XAFFAN,772845	True cif	423	s1	n.d.	n.d.	n.d.	n.d.	5263.2	2.100	13.42	11.93
162	DUT-4	10.1016/j.micromeso.2008.11.020	n.d.	n.d.	1360	s1	0.79	v1	8.5	d3	n.d.	n.d.	n.d.	n.d.
163	DUT-51(Zr)	10.1039/C2CC34246D	from CCDC,VEGBUG,872966	True cif	2106	s1	1.08	v1	18.8	d3	2775.5	1.100	24.61	9.08
164	DUT-52(Zr)	10.1039/C3CE41121D	from CCDC,OFAVUO,937877	False cif: unmodifiy excressive atom	1399	s1	0.54	v1	8.59	d3	n.d.	n.d.	n.d.	n.d.
165	DUT-53(Hf)	10.1039/C3CE41121D	from CCDC,OFAWAV,937878	True cif	1097	s1	0.31	v1	11.23	d3	2074.5	0.645	9.73	7.94
166	DUT-67	10.1021/Ja500330a	from RASPA	True cif	1560	s1	0.6	v1	16.6	d2	1808.2	0.535	17.05	6.73
167	DUT-67(Hf)	10.1021/cg301691d	from CCDC,XICZAM,902899	Clean cif: remove solvent	810	s1	0.33	v1	14.2	d3	1323.0	0.387	16.94	6.72
168	DUT-68(Hf)	10.1021/cg301691d	from CCDC,XICYOZ,902901	Clean cif: remove solvent	749	s1	0.34	v1	27.7	d3	928.1	0.266	28.07	6.15
169	DUT-68(Zr)	10.1021/cg301691d	from CCDC,XICYUF,902900	Clean cif: remove solvent	891	s1	0.41	v1	27.7	d3	1279.0	0.380	28.70	6.66
170	DUT-69(Hf)	10.1021/cg301691d	from CCDC,XICYEP,902903	False cif: unmodifiy excressive atom	450	s1	0.22	v1	5	d3	n.d.	n.d.	n.d.	n.d.
171	DUT-69(Zr)	10.1021/cg301691d	from CCDC,XICYIT,902902	False cif: unmodifiy excressive atom	560	s1	0.31	v1	5	d3	n.d.	n.d.	n.d.	n.d.
172	DUT-84(Zr)	10.1039/C3CE41121D	from CCDC,OFAWID,937880	False cif: unmodifiy excressive atom	637	s1	0.27	v1	11.14	d3	n.d.	n.d.	n.d.	n.d.
173	ED-ZIF-8	10.1002/Aic.13970	n.d.	n.d.	1428	s1	0.75	v1	45.3	d2	n.d.	n.d.	n.d.	n.d.
174	Et-MnCr	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
175	FeFFIVE-1-Ni	10.1126/science.aam8310	from CCDC,DAXPAW,1538218	Clean cif: remove solvent	324	s1	0.13	v1	n.d.	n.d.	0.0	0.000	4.66	2.30
176	HKUST-1-F	10.1002/bkcs.10087	from CCDE,EBAMUS,1020922	Clean cif: modify excressive H	1404	s1	n.d.	n.d.	n.d.	n.d.	1257.1	0.307	9.20	3.86
177	HV-MOF-1(Er)	10.1021/acs.inorgchem.8b03042	from CCDC,BIWDET,1864545	Clean cif: remove solvent	165	s2	n.d.	n.d.	24	d3	0.0	0.000	3.95	1.36
178	IPM-MOF-201(Ni)	10.1016/j.isci.2018.04.004	from CCDC,GEYQEJ,1561299	True cif	n.d.	n.d.	n.d.	n.d.	12.78	d3	1813.1	0.509	9.03	3.84
179	ISE-1(Ni)	10.1021/ja808444z	n.d.	n.d.	n.d.	n.d.	0.51	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
180	JUC-110	10.1039/C2cc33023g	from CCDC,XEFPUV,854096	True cif	n.d.	n.d.	n.d.	n.d.	4.5	d3	370.5	0.130	6.31	3.81

181	JUK-8(Zn)	10.5517/ccdc.csd.cc27ks9x	from CCDC,EDEQAJ,2072669	True cif	n.d.	n.d.	0.256	v1	n.d.	n.d.	0.0	0.000	3.44	2.34
182	kag-MOF-1(Zn)	10.1016/j.chempr.2017.09.002	from CCDC,ZEPDOQ,1491855	Clean cif: remove solvent	210	s1	0.12	v1	4.6	d2	224.0	0.081	5.55	4.62
183	KMF-1(Al)	10.1038/s41467-020-18968-7	from CCDC,KUZPUT,1984701	False cif: lake of H atom	1130	s1	0.473	v1	6	d1	n.d.	n.d.	n.d.	n.d.
184	La(pyzdc)L5	10.1002/chem.201403241	from CCDC,MOMJIJ,973063	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	2.05	0.95
185	LA^1-Zr6^12-shp	10.1021/jacs.9b02947	from CCDC,IPARID,1894279	False cif: unmodifiy excressive atom	2486	s1	0.94	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
186	LA^1-Zr6^8-csq	10.1021/jacs.9b02947	from CCDC,IPAQOI,1843117	True cif	3150	s1	2.18	v1	47	d3	3523.4	2.127	39.02	38.42
187	LA^1-Zr6^8-flu	10.1021/jacs.9b02947	from CCDC,TOGMIO,1843116	True cif	2850	s1	1.31	v1	38.6	d3	3434.9	0.890	9.94	7.99
188	LA^2-Zr6^12-shp	10.1021/jacs.9b02947	n.d.	n.d.	2250	s1	0.89	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
189	LA^2-Zr6^8-csq	10.1021/jacs.9b02947	n.d.	n.d.	n.d.	n.d.	2	v1	47	d3	n.d.	n.d.	n.d.	n.d.
190	LA^3-Zr6^8-flu	10.1021/jacs.9b02947	from CCDC,IPAQUO,1843118	True cif	2950	s1	1.01	v1	n.d.	n.d.	4092.7	1.717	19.43	10.46
191	Lanthanum Triazolyl Phosphonate MOF	10.1039/c5dt02651b	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	19	d2	n.d.	n.d.	n.d.	n.d.
192	LB^1-Zr6^8-flu	10.1021/jacs.9b02947	from CCDC,IPAQIC,1446339	True cif	2450	s1	0..94	v1	n.d.	n.d.	3268.9	1.100	11.64	7.56
193	LB^2-Zr6^8-csq	10.1021/jacs.9b02947	from CCDC,IPARAV,1843119	Clean cif: modify excressive atom	n.d.	n.d.	1.41	v1	n.d.	n.d.	3007.7	0.970	12.04	8.20
194	LB^2-Zr6^8-scu	10.1021/jacs.9b02947	n.d.	n.d.	n.d.	n.d.	0.96	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
195	LB^3-Zr6^8-flu	10.1021/jacs.9b02947	n.d.	n.d.	2542	s1	0.9	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
196	LC^1-Zr6^12-fcu	10.1021/jacs.9b02947	n.d.	n.d.	n.d.	n.d.	0.92	v1	34.5	d3	n.d.	n.d.	n.d.	n.d.
197	LC^2-Zr6^12-fcu	10.1021/jacs.9b02947	n.d.	n.d.	2105	s1	0.61	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
198	LC^3-Zr6^8-bcu	10.1021/jacs.9b02947	n.d.	n.d.	n.d.	n.d.	0.54	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
199	MAF-4.23-7.77	10.1002/adma.201004028	n.d.	n.d.	1870	s1	0.64	v1	11	d3	n.d.	n.d.	n.d.	n.d.
200	MAF-4.49-7.51	10.1002/adma.201004028	n.d.	n.d.	1870	s1	0.65	v1	11	d3	n.d.	n.d.	n.d.	n.d.
201	MAF-4.76-7.24	10.1002/adma.201004028	n.d.	n.d.	1870	s1	0.64	v1	11	d3	n.d.	n.d.	n.d.	n.d.
202	MAF-7(Zn)	10.1002/adma.201004028	from CCDC,EMAPAK,787579	Clean cif: remove solvent	1874	s1	0.67	v1	11.2	d3	1421.1	0.480	11.18	3.65
203	Me-FeCr	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
204	MFU-4	10.1039/B904280f	from CCDC,IGOCUD,723715	True cif	1611	s2	0.42	v2	n.d.	n.d.	0.0	0.000	12.13	2.27
205	Mg-CPO-27 (MOF-74)	10.1039/C4cs00078a	from RASPA	True cif	1400	s1	0.65	v1	11	d2	1707.7	0.667	11.87	11.05
206	Mg-CUK-1	10.5517/cc13d960	from CCDC,NUDLOP,1024711	True cif	580	s1	0.28	v1	13.4	d1	985.6	0.302	6.24	5.60
207	Mg-MOF-74©	10.5517/ccdc.csd.cc20k4pf	repeat with CPO-27-Mg	n.d.	1525	s1	0.62	v1	11	d2	n.d.	n.d.	n.d.	n.d.
208	MIL-100	10.1016/j.ijheatmasstransfer.2012.07.068	n.d.	n.d.	1600	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
209	MIL-100(Al)	10.1016/j.cej.2015.10.098	n.d.	n.d.	1786	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
210	MIL-100(Cr)	10.1021/acs.jpcc.5b06660	from RASPA	Clean cif: find symmetry	1871	s1	1.02	v1	29	d2	1918.3	0.844	26.60	8.94
211	MIL-100(Cr)(X=Cl)	10.1246/cl.2010.360	n.d.	n.d.	1522	s1	0.7	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
212	MIL-100(Cr)(X=SO4)	10.1246/cl.2010.360	n.d.	n.d.	1452	s1	0.7	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
213	MIL-100(Cr)-DEG	10.1016/j.ica.2013.07.024	n.d.	n.d.	580	s1	0.5	v1	12	d2	n.d.	n.d.	n.d.	n.d.
214	MIL-100(Cr)-EG	10.1016/j.ica.2013.07.024	n.d.	n.d.	710	s1	0.47	v1	12	d2	n.d.	n.d.	n.d.	n.d.

215	MIL-100(Cr)-EN	10.1016/j.ica.2013.07.024	n.d.	n.d.	640	s1	0.42	v1	15	d2	n.d.	n.d.	n.d.	n.d.
216	MIL-100(Cr)-TEG	10.1016/j.ica.2013.07.024	n.d.	n.d.	680	s1	0.53	v1	12	d2	n.d.	n.d.	n.d.	n.d.
217	MIL-100(Fe)	10.1016/j.ijheatmasstransfer.2012.07.068	from RASPA	True cif	1549	s1	0.82	v2	29	d2	1930.8	0.881	26.60	11.51
218	MIL-100V	10.1016/j.jcis.2015.06.036	n.d.	n.d.	1203	s1	0.74	v1	11	d1	n.d.	n.d.	n.d.	n.d.
219	MIL-101(Al)-NH2	10.1002/chem.201404654	n.d.	n.d.	3363	s1	1.67	v1	25	d2	n.d.	n.d.	n.d.	n.d.
220	MIL-101(Al)-URPh	10.1002/chem.201404654	n.d.	n.d.	1555	s1	0.83	v1	18	d2	n.d.	n.d.	n.d.	n.d.
221	MIL-101(Cr)-pCOOH	10.1039/C4TA04907A	n.d.	n.d.	2380	s1	1.26	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
222	MIL-101(Cr)-pMal	10.1039/C4TA04907A	n.d.	n.d.	1670	s1	0.89	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
223	MIL-101(Cr)-pUR2	10.1039/C4TA04907A	n.d.	n.d.	1330	s1	0.64	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
224	MIL-101-NH2	10.1016/j.micromeso.2012.01.015	n.d.	n.d.	2509	s1	1.27	v1	34	d2	n.d.	n.d.	n.d.	n.d.
225	MIL-101-SO3H	10.1016/j.micromeso.2012.01.015	n.d.	n.d.	1920	s1	0.94	v1	34	d2	n.d.	n.d.	n.d.	n.d.
226	MIL-101V	10.1016/j.jcis.2015.06.036	n.d.	n.d.	2705	s1	1.4	v1	21	d1	n.d.	n.d.	n.d.	n.d.
227	MIL-125	10.1016/j.cattod.2012.08.014	n.d.	n.d.	1510	s1	0.68	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
228	MIL-125(Ti)-NH3^3+Cl-	10.1016/j.cej.2019.05.121	n.d.	n.d.	1388	s1	0.5	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
229	MIL-125(Ti)-NHCyp	10.1021/acsami.7b15045	n.d.	n.d.	510	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
230	MIL-125(Ti)-NHMe	10.1021/acsami.7b15045	n.d.	n.d.	1047	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
231	MIL-125-NH2	10.1039/C4cs00078a	n.d.	n.d.	1220	s1	0.55	v1	12	d2	n.d.	n.d.	n.d.	n.d.
232	MIL-160	10.1002/adma.201502418	form CCDC,PIBZUY01,1969089	False cif: no atom	1070	s1	0.398	v1	5	d3	n.d.	n.d.	n.d.	n.d.
233	MIL-163	10.1002/anie.201507058	from CCDC,WUTBEU,1415776	Clean cif: remove solvent	170	s1	n.d.	n.d.	12	d3	2175.9	0.907	12.65	12.46
234	MIL-47(V)-F	10.1039/C3CP44204G	n.d.	n.d.	1078	s1	0.36	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
235	MIL-47(V)-F2	10.1016/j.micromeso.2013.07.030	n.d.	n.d.	987	s2	0.34	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
236	MIL-53(Al)-(OH)0.34(NH2)0.66	10.1002/asia.201301673	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
237	MIL-53(Al)-(OH)0.53(NH2)0.47	10.1002/asia.201301673	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
238	MIL-53(Al)-(OH)0.68(NH2)0.32	10.1002/asia.201301673	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
239	MIL-53(Al)-(OH)2	10.1021/ic201219g	n.d.	n.d.	n.d.	n.d.	0.07	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
240	MIL-53(Al)-Br	10.1021/ic201219g	n.d.	n.d.	n.d.	n.d.	0.14	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
241	MIL-53(Al)-CH3	10.1021/ic201219g	n.d.	n.d.	n.d.	n.d.	0.32	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
242	MIL-53(Al)-Cl	10.1021/ic201219g	n.d.	n.d.	n.d.	n.d.	0.32	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
243	MIL-53(Al)-F	10.1039/C3CP44204G	n.d.	n.d.	1137	s1	0.48	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
244	MIL-53(Al)-F2	10.1016/j.micromeso.2013.07.030	n.d.	n.d.	467	s2	0.16	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
245	MIL-53(Al)ht	10.1039/C3cc42287a	n.d.	n.d.	1489	s1	0.56	v1	8.5	d2	n.d.	n.d.	n.d.	n.d.
246	MIL-53(Al)it	10.1039/C3cc42287a	n.d.	n.d.	1031	s1	0.72	v1	34	d2	n.d.	n.d.	n.d.	n.d.
247	MIL-53(Al)-NH2	10.1039/C4NJ00076E	n.d.	n.d.	940	s1	0.37	v1	13	d3	n.d.	n.d.	n.d.	n.d.
248	MIL-53(Al)-NO2	10.1021/ic201219g	n.d.	n.d.	n.d.	n.d.	0.34	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
249	MIL-53(Al)-OH	10.1021/ja109810w	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
250	MIL-53(Al)-TDC	10.1039/C8TA04407D	n.d.	n.d.	1150	s1	0.48	v1	8.2	d3	n.d.	n.d.	n.d.	n.d.

251	MIL-53(Cr)	10.1021/ja1023282	from RASPA	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.06	2.47
252	MIL-53(Fe)-(COOH)2	10.1021/ja109810w	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
253	MIL-53(Ga)	10.5517/ccrnhb6	from CCDC,QOVWOO,704888	Clean cif: remove solvent	1230	s1	0.47	v1	20	d3	0.0	0.000	3.16	2.83
254	MIL-53(Ga)-NH2	10.1039/C4NJ00076E	n.d.	n.d.	210	s1	n.d.	n.d.	20	d3	n.d.	n.d.	n.d.	n.d.
255	MIL-68(In)	10.5517/ccdc.csd.cc1ytby1	from CCDC,VIFPUY,1811824	True cif	1110	s1	0.42	v1	16	d3	1324.7	0.569	14.84	14.54
256	MIL-68(In)-NH2	10.5517/ccdc.csd.cc1z7p41	from CCDC,MIQXIW,1824633	False cif: unmodifiy excressive atom	850	s1	0.3	v1	16	d3	n.d.	n.d.	n.d.	n.d.
257	MIL-91(Ti)	10.1039/C5TA09349J	n.d.	n.d.	403	s1	0.16	v1	4	d3	n.d.	n.d.	n.d.	n.d.
258	MIP-200	10.1038/s41560-018-0261-6	from CCDC,MIHZIP,1834834	True cif	1000	s1	0.4	v1	13	d1	1262.6	0.446	14.85	13.19
259	Mn2(Gd-H-DOTA-4AmP)(H2O)7	10.1039/C6CC02908F	from CCDC,PEHFUG,1471149	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1041.2	0.273	6.88	5.47
260	Mn2Cl2(BTDD)	10.1021/acscentsci.7b00186	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	22	d1	n.d.	n.d.	n.d.	n.d.
261	MOF-1(Ce,Eu)	10.1002/adma.201701804	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
262	MOF-303(Al)	10.5517/ccdc.csd.cc27s2dj	from CCDC,CAMTET,2078717	True cif	1119	s1	0.58	v1	n.d.	n.d.	1404.7	0.428	6.54	5.76
263	MOF-74(Ni)-BPP	10.1021/jacs.7b04872	n.d.	n.d.	n.d.	n.d.	0.88	v1	17	d2	n.d.	n.d.	n.d.	n.d.
264	MOF-74(Ni)-TPP	10.1021/jacs.7b04872	n.d.	n.d.	n.d.	n.d.	1.14	v1	23	d2	n.d.	n.d.	n.d.	n.d.
265	MOS-1(Co)	10.1021/acssuschemeng.7b00460	n.d.	n.d.	1112	s1	n.d.	n.d.	13.9	d3	n.d.	n.d.	n.d.	n.d.
266	MOS-2(Co)	10.1021/acssuschemeng.7b00460	n.d.	n.d.	76	s1	n.d.	n.d.	7.6	d3	n.d.	n.d.	n.d.	n.d.
267	MOS-3(Co)	10.1021/acssuschemeng.7b00460	n.d.	n.d.	27	s1	n.d.	n.d.	7.5	d3	n.d.	n.d.	n.d.	n.d.
268	MUF-77(Zn)-butyl	10.1021/jacs.5b00365	from CCDC,YUKBIR,1409924	True cif	3250	s1	1.21	v1	13.6	d2	3714.4	0.940	14.59	6.22
269	MUF-77(Zn)-decyl	10.1021/jacs.5b00365	from CCDC,YUKCAK,1409927	True cif	1170	s1	0.48	v1	n.d.	n.d.	4343.1	1.171	16.26	6.43
270	MUF-77(Zn)-ethyl	10.1021/jacs.5b00365	from CCDC,YUKMUO,149923	False cif: unmodifiy excressive atom	3600	s1	1.55	v1	18.5	d2	n.d.	n.d.	n.d.	n.d.
271	MUF-77(Zn)-hexyl	10.1021/jacs.5b00365	from CCDC,YUKBOX,1409925	True cif	2170	s1	1	v1	11.2	d2	4357.7	1.163	16.41	6.25
272	MUF-77(Zn)-methyl	10.1021/jacs.5b00365	from CCDC,YUKMOI,1409922	True cif	3600	s1	1.85	v1	21.1	d2	4437.3	1.677	21.78	7.63
273	MUF-77(Zn)-octyl	10.1021/jacs.5b00365	from CCDC,YUKBUD,1409926	True cif	1570	s1	0.65	v1	n.d.	n.d.	4293.4	1.163	16.71	6.33
274	MUF-7a(Zn)	10.5517/cc12mr4l	from CCDC,BOCNAK,1002079	False cif: unmodifiy excressive atom	4450	s1	2.16	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
275	NBu4	10.1039/C4cs00078a	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
276	NENU-11	10.1021/Ja109659k	from CCDC,EWESEF,715939	Clean cif: remove solvent	572	s1	0.39	v1	n.d.	n.d.	1111.0	0.328	11.15	6.65
277	Ni(BTTB)	10.1039/C4TA01372G	n.d.	n.d.	391	s1	0.2	v1	4.3	d1	n.d.	n.d.	n.d.	n.d.
278	Ni(dpip)2.5DMF	10.1021/acsami.0c21554	from CCDC,BALWUK,2047212	True cif	1441.6	s2	n.d.	n.d.	10	d2	2100.6	0.589	9.83	7.70
279	Ni25Zn75-MOF-74	10.1002/ejic.201800042	n.d.	n.d.	1160	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
280	Ni2Cl2(BTDD)	10.1021/acscentsci.7b00186	n.d.	n.d.	1762	s1	n.d.	n.d.	22	d1	n.d.	n.d.	n.d.	n.d.
281	Ni2Cl2BBTA	10.1021/jacs.8b09655	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	13	d3	n.d.	n.d.	n.d.	n.d.
282	Ni3C87H118N12O29	10.1021/Ic200381f	from CCDE,EZOFOP,802891	True cif	n.d.	n.d.	0.68	v1	16	d2	0.0	0.000	16.10	1.41
283	Ni50Zn50-MOF-74	10.1002/ejic.201800042	n.d.	n.d.	1190	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
284	Ni75Zn25-MOF-74	10.1002/ejic.201800042	n.d.	n.d.	1200	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
285	Ni8(L1)6	10.1002/anie.201303484	from CCDC,BIBYES,931408	False cif: unmodifiy	205	s1	0.52	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

				excressive atom										
286	Ni8(L2)6	10.1002/anie.201303484	from CCDC,BIBYAO,931409	False cif: unmodifiy excressive atom	990	s1	0.52	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
287	Ni8(L3)6	10.1002/anie.201303484	from CCDC,BIBXUH,931410	Clean cif: remove solvent	1770	s1	1.21	v1	n.d.	n.d.	2526.2	0.818	14.76	4.99
288	Ni8(L4)6	10.1002/anie.201303484	from CCDC,BIBXOB,931411	Clean cif: remove solvent	1920	s1	0.97	v1	n.d.	n.d.	5069.4	1.917	19.73	7.76
289	Ni8(L5-(CF3)2)6	10.1002/anie.201303484	from CCDC,BIBXIV,931412	False cif: unmodifiy excressive atom	2195	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
290	NI8(L5-(CH3)2)6	10.1002/anie.201303484	n.d.	n.d.	1985	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
291	Ni-CUK-1	10.1021/acsami.9b02605	n.d.	n.d.	520	s1	0.26	v1	13.4	d1	n.d.	n.d.	n.d.	n.d.
292	Ni-DOBDC	10.5517/ccdc.csd.cc1m5dsz	from CCDC,ORIVUI ,1494751	Clean cif: remove solvent	639	s1	0.362	v1	11	d2	1240.5	0.493	11.85	11.05
293	Ni-MOF	10.1039/C8CC05428B	n.d.	n.d.	1960	s1	0.71	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
294	NU-1000(Zr)	10.1021/ja408959g	from CCDC,1459134	True cif	2320	s1	1.4	v1	31	d2	3327.3	1.749	31.07	30.38
295	NU-1000(Zr)-SALI-1	10.1021/ja408959g	n.d.	n.d.	1710	s1	1	v1	30	d2	n.d.	n.d.	n.d.	n.d.
296	NU-1000(Zr)-SALI-7	10.1021/ja408959g	ftom CCDC,1459133	True cif	900	s1	0.6	v1	28	d2	2407.5	0.792	17.35	14.34
297	NU-1000(Zr)-SALI-9	10.1021/ja408959g	n.d.	n.d.	870	s1	0.6	v1	28	d2	n.d.	n.d.	n.d.	n.d.
298	NU-1000(Zr)-TFA	10.1021/acsanm.1c00638	n.d.	n.d.	1880	s1	n.d.	n.d.	31	d3	n.d.	n.d.	n.d.	n.d.
299	NU-901(Zr)-TFA	10.1021/acsanm.1c00638	n.d.	n.d.	1980	s1	n.d.	n.d.	11	d3	n.d.	n.d.	n.d.	n.d.
300	NU-905(Zr)-TFA	10.1021/acsanm.1c00638	n.d.	n.d.	2055	s1	n.d.	n.d.	20	d3	n.d.	n.d.	n.d.	n.d.
301	PCP-1(La)	10.1039/C3SC52177J	from CCDC,CIQQIE,946972	Clean cif: remove solvent	n.d.	n.d.	0.1218	v1	n.d.	n.d.	597.3	0.135	6.88	3.67
302	Pip-CPO-27-Ni	10.1039/C2dt31112g	n.d.	n.d.	46.7	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
303	PIZOF-2	10.1021/Ja500330a	n.d.	n.d.	2080	s1	0.88	v1	17.6	d2	n.d.	n.d.	n.d.	n.d.
304	pretreated a-Al	10.1039/c5ce00789e	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
305	pretreated m-Al	10.1039/c5ce00789e	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
306	SALI-5(Zr)	10.1039/C5SC01784J	n.d.	n.d.	1270	s1	0.85	v1	29	d2	n.d.	n.d.	n.d.	n.d.
307	SALI-9(Zr)	10.1039/C5SC01784J	n.d.	n.d.	900	s1	0.63	v1	27.5	d2	n.d.	n.d.	n.d.	n.d.
308	SALI-9'(Zr)	10.1039/C5SC01784J	n.d.	n.d.	1190	s1	0.87	v1	29.6	d2	n.d.	n.d.	n.d.	n.d.
309	SALI-BA(Zr)	10.1039/C5SC01784J	n.d.	n.d.	2005	s1	1.21	v1	27.8	d2	n.d.	n.d.	n.d.	n.d.
310	SIFSIX-14-Cu-i	10.1021/jacs.7b01682	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
311	SIFSIX-1-Cu	10.1021/jacs.7b01682	from CCDC,XEBTAC,1525206	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	3.75	3.52
312	SIFSIX-2-Cu-i	10.1021/jacs.7b01682	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
313	SIFSIX-3-Ni	10.1021/jacs.7b01682	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
314	SIM-1	10.1039/C4cs00078a	n.d.	n.d.	470	s1	0.23	v1	6	d2	n.d.	n.d.	n.d.	n.d.
315	S-MIL-53(Al)	10.5517/cc7df56	from CCDC,SABWAU,220477	False cif: disorder structure	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
316	SNU-80	10.1002/chem.201103078	from CCDC,RAKJIY,842625	False cif: unmodifiy excressive atom	456	s1	0.18	v1	7	d3	n.d.	n.d.	n.d.	n.d.
317	STAM-17(Cu)-Oet	10.1038/s41557-018-0104-x	from CCDC,ZIFVOC,1566115	True cif	58.42	s1	n.d.	n.d.	n.d.	n.d.	0.0	0.000	5.26	3.57
318	TAF-1a	10.1002/chem.201204458	from CCDC,GEZRAG,886640	False cif: unmodifiy excressive atom	268.5	s1	n.d.	n.d.	4.6	d2	n.d.	n.d.	n.d.	n.d.

319	ThrZnOAc	10.1039/C3CE41083H	from CCDC,KIGCEK,943050	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	636.5	0.192	7.60	7.42
320	Ti(pyradine-2-carboxylic acid)	10.1002/bkcs.10087	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
321	TUC-110(Cd)	10.1039/C2CC33023G	from CCDC,XEFPUV,854096	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	370.5	0.130	6.31	3.81
322	UiO-66	10.1021/Ja500330a	from RASPA	True cif	1290	s1	0.49	v1	8.4	d2	1059.0	0.320	8.46	3.81
323	UiO-66(Hf)-(OH)2	10.1002/aic.15837	n.d.	n.d.	920	s1	0.4	v1	5.85	d2	n.d.	n.d.	n.d.	n.d.
324	UiO-66(Zr)-(C2H5)2	10.1039/C5DT02908B	n.d.	n.d.	340	s1	0.16	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
325	UiO-66(Zr)-(CF3)2	10.1039/C5DT02908B	n.d.	n.d.	630	s1	0.3	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
326	UiO-66(Zr)-(CH3)2	10.1039/C5DT02908B	n.d.	n.d.	790	s1	0.35	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
327	UiO-66(Zr)-(COOH)2	10.1002/anie.201302682	n.d.	n.d.	415	s1	0.21	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
328	UiO-66(Zr)-(OH)2	10.1002/aic.15837	n.d.	n.d.	1230	s1	0.56	v1	5.85	d2	n.d.	n.d.	n.d.	n.d.
329	UiO-66(Zr)-1,4-Napthyl	10.1021/la3035352	n.d.	n.d.	757	s1	0.4	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
330	UiO-66(Zr)-2,5-(oMe)2	10.1021/la3035352	n.d.	n.d.	868	s1	0.38	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
331	UiO-66(Zr)-C2F5	10.1039/C5DT02908B	n.d.	n.d.	570	s1	0.26	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
332	UiO-66(Zr)-CF3	10.1039/C5DT02908B	n.d.	n.d.	815	s1	0.36	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
333	UiO-66(Zr)-CH3	10.1021/jp308657x	n.d.	n.d.	1065	s1	0.51	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
334	UiO-66(Zr)-NH3^3+Cl-	10.1016/j.cej.2019.05.121	n.d.	n.d.	1007	s1	0.35	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
335	UiO-66(Zr)-NO2	10.1021/la3035352	n.d.	n.d.	792	s1	0.42	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
336	UiO-66(Zr4+) with high concentration stearic acid	10.1021/acs.chemmater.5b00665	n.d.	n.d.	n.d.	n.d.	0.574	v1	6.5	d2	n.d.	n.d.	n.d.	n.d.
337	UiO-66(Zr4+) with metal/ligand ratio 6:3	10.1021/acs.chemmater.5b00665	n.d.	n.d.	n.d.	n.d.	0.45	v1	6	d2	n.d.	n.d.	n.d.	n.d.
338	UiO-66D(Zr)	10.1039/C5DT02908B	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
339	UiO-66D(Zr)-(CF3)2	10.1039/C5DT02908B	n.d.	n.d.	2180	s1	0.88	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
340	UiO-66-NH2	10.1021/Ie202327p	n.d.	n.d.	1040	s1	0.57	v1	6	d2	n.d.	n.d.	n.d.	n.d.
341	UiO-67(Zr)	10.1039/C3TA10662D	from RASPA	True cif	2145	s1	n.d.	n.d.	n.d.	n.d.	2747.3	0.787	12.20	6.25
342	UIO-67(Zr)-BIPY	10.1039/C3TA10662D	n.d.	n.d.	2385	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
343	UiO-67(Zr)-BN	10.1021/acs.inorgchem.5b02257	from CCDC,QAJPEZ01,1422390	False cif: unmodifiy excressive atom	1416	s1	0.548	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
344	UMCM-1	10.1021/Ie202328p	n.d.	n.d.	6010	s1	2.41	v1	32	d2	n.d.	n.d.	n.d.	n.d.
345	untreated a-Al	10.1039/c5ce00789e	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
346	untreated m-Al	10.1039/c5ce00789e	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
347	ValZnCl	10.1039/C3CC41842A	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	12.2	d3	n.d.	n.d.	n.d.	n.d.
348	ValZnOAc	10.1039/C3CE41083H	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
349	Y-fum-fcu-MOF	10.1002/anie.201506345	from CCDC,ZAFXAI,1411424	True cif	691	s1	0.28	v1	8	d2	0.0	0.000	5.93	3.64
350	Y-shp-MOF-5	10.1021/jacs.7b04132	from CCDC,HEJFUA ,1545604	False cif: unmodifiy excressive atom	1550	s1	0.63	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
351	ZIF-412(Zn)	10.1021/jacs.7b02272	from CCDC,NEHNAS,1423165	False cif: too many atom	1520	s1	n.d.	n.d.	38.1	d2	n.d.	n.d.	n.d.	n.d.
352	ZIF-71(Zn)	10.5517/ccqj9r8	from CCDC,GITVIP,671080	Clean cif: remove solvent	1183	s1	0.39	v1	n.d.	n.d.	879.3	0.295	17.46	5.71

353	ZIF-8	10.1021/ic200937u	from RASPA	True cif	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	11.39	3.41
354	ZIF-8_50-90_50	10.1021/acssuschemeng.7b02604	n.d.	n.d.	1350	s1	0.61	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
355	ZIF-8_55-71_45	10.1021/acssuschemeng.7b02604	n.d.	n.d.	630	s1	0.29	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
356	ZIF-8_70-90_30	10.1021/acssuschemeng.7b02604	n.d.	n.d.	1310	s1	0.61	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
357	ZIF-90(Zn)	10.5517/ccr8r2t	from CCDC,WOJGEI,693596	False cif: unmodifiy excressive atom	1280	s1	0.49	v1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
358	Zn(BTTB)	10.1039/C4TA01372G	n.d.	n.d.	447	s1	0.25	v1	4.47	d1	n.d.	n.d.	n.d.	n.d.
359	Zn(BTTB)(AZPY)	10.1039/C4TA01372G	n.d.	n.d.	647	s1	0.36	v1	4.94	d1	n.d.	n.d.	n.d.	n.d.
360	Zn(BTTB)(BDC)	10.1039/C4TA01372G	from CCDC,GOSDID,986373	Clean cif: remove solvent	441	s1	0.21	v1	4.24	d1	949.8	0.253	7.14	3.96
361	Zn(BTTB)(BPY)	10.1039/C4TA01372G	from CCDC,GOSDUP,986374	False cif: unmodifiy excressive atom	841	s1	0.38	v1	4.06	d1	n.d.	n.d.	n.d.	n.d.
362	Zn(BTTB)(DMBPY)	10.1021/la503269f	n.d.	n.d.	749	s1	0.27	v1	4.41	d1	n.d.	n.d.	n.d.	n.d.
363	Zn(DM)0.5(AT)	10.1021/ic402095u	from CCDC,PITRIV,976591	Clean cif: remove solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0	0.000	4.42	3.00
364	Zn(II)-MOF [Zn(HPylmDC)(DMA)]n	10.1039/C4dt00230j	n.d.	n.d.	185.6	s1	n.d.	n.d.	4.425	d1	n.d.	n.d.	n.d.	n.d.
365	Zn(L)(tdca)*1.5DMF	10.1080/00958972.2014.957689	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	6.6	d3	n.d.	n.d.	n.d.	n.d.
366	Zn(NDI-H)	10.1039/C3ee40876k	n.d.	n.d.	1460	s1	n.d.	n.d.	16	d3	n.d.	n.d.	n.d.	n.d.
367	Zn(NDI-NHEt)	10.1039/C3ee40876k	n.d.	n.d.	1236	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
368	Zn(NDI-SEt)	10.1039/C4cs00078a	n.d.	n.d.	888	s1	n.d.	n.d.	16	d2	n.d.	n.d.	n.d.	n.d.
369	Zn(NDI-SO2Et)	10.1039/C4cs00078a	n.d.	n.d.	764	s1	n.d.	n.d.	16	d2	n.d.	n.d.	n.d.	n.d.
370	Zn(NDI-SOEt)	10.1039/C4cs00078a	n.d.	n.d.	927	s1	n.d.	n.d.	16	d2	n.d.	n.d.	n.d.	n.d.
371	Zn(NO3)2*6H2O	10.1002/chem.200500963	from CCDC,CEKNIQ,260571	True cif	n.d.	n.d.	0.17	v1	17.3	d3	3634.1	1.670	19.35	12.34
372	Zn2(bptc)	10.1021/ja060946u	from CCDC,HENYUV,623824	Clean cif: remove solvent	313	s1	0.15	v1	n.d.	n.d.	0.0	0.000	4.24	2.98
373	Zn2C14N2O8H4	10.1021/Ja060946u	from CCDC,HESVOR,623825	True cif	312.7	s1	0.146	v1	5.2	d2	0.0	0.000	4.41	3.00
374	Zn2Co3(MFU-4I)	10.1039/C8SC00112J	n.d.	n.d.	3544	s1	n.d.	n.d.	16.2	d2	n.d.	n.d.	n.d.	n.d.
375	Zn3(TCPB)2(H2O)2	10.1039/C3dt50896j	from CCDC,ZESQIZ01,924304	True cif	284	s1	n.d.	n.d.	4.3	d2	982.0	0.265	4.71	4.17
376	Zn3Co2(MFU-4I)	10.1039/C8SC00112J	n.d.	n.d.	3037	s1	n.d.	n.d.	16.1	d2	n.d.	n.d.	n.d.	n.d.
377	Zn3L2	10.1021/cg301559s	from CCDC,SEQRUD,855035	True cif	535	s1	n.d.	n.d.	4.5	d3	884.9	0.225	4.70	3.97
378	Zn4O(dmcapz)3	10.1021/Ja2042113	from CCDC,OYODIQ,817665	False cif: unmodifiy excressive atom	840	s1	0.45	v2	6	d2	n.d.	n.d.	n.d.	n.d.
379	Zn5(MFU-4I)	10.1039/C8SC00112J	n.d.	n.d.	3525	s1	n.d.	n.d.	16.5	d2	n.d.	n.d.	n.d.	n.d.
380	Zn-BTTB-DMBPY	10.1021/La503269f	n.d.	n.d.	749	s1	0.269	v1	4.41	d2	n.d.	n.d.	n.d.	n.d.
381	ZnCo4(MFU-4I)	10.1039/C8SC00112J	n.d.	n.d.	3091	s1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
382	Zn-MOF-74(cycle 1)	10.5517/ccdc.csd.cc20k4mc	from CCDC,TODZAQ,1863522	True cif: save bound solvent	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	78.1	0.029	4.59	3.87
383	Zn-Trimesate	10.1021/jp4036327	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	5	d1	n.d.	n.d.	n.d.	n.d.
384	Zr-Fum HT	10.1021/acsami.0c15901	n.d.	n.d.	1020	s1	0.553	v1	7.5	d2	n.d.	n.d.	n.d.	n.d.
385	Zr-MOF-801-P	10.1021/Ja500330a	from CCDC,BOHKAM,1002678	True cif	990	s1	0.45	v1	7.4	d2	0.0	0.000	7.65	3.33

386	Zr-MOF-801-SC	10.1021/Ja500330a	from CCDC,BOHJOZ,1002676	Clean cif: remove solvent	690	s1	0.27	v1	7.4	d2	0.0	0.000	7.47	3.42
387	Zr-MOF-802	10.1021/Ja500330a	from CCDC,BOHXED,1002674	False cif: unremove solvent	20	s1	0.01	v1	5.6	d2	n.d.	n.d.	n.d.	n.d.
388	Zr-MOF-804	10.1021/Ja500330a	n.d.	n.d.	1145	s1	0.46	v1	7.2	d2	n.d.	n.d.	n.d.	n.d.
389	Zr-MOF-805	10.1021/Ja500330a	n.d.	n.d.	1230	s1	0.48	v1	9.5	d2	n.d.	n.d.	n.d.	n.d.
390	Zr-MOF-806	10.1021/Ja500330a	from CCDC,BOHXAZ,1002673	False cif: unmodifiy excressive atom	2220	s1	0.85	v1	12.6	d2	n.d.	n.d.	n.d.	n.d.
391	Zr-MOF-808	10.1021/Ja500330a	from CCDC,BOHWUS,1002672	False cif: unmodifiy excressive atom	2060	s1	0.84	v1	18.4	d2	n.d.	n.d.	n.d.	n.d.
392	Zr-MOF-841	10.1021/Ja500330a	from CCDC,BOHWIG,1002670	True cif	1390	s1	0.53	v1	9.2	d2	976.1	0.282	9.00	3.89

n.d. represents no data.

For Exp. S_a Note: s1 represents BET surface area, s2 represents Langmuir surface area, while default (no superscript) is BET surface area.

For Exp. V_a Note: v1 represents pore volume measured based on pore volume based on N_2 adsorption while v2 is based on H_2O adsorption.

For Exp. D_p Note: d1 represents average pore diameter, d2 represents dominant pore size obtained according to pore size distribution, d3 represents largest cavity diameter.

S2. LGCMC and force field parameters

The introduction of input and output files of LGCMC

To execute the LGCMC simulation, there are two requisite input files to build the discretized free energy model. One is a three-dimensional grid model that stores the adsorbent-water interaction, and another is discretized coarse-grained water-water interaction in specific adsorbents. Besides, the operating conditions of water adsorption including temperature and pressure were converted equivalently to the initial chemical potential of water for subsequent LGCMC simulation. Output files including water uptake, the heat of adsorption and water distribution in adsorbents can be obtained.

The force field parameters of water and MOFs in this work

Table S2. The force field parameters of Tip4p water [7]

Molecule	Interaction site	σ (Å)	ε (kJ/mol)	q (eV)
Tip4p water	O	3.154	0.649	0
	H	0	0	0.52
	M	0	0	-1.04

Table S3. The force field parameters of mW water in Eq.1 [8]

Parameter	A	B	p	q	γ
Value	7.049556277	0.6022245584	4	0	1.2
Parameter	a	θ_0 (°)	λ	ε (kcal/mol)	σ (Å)
Value	1.8	109.47	23.15	6.189	2.3925

In molecular simulations, accurate charge assignments to the framework atoms are essential. Accurate charges calculated by the DDEC method (DFT-computed charges)[9] were admitted and usually preferred to use in simulations. However, these calculations are expensive, which could take a few days using tens of CPU cores for each adsorbent (e.g., MOFs). Recently, Zou et al. developed a charge calculation method named the multilayer connectivity-based atom contribution (mCBAC) approach

[10], in essence, which is an automatic procedure of supervised machine learning (ML) for predicting charges according to the type and connectivity of atoms in MOFs. In the mCBAC approach, the ML model is trained from the available DDEC charges of ~2900 Core MOFs, which contributes to the comparable accuracy of mCBAC and DDEC charges while the calculated time of just seconds was required. It has been demonstrated that the accurate charge assignments from mCBAC lead to reliable predictions CO_2 and water adsorption in a large number of MOFs. [10-11] In this work, the usability validation of mCBAC was executed in some typical MOFs (i.e., ZIF-8-Zn, Cu-BTC, CAU-10-Al+H, MIL-53-Cr-lt, UiO-66-Zr and MIP-200-Zr) with different metal sites. The high level of similarity between mCBAC and DDEC charges (Figure S2 about the comparative distribution of mCBAC and DDEC charges of six typical MOFs) proved the accurate and efficient charge assignments for MOFs by mCBAC method. Therefore, mCBAC charges were adopted for all atoms of selected MOFs in this work.

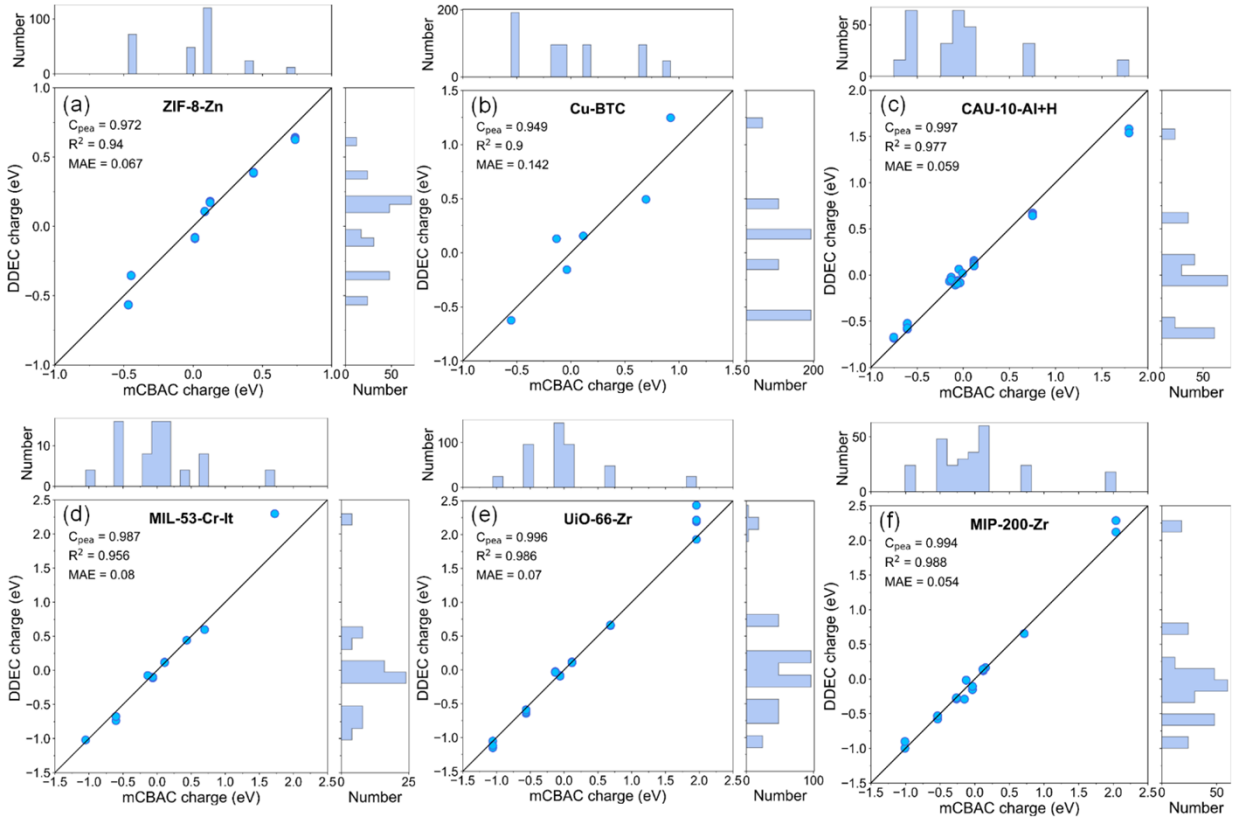

Figure S2. Comparative distribution of mCBAC and DDEC charges of six typical MOFs. (a) ZIF-8-Zn, (b) Cu-BTC, (c) CAU-10-Al+H, (d) MIL-53-Cr-lt, (e) UiO-66-Zr and (f) MIP-200-Zr.

S3. Supplementary results of lattice GCMC (LGCMC) simulation

Table S4. The chemical potentials (μ) for experimental water and mW model corresponding to various relative pressures at 298 K

T (K)	P (Pa)	P/P_0	μ_{exp} (kJ/mol)	μ_{mW} (kJ/mol)
298	315.8	0.1	-51.247	-60.757
298	631.6	0.2	-49.530	-59.039
298	947.4	0.3	-48.526	-58.035
298	1263.2	0.4	-47.813	-57.322
298	1579	0.5	-47.260	-56.770
298	1894.8	0.6	-46.809	-56.318
298	2210.6	0.7	-46.427	-55.936
298	2526.4	0.8	-46.096	-55.605
298	2842.2	0.9	-45.804	-55.314
298	3158	1	-45.543	-55.053
298	6316	2	-43.827	-53.336
298	9474	3	-42.824	-52.333
298	12632	4	-42.112	-51.621
298	15790	5	-41.561	-51.070
298	18948	6	-41.110	-50.619
298	22106	7	-40.729	-50.239

Table S5. The size of crystal unit cell for six MOFs used in this work

Adsorbents	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	No. of sub-cells (1 Å grid size)
MOF-74-Mg	26.14	26.14	6.94	90	90	120	15309

Al(OH)-(1,4-NDC)	21.10	21.10	6.61	90	90	90	9680
MUF-77-Zn+methyl	29.95	29.95	29.95	90	90	90	27000
MIL-100-Fe	51.55	51.55	51.55	120	120	90	140608
MIL-101-Cr	62.84	62.84	62.84	90	60	120	250047
DUT-67-Zr	39.12	39.12	39.12	90	90	90	64000

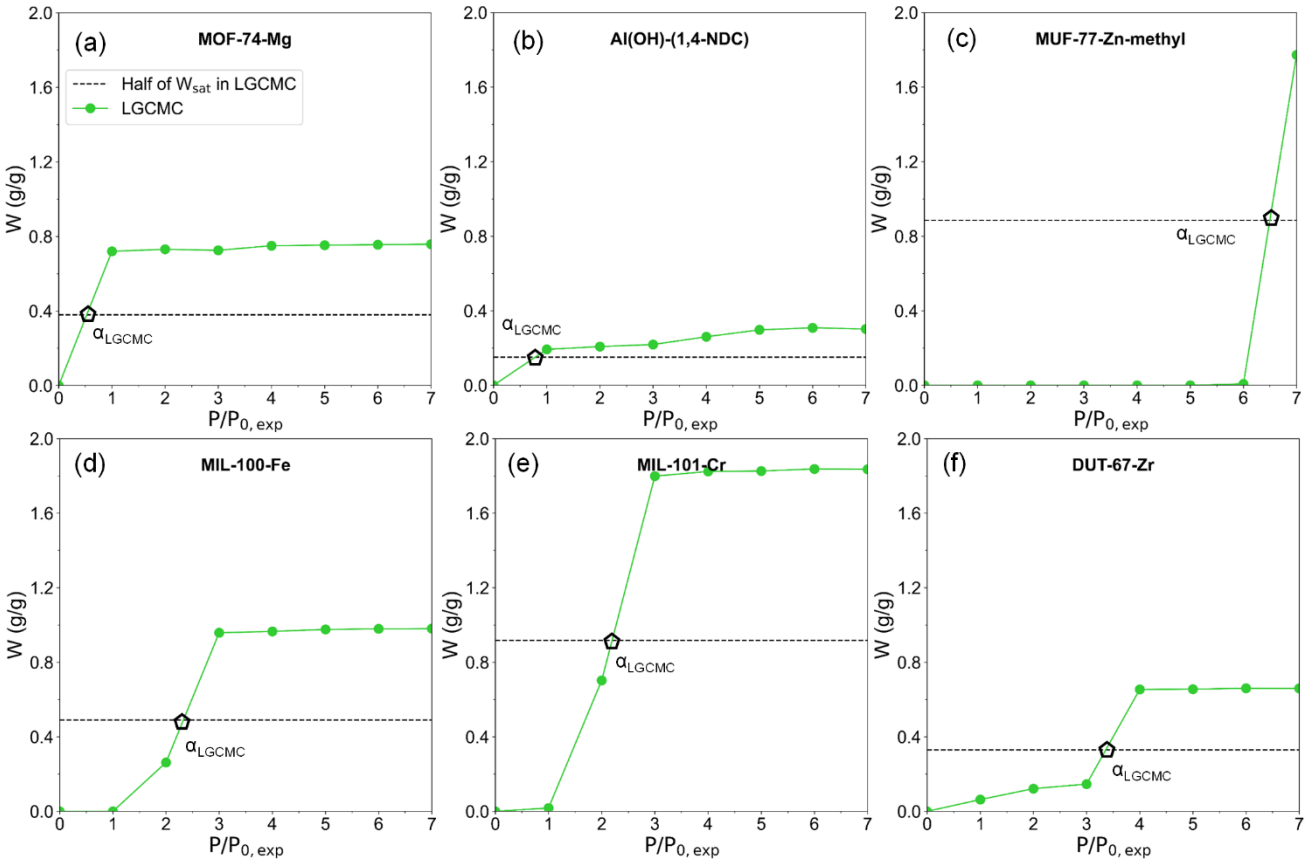

Figure S3. Simulated water adsorption isotherms of used MOFs by LGCMC. The step position of isotherms (α_{LGCMC}, which is considered equal to $P_{c,mW}/P_{0,exp}$ in this work) was defined as the relative pressure when the half of saturation water uptake was reached. α_{LGCMC} of (a) MOF-74-Mg, (b) Al(OH)-(1,4,-NDC), (c) MUF-77-Zn-methyl, (d) MIL-100-Fe, (e) MIL-101-Cr and (f) DUT-67-Zr is regarded as 0.5, 0.5, 6.5, 2.5, 2.5 and 3.5, respectively.

Table S6. The parameter for calculating the corrected chemical potential difference (Δμ) of used MOFs

Adsorbents	LCD (Å)	θ (°)	$P_{c,Kelvin}/P_{0,exp}$	$P_{c,mW}/P_{0,exp}$	Δμ

MOF-74-Mg	11.87	9.5	0.172	0.5	2.650
Al(OH)-(1,4-NDC)	7.48	9.5	0.061	0.5	5.213
MUF-77-Zn+methyl	21.78	82.9	0.887	6.5	4.936
MIL-100-Fe	26.6	24.4	0.484	2.5	4.070
MIL-101-Cr	33.66	24.4	0.563	2.5	3.692
DUT-67-Zr	17.05	63.4	0.573	3.5	4.484

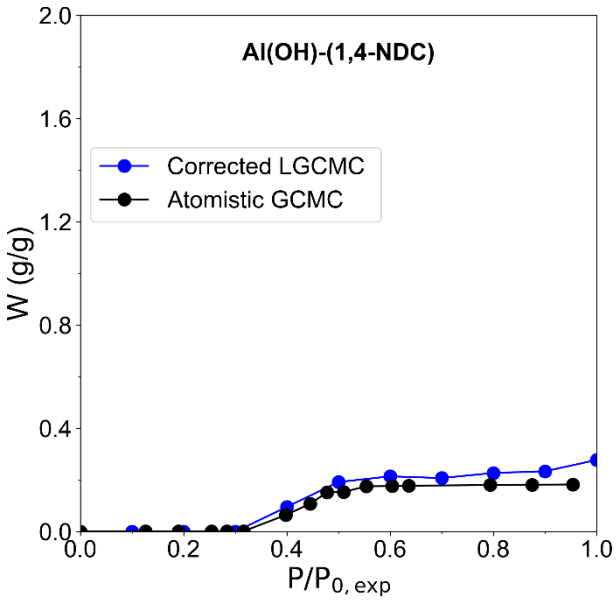

Figure S4. Simulated water adsorption isotherms of MOFs by corrected LGCMC and atomistic GCMC simulation[12] using the same force filed parameters of Al(OH)-(1,4-NDC).

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