Supplementary Material

for

Screening of Metal−Organic Frameworks for Adsorption Heat Transformation under the Guidance of the Structure−Property Relationship

Min Xu[a,b,*], Zhangli Liu[a,b], Xiulan Huai[a,b], Lanting Lou[a,b], Jiangfeng Guo[a,b]

[a] Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing, 100190, China

b University of Chinese Academy of Sciences, Beijing 100049, China

*Corresponding authors. Tel/Fax.: +86-10-82543035;

*E-mail address: xumin@iet.cn

Table S1 Experimental and calculated water adsorption capacities obtained for the MOFs investigated.

Samples	α	q_{max} g/g-1	*q g/g-1*			*Q*a kJ/mol	V_{tot} cm3g−1	S_{BET} m^2/g	ref
			p/p_0=0.1	p/p_0=0.3	p/p_0=0.9				
MIL-101(Cr)	0.45	1	0.063	0.104	0.973				1
MIL-101(Cr)-NH_2	0.42	1.05	0.06	0.14	1.04		1.6	2690	1
MIL-101(Cr)-pNH_2	0.41	1	0.058	0.151	0.998		1.3	2495	1
MIL-101(Cr)-NO_2	0.5	0.45	0.018	0.054	0.416		0.6	1245	1
MIL-101(Cr)-pNO_2	0.48	0.6	0.045	0.109	0.594		1	2195	1
MIL-101(Cr)	0.44	1	0.054	0.1	0.99		1.1	2059	2
MIL-101(Cr)	0.43	1.6				75	1.7	4150±100	3
MIL-101(Cr)	0.46	1.3	0.095	0.14	1.3		1.6	3017	4
MIL-101(Cr)	0.48	1.4	0.076	0.14	1.365	70	1.58	3124	5
MIL-101(Cr)-NH_2	0.42	0.95	0.043	0.087		65	1.27	2146	5
MIL-101(Cr)-NO_2	0.48	0.65	0.013	0.067		40	1.19	2509	5
MIL-101(Cr)-SO_3H	0.28	0.95	0.12	0.371		60	0.94	11920	5
MIL-101(Cr)	0.47	0.87	0.052	0.099	0.87	78	1.22	2500	6
MIL-101(Cr)-NH_2	0.35	0.9	0.076	0.142	0.9		0.97	2080	6
MIL-101(Cr)-NO_2	0.45	0.7	0.037	0.081			0.95	2000	6
MIL-101(Cr)	0.45	0.4	0.087	0.14					7
MIL-101(Al)-NH_2	0.35	0.43	0.37				1.67	3363	8
MIL-101(Al)-URPh	0.4	0.36	0.274	0.344	0.36		0.83	1555	8
MIL-100(Cr)	0.36	0.4	0.044	0.103	0.395		0.77	1330	9
grafted with EG	0.35	0.43	0.037	0.13	0.422		0.47	710	9
grafted with DEG	0.35	0.42	0.037	0.118	0.407		0.5	580	9
grafted with TEG	0.35	0.33	0.033	0.087	0.33		0.53	680	9

grafted with EN	0.35	0.37	0.037	0.148	0.323		0.42	640	9
MIL-100(Cr)	0.45	1.05	0.02	0.04	1.05	82	1.59	3402	74
Li-MIL-100(Cr)	0.38	0.96	0.08	0.19	0.96		0.94	2054	74
Na-MIL-100(Cr)	0.38	0.88	0.02	0.05	0.88		0.91	2001	74
K-MIL-100(Cr)	0.4	0.76	0.02	0.08	0.76		0.72	1547	74
MIL-100(Cr)	0.42	1.22	0.1	0.2	1.22		1.32	2789	75
MIL-100(Cr)/GO-6	0.45	1.58	0.1	0.2	1.58		1.78	3522	75
MIL-100(Cr)	0.45	1.47	0.1	0.12	1.46		1.753	3460	76
MIL-100(Cr)/2%GrO	0.45	1.55	0.1	0.12	1.5		2.14	3674	76
MIL-100(Cr)(X=F)	0.3	0.8	0.093	0.317	0.794		0.93	1517	10
MIL-100(Cr)(X=Cl)	0.31	0.6	0.085	0.283		48	0.7	1522	10
MIL-100(Cr)(X=SO_4)	0.25	0.6	0.093	0.34		48	0.7	1456	10
MIL-100(Fe)	0.35	0.79	0.087	0.258	0.783	82	0.82	1549	4
MIL-100(Fe)	0.29	0.75	0.091	0.398	0.75	92	0.85	1917	11
MIL-100(Fe)	0.38	0.87					0.92	2300±100	3
MIL-100(Al)	0.28	0.5	0.093	0.287	0.5	78	0.8	1814	11
MIL-125(Ti)	0.25	0.36	0.031	0.301	0.357		0.47	1160	6
MIL-125(Ti)-NH_2	0.2	0.45	0.043	0.357	0.441		0.51	1230	6
MIL-125(Ti)-NH_2	0.19	0.35	0.017	0.307	0.35	40	0.45	1220	12
MIL-125(Ti)	0.35	0.3	0.003	0.012	0.295		0.6	1510	13
MIL-125(Ti)-NH_2	0.2	0.52	0.036	0.433	0.518		0.67	1492	13
MIL-125(Ti)-NH_2	0.23	0.683	0.03	0.55	0.65		0.66	1509	73
MIL-91(Ti)	0.02	0.22	0.16	0.18	0.2				82
Mil-127(Fe)	0.3	0.7	0.2	0.35	0.65				82
CAU-1(Al)	0.38	0.55	0.015	0.026	0.387		0.64	1530	14
CAU-1(Al)-$NHCH_3$	0.48	0.4	0.026	0.068	0.522		0.53	1340	14

CAU-1(Al)-$NHCOCH_3$	0.26	0.25	0.045	0.12	0.252		0.3	680	14
UiO-66(Zr)	0.33	0.36	0.051	0.159	0.348	45	0.41	1030	6
UiO-66(Zr)-NH_2	0.15	0.36	0.139	0.267	0.36	89.2	0.35	830	6
UiO-66(Zr)	0.25	0.45	0.075	0.293	0.443		0.52	1160	15
UiO-66(Zr)-NH_2	0.16	0.36	0.132	0.292	0.351		0.57	1040	15
UiO-66(Zr)	0.25	0.5	0.047	0.163	0.494	20	0.77	1032	12
UiO-66(Zr)-NH_2	0.15	0.45	0.036	0.104	0.323	38	0.7	1328	12
UiO-67(Zr)	0.6	0.18	0.014	0.025	0.169	10	0.97	2064	12
UiO-67(Zr)	0.5	0.29	0.024	0.042	0.29			2145	16
UiO-66(Zr)-BIPY	0.2	0.23	0.059	0.16	0.23			2385	16
UiO-66(Zr)	0.34	0.43	0.016	0.1	0.528		0.49	1290	17
UiO-66(Zr)	0.35	0.37	0.025	0.121	0.404		0.52		18
UiO-66(Zr)-CH_3	0.29	0.31	0.024	0.18	0.309		0.51	1065	18
UiO-66(Zr)-$(CH_3)_2$	0.43	0.23	0.008	0.104	0.224		0.4	811	19
UiO-66(Zr)	0.26	0.45	0.019	0.33	0.446		0.55	1120 1089	20
UiO-66(Zr)-NH_2	0.16	0.34	0.137	0.325	0.339		0.52	1187 1059	20
UiO-66(Zr)-1,4-naphthyl	0.25	0.26	0.024	0.141	0.26		0.4	766 747	20
UiO-66(Zr)-NO2	0.18	0.37	0.082	0.323	0.37		0.42	765 819	20
UiO-66(Zr)-2,5-$(OMe)_2$	0.2	0.42	0.103	0.352	0.42		0.38	899 837	20
UiO-66(Zr)-$(COOH)_2$	0.15	0.27	0.036	0.099	0.201		0.21	415	21
MOF-801(Zr)	0.09	0.36	0.224	0.304	0.36	49.33	0.45	990	17
MOF-802(Zr)	0.4	0.09	0.028	0.056	0.088		<0.01	＜20	17
MOF-804(Zr)	0.4	0.23	0.128	0.188	0.23		0.46	1145	17
MOF-805(Zr)	0.31	0.33	0.02	0.128	0.33		0.48	1230	17

MOF-806(Zr)	0.1	0.34	0.024	0.048	0.34		0.85	2220	17
MOF-808(Zr)	0.3	0.59	0.044	0.128	0.588		0.84	2060	17
MOF-841(Zr)	0.22	0.51	0.008	0.44	0.51	45.67	0.53	1390	17
PIZOF-2(Zr)	0.75	0.68	0.003	0.006	0.68		0.67	2080	17
DUT-67(Zr)	0.22	0.5	0.08	0.312	0.5		0.6	1560	17
DUT-51(Zr)	0.63	0.55	0.015	0.031			1.08		22
DUT-52(Zr)	0.35	0.24	0.003	0.035	0.237		0.54	1399	23
DUT-84(Zr)	0.38	0.12	0.004	0.032	0.119		0.27	637	23
DUT-53(Hf)	0.38	0.22	0.004	0.028	0.22		0.31	782	23
DUT-67(Zr)	0.35	0.41	0.034	0.108	0.29		0.44	1767	24
DUT-67(Hf)	0.35	0.29	0.034	0.108	0.29		0.33	1221	24
DUT-68(Zr)	0.4	0.34	0.041	0.112	0.278		0.41	1786	24
DUT-68(Hf)	0.38	0.29	0.041	0.112	0.278		0.34	1299	24
DUT-69(Zr)	0.3	0.26	0.049	0.106	0.185		0.31	1110	24
DUT-69(Hf)	0.28	0.2	0.049	0.106	0.185		0.22	843	24
NU-1000(Zr)	0.75	1					1.4	2320	25
MIP-200(Zr)	0.18	0.45	0.125	0.39	0.45		0.4	1000	79
MIL-163(Zr)	0.55	0.648	0.05	0.108	0.576			90-170	81
MIL-53(Cr)	0.15	0.1	0.009	0.067	0.103			1626	26
MIL-53(Al)	0.09	0.14	0.009	0.074	0.095		0.51	1040	6
MIL-53(Al)-NH_2	0.08	0.04					0.37	940	6
MIL-53(Ga)	0.05	0.02					0.47	1230	6
MIL-53(Ga)-NH_2		0.02						210	6
MIL-53(Al)	0.3	0.09							27
MIL-53(Fe)-$(COOH)_2$	0.05	0.16							27
MIL-53(Al)-OH	0.75	0.4							27

MIL-53(Al)-$(OH)_{0.68}(NH2)_{0.32}$	0.8	0.36							28
MIL-53(Al)-$(OH)_{0.53}(NH2)_{0.47}$	0.88	0.23							28
MIL-53(Al)-$(OH)_{0.34}(NH2)_{0.66}$	0.02	0.11							28
MIL-53(Al)-Cl	0.18	0.14	0.028	0.085	0.14		0.32		29
MIL-53(Al)-Br	0.5	0.11	0.017	0.052	0.11		0.14		29
MIL-53(Al)-CH_3	0.25	0.11	0.018	0.056	0.108		0.32		29
MIL-53(Al)-NO_2	0.1	0.12	0.056	0.07	0.12		0.34		29
MIL-53(Al)-$(OH)_2$	0.65	0.42	0.102	0.128	0.42		0.07		29
MIL-53(Al)-F	0.8	0.07	0.027	0.031	0.059		0.48	1137	30
MIL-53(Al)-F_2	0.7	0.23	0.001	0.004	0.202		0.16	467	31
MIL-47(V)-F	0.6	0.18	0.07	0.164	0.179		0.36	1078	30
MIL-47(V)-F_2	0.7	0.18	0.003	0.008	0.179		0.34	987	31
MIL-53(Al)-NH_2	0.02	0.09							27
MIL-53(Al)ionothermal	0.15	0.08	0.002	0.01	0.076		0.36	1031	32
MIL-53(Al)-SO_3H	0.45	0.45							33
Al(OH)-(1,4-NDC)	0.45	0.16	0.008	0.024	0.153		0.22	546	34
DUT-4(Al)	0.65	0.52	0.005	0.014	0.431		0.79	1360	4
MIL-68(In)	0.58	0.32	0.004	0.004	0.3		0.42	1100	6
MIL-68(In)-NH_2	0.44	0.32	0.009	0.021	0.32		0.3	850	6
MIL-160(Al)	0.08	0.356	0.25	0.35	0.355	65	0.398	1070	80
CAU-10(Al)-H	0.18	0.35	0.007	0.292	0.347	50	0.27	525	35
CAU-10(Al)-H	0.18	0.38	0.007	0.31	0.371		0.28	635	36
CAU-10(Al)-CH_3	0.45	0.18	0.014	0.026	0.18				36
CAU-10(Al)-OCH_3	0.25	0.08	0.002	0.074					36
CAU-10(Al)-NO_2	0.32	0.17	0.001	0.05			0.21	440	36
CAU-10(Al)-NH_2	0.16	0.23	0.093	0.192					36

CAU-10(Al)-OH	0.16	0.3	0.042	0.235	0.3				36
CAU-13(Al)	0.22	0.16	0.01	0.102	0.143		0.15	380 450	37
Al-fumarate	0.27	0.45	0.027	0.106	0.353		0.48	1021	38
CAU-23(Al)	0.28	0.425	0.03	0.375	0.4			1250	78
Li-rho-ZMOF	0.01	0.342	0.207	0.342		159*			77
Na-rho-ZMOF	0.01	0.324	0.185	0.324		130*			77
Cs-rho-ZMOF	0.01	0.261	0.144	0.261		105*			77
MOF-74(Mg)	0.02	0.63	0.534	0.576	0.625	76	0.65	1400	15
MOF-74(Mg)	0.05	0.6	0.55	0.605	0.75		0.53	1250	17
MOF-74(Ni)	0.05	0.51	0.505	0.565	0.63		0.49	1040	17
MOF-74(Co)	0.05	0.49	0.49	0.545	0.615		0.46	1130	17
MOF-74(Ni)	0.02	0.54	0.024	0.025	0.026				39
ZIF-8(Zn)						10	0.49		40
SIM-1(Zn)	0.27	0.14	0.017	0.073	0.129		0.3	570	6
MAF-4(ZIF-8)			0.003	0.005	0.009		0.65	1870	40
MAF-47-0.76	0.85	0.4	0.002	0.006	0.293		0.64		40
MAF-47-0.49	0.62	0.43	0.002	0.007	0.427		0.65		40
MAF-47-0.23	0.37	0.43	0.004	0.009	0.43		0.64		40
MAF-7(Zn)	0.27	0.43	0.006	0.102	0.43		0.65	1870	40
ZIF-71(Zn)			0.001	0.002	0.004		0.39		41
ZIF-90(Zn)	0.35	0.32	0.003	0.011	0.33		0.49		41
ZIF-93(Zn)	0.5	0.41	0.02	0.07	0.4				82
CoNIm	0.55	0.16	0.008	0.074	0.153			1858	42
DMOF(Zn)	0.3	0.09	0.002	0.061	0.047		0.75	1960	15
DMOF(Zn)-NH_2	0.3	0.08	0.022	0.049			0.58	2010	15
DMOF(Zn)-Br	0.45	0.05	0.013	0.031	0.05		0.53	1315	43

DMOF(Zn)-Cl_2	0.35	0.07	0.003	0.01	0.07		0.45	1175	43
DMOF(Zn)-OH	0.3	0.11	0.021	0.051	0.097		0.54	1130	43
DMOF(Zn)-NO_2	0.4	0.14	0.034	0.039	0.133		0.53	1310	43
DMOF(Zn)-N			0.002	0.01	0.019		0.57	1420	43
DMOF(Zn)-A	0.3	0.27	0.003	0.137	0.27		0.33	760	43
DMOF-TM1(Zn) (mixed linker)	0.44	0.27	0.007	0.044	0.271		0.53	1980	43
DMOF-TM2(Zn)	0.26	0.43	0.002	0.003	0.374		0.51	1050	44
DMOF-TM(Co)	0.35	0.4					0.49	1738	45
DMOF-TM(Ni)	0.45	0.4					0.48	1434	45
DMOF-TM(Cu)	0.55	0.42					0.46	1471	45
$Cd(BTTB)_n$	0.5	0.27	0.036	0.075	0.252		0.19	415	46
Zn(BTTB)n	0.7	0.22	0.019	0.044	0.201		0.25	447	46
$Zn(BTTB)\ (BDC)_n$	0.5	0.09	0.018	0.037	0.087		0.21	441	46
Ni(BTTB)n	0.8	0.02	0.007	0.008	0.019		0.2	391	46
Co(BTTB) (BPY)	0.3	0.01	0.001	0.007	0.009		0.4	843	46
Zn(BTTB) (BPY)	0.7	0.27	0.013	0.034	0.252		0.38	841	46
Co(BTTB) (AZPY)	0.55	0.25	0.012	0.102	0.22		0.39	805	46
Zn(BTTB) (AZPY)	0.55	0.2	0.019	0.133	0.193		0.36	647	46
Co(BTTB) (DMBPY)	0.85	0.2					0.29		45
Zn(BTTB) (DMBPY)	0.85	0.22					0.27		45
$Cu2(pzdc)_2pyz$	0.1	0.12	0.061	0.079					47
$Cu2(pzdc)_2bpy$	0.09	0.17	0.119	0.148	0.167				47
$Cu2(pzdc)_2bpe$	0.08	0.29	0.173	0.227					47
CuBTC	0.1	0.5	0.013	0.024	0.033	10	0.62	6010	15,48
CuMBTC	0.3	0.18	0.072	0.09	0.162		0.5	1471	48
CuEBTC	0.15	0.18	0.09	0.126	0.162		0.46	1434	48

Cu-BTC	0.15	0.54		0.283			1635	49
Cu-BTC	0.1	0.5	0.218	0.443	0.5	0.72	1340	4
Cu-BTC	0.5	0.72	0.234	0.27	0.702			39
$Cu2(dmcapz)_2$	0.33	0.22				0.23	539	50
$Cu2(pmpmd)_2(CH_3OH)_4(opd)_2$	0.15	0.2						51
CAU-14(Cu)	0.2	0.297	0.054	0.234	0.27	0.27	647	83
Zn-trimesate	0.1	0.2						52
Zn2(bptc)	0.18	0.16						53
MFU-4(Zn)	0.25	0.55	0.122	0.302	0.54		1611	54
ThrZnOAc	0.25	0.15	0.009	0.065	0.14			55
AlaZnOAc	0.88	0.25	0.002	0.105	0.234			55
AlaZnCl	0.25	0.16	0.019	0.071	0.16			56
AlaZnBr	0.6	0.14	0.006	0.013				56
ValZnOAc	0.78	0.25			0.243			55
ValZnCl	0.45	0.07	0.011	0.02				56
$(H_2dab)[Zn_2(ox)_3]$	0.7	0.23						57
Zn(NDI-H)	0.45	0.45		0.023	0.42	0.65	1236	58
Zn(NDI-SEt)	0.41	0.25		0.042	0.243	0.39	1236	58
Zn(NDI-SOEt)	0.26	0.3	0.043	0.161	0.291	0.38	888	58
$Zn(NDI\text{-}SO_2Et)$	0.35	0.25	0.028	0.075	0.243	0.31	888	58
$Zn4O(dmcapz)_3$	0.85	0.45	0.008	0.016	0.324	0.43	840	59
$Zn4O(bfbpdc)_3(bpy)_{0.5}$	0.92	0.5	0.001	0.002	0.184	0.59	1450	60
Zn2(bptc)	0.18	0.16	0.018	0.107	0.153		312.7	53
CAU-3(Al)	0.63	0.51	0.026	0.038	0.51	0.64	1550	61
$CAU\text{-}3(Al)\text{-}NH_2$	0.67	0.5	0.05	0.086	0.5	0.53	1250	61
CAU-6(Al)	0.09	0.4	0.238	0.288	0.378	0.25	620	62

CALF-25(Ba)	0.6	0.09					385	63
ISE-1(Ni)	0.15	0.18				0.51		64
JUC-110(Cd)	0.2	0.11	0.003	0.032	0.107			65
NOTT-400	0.35	0.449	0.02	0.05	0.43		1356	87
NOTT-401	0.38	0.112	0.018	0.032	0.102		1504	88
Ni8(L1)6	0.9	0.45				0.52	205	66
Ni8(L2)6	0.8	0.63				0.52	990	66
Ni8(L3)6	0.4	0.99				1.21	1770	66
Ni8(L4)6	0.45	0.9				0.97	1920	66
Ni8(L5)6	0.7	1.12	0.02	0.043	1.004	1.25	2215	66
Ni8(L5-$(CH_3)_2)_6$	0.72	0.7	0.02	0.039	0.621		1985	66
Ni8(L5-$(CF_3)_2)_6$	0.85	0.86	0.014	0.031	0.781		2195	66
([Ni$(L6)_2$]·$4H_2O$)n	0.11	0.12	0.029	0.105	0.117		321	67
[Cd(L′1) (Cl)]$(H_2O)_{1a}$	0.9	0.38	0.003	0.01	0.394			68
[Cd(L′2) (Cl)]$(H_2O)_{2a}$	0.1	0.09	0.042	0.083	0.093			68
[Cd2$(L′2)_2(Br)_2$]$(H_2O)_{32b}$	0.5	0.04	0.007	0.014	0.034			68
[Cd(L′3) (Cl)]$(H_2O)_{23a}$	0.15	0.11		0.094	0.109			68
[Cd(L7) (DMF)]	0.1	0.15	0.063	0.101	0.143		224.4	69
[Co(DPE)]·0.5DPE	0.45	0.2	0.012	0.021	0.17	0.14	310	70
[Dy(ox) (Bpybc)(H_2O)]	0.6	0.25						71
[PbL2]·2DMF·$6H_2O$	0.8	0.24	0.022	0.042	0.174			72
[$Cd_2(sdb)_2(pcih)_{2]}$·2DMF·H_2O	0.23	0.185	0.008	0.148	0.185	0.22	120	84
[Co4L3(μ3-OH)$(H_2O)_3$](SO_4)0.5·xH_2O	0.08	0.189	0.147	0.172	0.185			85
[La3L4(H2O)6]-Cl·xH_2O	0.21	0.271	0.09	0.246	0.27			86

q_{max} (maximum water adsorption capacity), α(relative pressure for which capacity is 50% of q_{max}), Vtot (total pore volume), Qa (heats of adsorption at zero adsorption), S_{BET}(BET surface area)

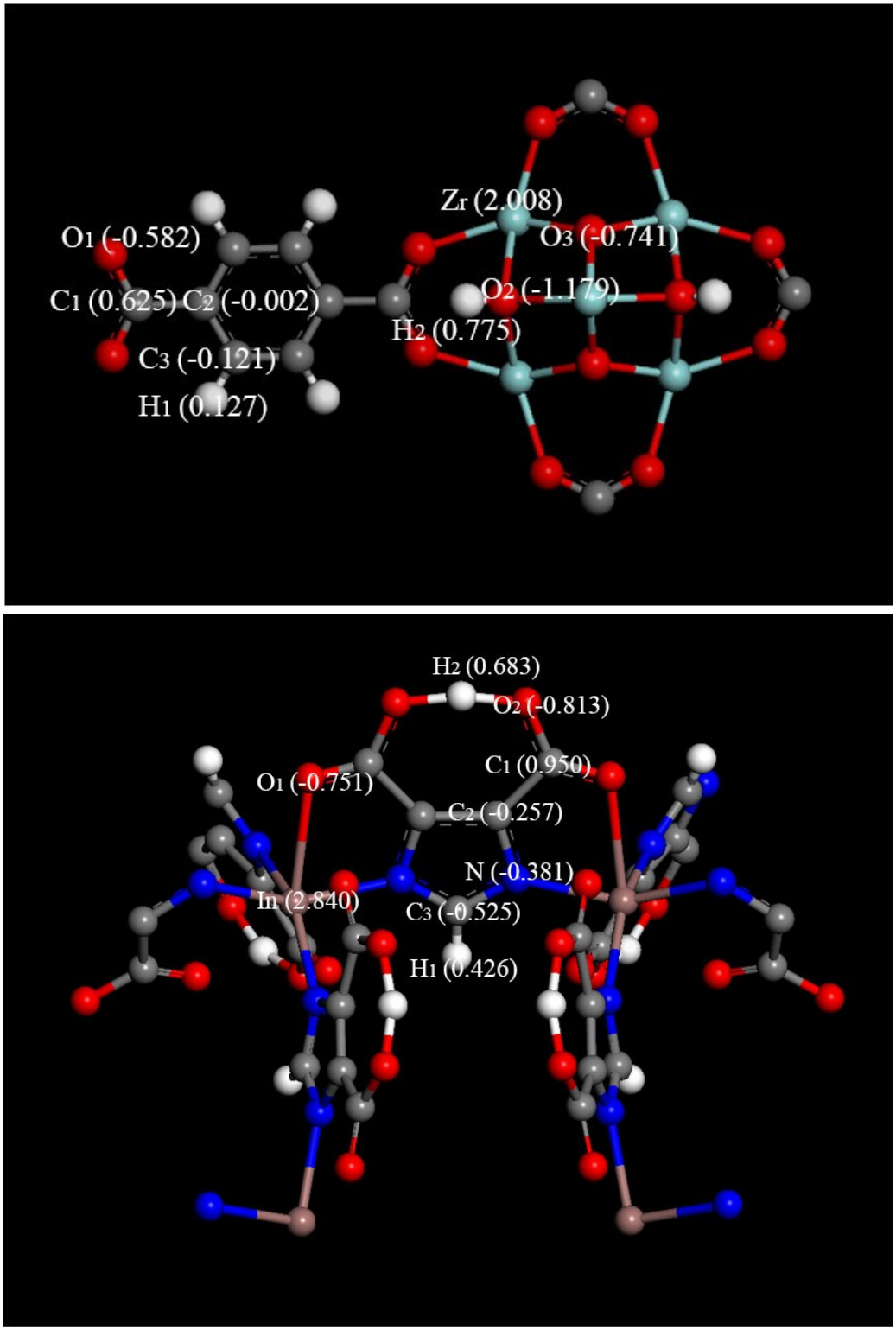

Figure S1 Partial charges for each atoms of UiO-66(Zr) and rho-ZMOF

Table S2. LJ potential parameters for the atoms of the H_2O, UiO-66(Zr) and Na-rho-ZMOF.

Elements	**σ (Å)**	**ε/k_B (K)**
Zr	2.783	34.724
In	3.976	301.417
Na+	2.658	15.096
C	3.473	47.859
O	3.033	48.161
H	2.846	7.649
N	3.263	38.951
OW(for Na-rho-ZMOF)	3.1506	76.54
OW(for UiO-66(Zr))	3.154	78.02
HW	0	0

Synthesis and activation methods

Materials

All materials were purchased from Shanghai Macklin Biochemical Co., Ltd and used directly without further purification.

Synthesis of MOAAF-1(Zn)

1,3,5-benzenetricarboxylic acid (H_3btc 0.30 g, 1.4 mmol) was dissolved in DMF (10 mL) in a 20 mL glass vial. Then, Triethanolamine (TEOA, 1.16 g, 7.8 mmol) and solid $ZnCl_2$ (0.3 g, 2.2 mmol) were added to the reaction mixture, and the resulting solution was sealed and heated at 100 °C for 24h. After cooling to room temperature, the resultant crystals were formed.

Synthesis of MOF-107(Cu)

2,5-thiophenedicarboxylic acid, ($TDCH_2$) (18.0 mg, 0.010 mmol), and $Cu(NO_3)_2{\cdot}2.5H_2O$, (23.5 mg, 0.010 mmol) was dissolved in N,N'-diethylformamide (DEF)/ethanol (1.6 ml/0.4 ml). The solution was placed in a Teflon-lined stainless-steel autoclave. The reactor was sealed and heated to 80°C for 20 h at a rate of 2.0°C/min, then cooled to room temperature at a rate of 1.0°C/min. The resultant blue crystals were filtered.

Synthesis of Zn(BTCPyrol)

The mixture of $Zn(OAc)_2 \cdot 2H_2O$ (0.1467 g, 0.6 mmol), 1,3,5-benzenetricarboxylic acid (H3btc, 0.0803 g, 0.4 mmol) and 1.5 mL 2-pyrrolidinone (pyrol) was sealed and heated to 100°C for 5 days. After cooling to room temperature, colorless crystals were obtained.

Synthesis of Zn(NH_2BDC)

A mixture of $Zn(NO_3)_2 \cdot 6\ H_2O$ (0.0595 g, 0.2 mmol) and H_2NH_2BDC (0.0362 g, 0.2 mmol) was dissolved in DMF/H_2O (10 ml, 2:1), then Triethylamine (Et_3N 0.05 ml) was added. The mixture was stirred for 2 h in air and then filtrated. The yellow filtrate was kept at room temperature for two weeks, yellow block crystals were obtained.

Activation of the samples

All samples were filtrated first, and washed three times by DMF. Then, the samples were put into the DMF solution and heated to 80°C. The mixture was stirred for 4 h, followed by washing three times with methanol. The obtained materials were soaked in methanol for 5 days at room temperature. The filtrated samples were dried at 80°C overnight under vacuum, and then calcination at 180°C for 24 h.

Characterization

The X-ray diffraction (XRD) patterns were recorded at room temperature under ambient conditions with a BRUKER instrument (D8 Focus, Cu Kα with k = 1.5418 Å). The morphologies of samples were also characterized by scanning electron microscopy (SEM) on a Hitachi S4800. Specific surface area and pore volume of composites were obtained by nitrogen gas adsorption at a low temperature of about 77 K using a gas adsorption analyzer (Quantachrome Quadrasorb SI-MP). Water sorption analysis was performed by a 3H-2000PW gravimetric analyzer (Beishide Instrument Technology Co., Ltd.). Water sorption isotherms were performed at 25℃ in the relative-pressure range from 0 to 0.9. Prior to measurements, the samples were degassed at 150℃ to a constant weight.

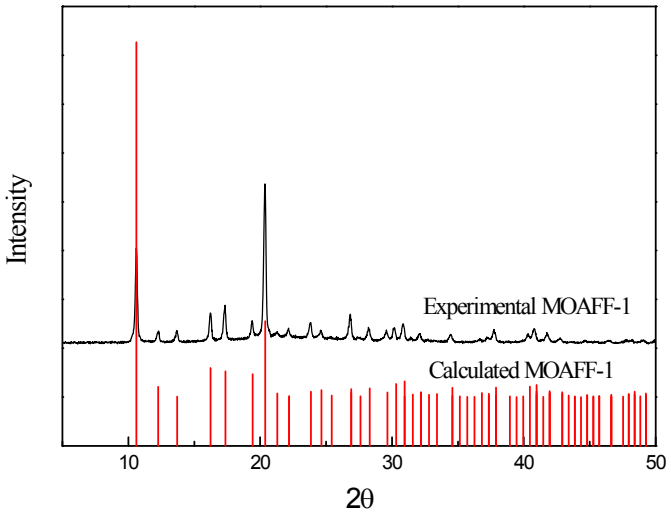

Figure S2 XDR pattern of MOAAF-1

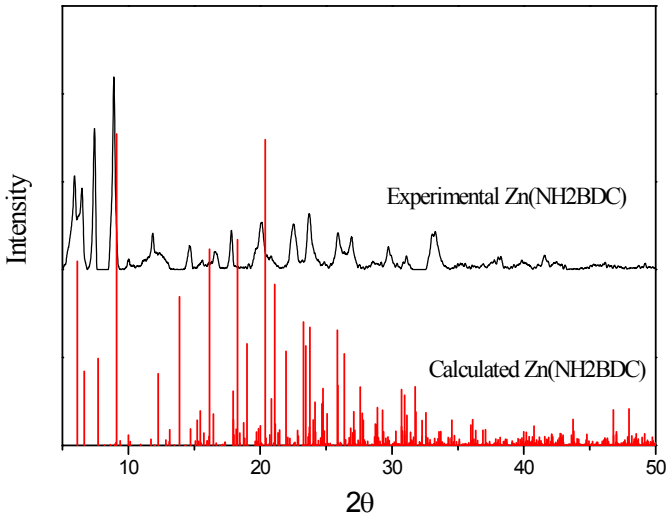

Figure S3 XDR pattern of $Zn(NH_2BDC)$

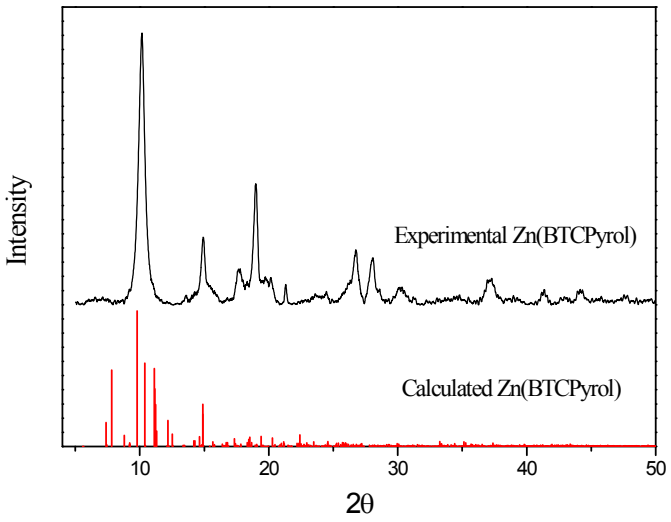

Figure S4 XDR pattern of Zn(BTCpyrol)

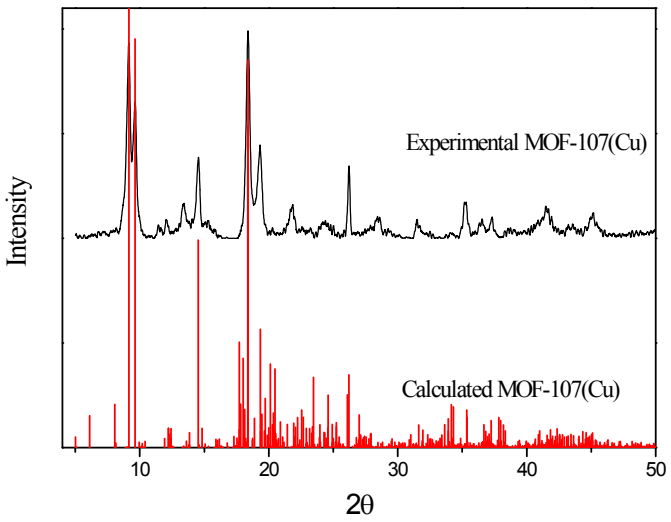

Figure S5 XDR pattern of MOF-107(Cu)

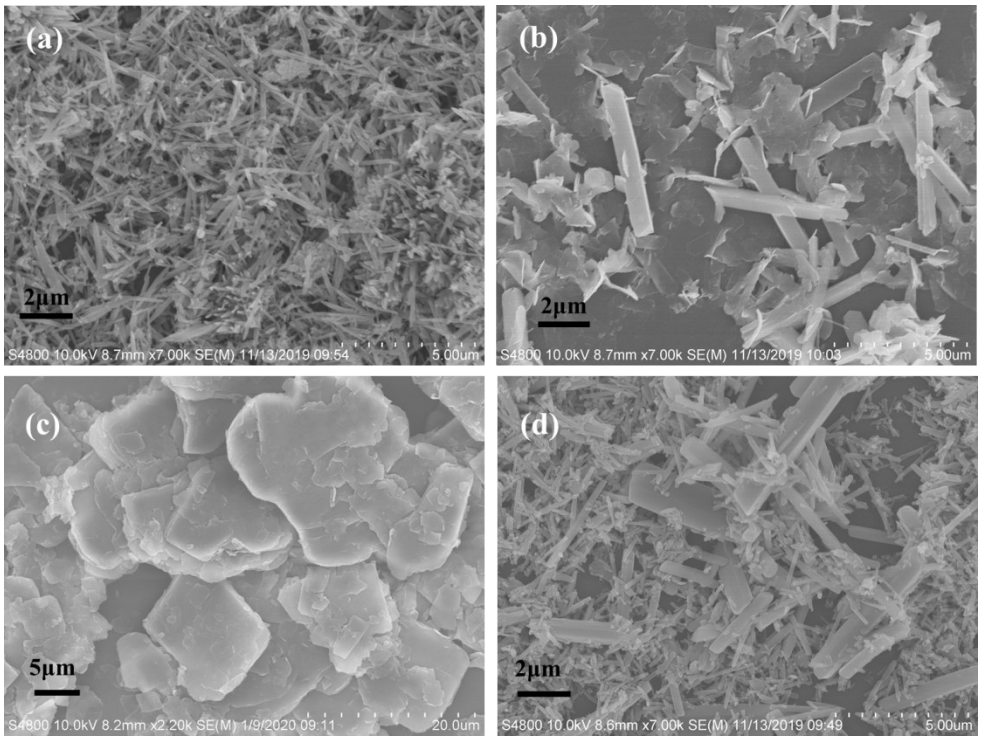

Figure S6. SEM of MOAAF-1(a), Zn(BTCPyrol)(b); MOF-107(c); and Zn(NH_2BDC)

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