Supporting Information

Gradient boosted machine learning model to predict H_2, CH_4 and CO_2 uptake in metal organic frameworks using experimental data

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Table S1: MOF structures with literature H_2 uptakes

MOF Name	Common Name	Pressure (Bar)	Temperature (K)	Uptake (%wt)	Reference
$Be_{12}(OH)_{12}(BTB)_4$		1	77	1.6	Sumida et al., 2009[1]
		20	77	6	
		100	77	9.2	
		95	298	2.3	
Cd4(TCPM)2		1	77	2.8	Chun et al., 2004[2]
Co(BDP)		30	77	3.1	Jin Choi, Dincă and Long, 2008[3]
Co(BTC)(4,4'-bpy)		72	77	2.05	Li.Y et al., 2008[4]
Co2(BDC)2(dabco)		44.2	77	4.11	Suh et al, 2012[5]
Co3(bpdc)3(4,4'-bpy)		1	77	1.98	Lee et al., 2005[6]
Co3(NDC)3(dabco)		1	77	2.45	Chun et al., 2008[7]
Co3[(Co4Cl)3(BTT)8(H2O)12]2		1	77	1.8	Liao et al., 2013[8]
Cr3(BTC)2		1	77	1.9	Sumida, Her, et al., 2011[9]
Cu(dccptp)(NO3)		20	77	1.91	Yang et al., 2008[10]
Cu(peip)		1	77	2.51	Liu, Oh and Soo Lah, 2011[11]
		40	77	4.14	
Cu(pmip)		1	77	2.36	Liu, Oh and Soo Lah, 2011[11]
Cu(TZI)3		1	77	2.4	Nouar et al., 2008[12]
Cu2(BDC)2(dabco)		1	77	1.8	Lee et al., 2007[13]
		33.7	77	2.7	
Cu2(BDDC)		0.95	77	1.64	Bing Zheng et al., 2010[14]
		17	77	3.98	
Cu2(dhtp)	Cu-MOF-74	5	77	2.22	García-Holley et al., 2018[15]
		100	77	3.15	
		100	160	2.87	
Cu2(DAIA)(H2O)2	Cu-MOPF	1	77	2.8	Maity, Karan and Biradha, 2018[16]
Al(OH)(SDC)	CYCU-3-Al	5	77	3.37	García-Holley et al., 2018[15]

		100	77	8.24	
		100	160	7.92	
Fe3(OH)(pbpc)2		1	77	1.6	Jia et al., 2007[17]
		20	77	3.05	
Fe4O2(BTB)8/3		1	77	2.1	Choi et al., 2007[18]
Zn6(BTB)4(4,4’-bpy)3	FJI-1	37	77	6.52	Han et al., 2011[19]
HCu[(Cu4Cl)3(BTT)8]	Cu-BTT	1.2	77	2.42	Dincă et al., 2007[20]
		20	77	4.1	
Cu3(BTC)2	HKUST-1	5	77	3.53	García-Holley et al., 2018[15]
		100	77	5.31	
		100	160	4.91	
Zn4O(CH3PhTDC)3	IFMC-29	1	77	1.75	Cheng et al., 2018[21]
Zn4O(dobdc)2	IRMOF-6	45	77	4.63	Wong-Foy, Matzger and Yaghi, 2006[22]
Zn4O(NDC)3	IRMOF-8	1	77	1.5	Rowsell et al., 2004[23]
Zn4O(HPDC)2	IRMOF-11	1	77	1.62	Rowsell et al., 2004[23]
		33.7	77	3.4	Wong-Foy, Matzger and Yaghi, 2006[22]
Zn4O(pyrdc)2	IRMOF-13	1	77	1.73	Rowsell and Yaghi, 2006[24]
Zn4O(ttdc)2	IRMOF-20	77.6	77	6.25	Wong-Foy, Matzger and Yaghi, 2006[22]
Cd3(bpdc)3	JUC-48	40	77	2.8	Fang et al., 2007[25]
Cu3(BTAT)	MFM-132a	1	77	2.83	Yan et al., 2018[26]
		20	77	6.3	
Mg2(dobdc)	Mg-MOF-74	1	77	2.2	Sumida, Brown, et al., 2011[27]
		100	77	4.9	
Al(OH)(bdc)	MIL-53(Al)	16	77	3.8	Férey et al., 2003[28]
Cr(OH)(bdc)	MIL-53(Cr)	16	77	3.1	Férey et al., 2003[28]
Cr3OF(BTC)2	MIL-100	26.5	77	3.28	Latroche et al., 2006[29]
Cr3O(BDC)2	MIL-101(Cr)	1	77	1.92	Ren et al., 2014[30]
Mn3[(Mn4Cl)3(BTT)8]2	Mn(BTT)	1.2	77	2.2	Dincă et al., 2007[20]
		90	77	6.9	
Zn4O(bdc)3	MOF-5, IRMOF-1	50	77	4.7	Panella et al., 2006[31]

Pd(bdc)	MOF-5 (Pd)	1	77	1.86	Sabo et al., 2007[32]
Zn2(dhtp)	Zn-MOF-74, CPO-27-Zn	1	77	1.77	Rowsell and Yaghi, 2006[24]
		30	77	2.8	Liu et al., 2008[33]
		70	77	7.5	Wong-Foy, Matzger and Yaghi, 2006[22]
Zn4O(BBC)2(H2O)3	MOF-200	80	77	7.4	Furukawa et al., 2010[34]
Zn4O(BTB)4/3(NDC)	MOF-205	80	77	7	Furukawa et al., 2010[34]
Zn4O(BTE)4/3(bpdc)	MOF-210	80	77	8.6	Furukawa et al., 2010[34]
Cu2(bptc)	MOF-505, NOTT-100	1	77	2.47	Chen et al., 2005[35]
		20	77	4.02	Lin et al., 2009[36]
Zn4O(AZD)3	MOF-646	1	77	1.75	Barman et al., 2010[37]
	MOF-808	1	77	2.78	Xia et al, 2016[38]
Ni(dhtp)2	Ni-MOF-74	70	77	1.8	Dietzel et al., 2006[39]
Ni(BTC)(4,4'-bpy)		72	77	3.42	Y. Li et al., 2008[4]
Ni3(OH)(pbpc)3		1	77	1.99	Jia et al., 2007[17]
		20	77	4.15	
Ni3[(Co4Cl)3(BTT)8(H2O)12]2		1	77	1.5	Liao et al., 2013[8]
NJU-bai12-ac		1	77	1.91	Zheng et al., 2013[40]
		20	77	5.9	
Cu2(tptc)	NOTT-101	1	77	2.52	Lin et al, 2009[36]
		20	77	6.06	
		60	77	6.6	
Cu2(qptc)	NOTT-102	1	77	2.24	Lin et al, 2009[36]
		20	77	6.07	
		60	77	7.2	
Cu2(NddIP)	NOTT-103	1	77	2.63	Lin et al, 2009[36]
		20	77	6.51	
		60	77	7.78	
Cu2(DFTP)	NOTT-105	1	77	2.52	Lin et al, 2009[36]

		20	77	5.4	
Cu2(DMTP)	NOTT-106	1	77	2.29	Lin et al, 2009[36]
		20	77	4.5	
Cu2(TMTP)	NOTT-107	1	77	2.26	Lin et al, 2009[36]
		20	77	4.46	
Cu2(ndip)	NOTT-109	1	77	2.33	Lin et al, 2009[36]
		20	77	4.15	
Cu2(pdip)	NOTT-110	1	77	2.64	Yang et al., 2009[41]
		20	77	6.59	
		55	77	7.62	
Cu2(dpdip)	NOTT-111	1	77	2.56	Yang et al., 2009[41]
		20	77	6.48	
		48	77	7.36	
Cu3(BDDC)	NOTT-112	1	78	2.3	Yan et al., 2009[42]
		37.5	77	7.07	
		100	77	8.74	García-Holley et al., 2018[15]
		100	160	8.31	
Cu3(tbtt)	NOTT-113	1	78	2.39	Yan, Blake, et al., 2011[43]
		30	78	5.1	
Cu3(abtt)	NOTT-114	1	78	2.39	Yan, Blake, et al., 2011[43]
		30	78	5	
Cu3(NTBD)	NOTT-115	1	78	2.39	Yan, Blake, et al., 2011[43]
		33	78	5.6	
Cu3(btti)	NOTT-119, PCN-69	1	77	1.44	Yan, Yang, et al., 2011[44]
		44	77	5.6	
Cu4(TDTM)	NOTT-140	1	77	2.5	Tan.C et al., 2011[45]
		20	77	6	
Sc2(bptc)(OH)2	NOTT-400	1	77	2.14	Ibarra et al., 2011[46]
		20	77	3.84	
Sc(TDA)(OH)	NOTT-401	1	77	2.31	Ibarra et al., 2011[46]

		20	77	4.44	
Cu3(ttei)	NU-100	1	77	1.82	Farha et al., 2010[47]
		56	77	9.95	
Cu3(TIPTB)	NU-125, NOTT-122	1	77	2.61	Yan et al., 2014[48]
		5	77	4.6	García-Holley et al., 2018[15]
		100	77	8.2	
		100	160	7.76	
Zr(TBAPy)2	NU-1000	5	77	3.37	García-Holley et al., 2018[15]
		100	77	7.98	
		100	160	7.62	
Zr(Py-XP)	NU-1101	100	77	9.5	Gómez-Gualdrón et al., 2017[49]
Zr(Por-PP)	NU-1102	100	77	9.9	Gómez-Gualdrón et al., 2017[49]
Zr(Py-PTP)	NU-1103	100	77	13	Gómez-Gualdrón et al., 2017[49]
Cu3(TATB)2 (catenated)	PCN-6	1	77	1.9	Sun, Ma, et al., 2006[50]
		50	77	7.2	S. Ma et al., 2008[51]
Cu2(aobtc)	PCN-10	1	77	2.34	X.-S. Wang, Ma, Rauch, et al., 2008[52]
		3.5	30	6.84	
		45	77	5.23	
Cu2(sbtc)	PCN-11	1	77	2.55	X.-S. Wang, Ma, Rauch, et al., 2008[49]
		3.5	30	7.89	
		45	77	5.97	
Cu2(mdip)	PCN-12	1	77	3.05	X.-S. Wang, Ma, Forster, et al., 2008[49]
Cu2(adip)	PCN-14	1	77	2.7	Ma et al., 2009[53]
		45	77	4.42	
Cu2(ebdc)	PCN-16	1	77	2.6	Sun et al., 2010[54]
		45	77	5.1	
Cu2(PMTB)	PCN-21	1	77	1.6	Zhuang et al., 2010[55]
Cu2(bdi)	PCN-46	1	77	1.95	Zhao et al., 2010[56]
		32	77	5.31	

Cu3(btei)	PCN-61	1	77	2.25	Yuan et al., 2010[57]
		33	77	6.24	
Cu3(ntei)	PCN-66	1	77	1.79	Yuan et al., 2010[57]
		45	77	6.65	
Cu3(ptei)	PCN-68, NOTT-116	1	77	1.87	Yuan et al., 2010[57]
		50	77	7.32	
Fe2(abtc)	PCN-250	5	77	3.77	García-Holley et al., 2018[15]
		100	77	5.37	
		100	160	4.93	
Cu2(bdpb)	PMOF-3	1	77	2.47	Zhang et al., 2011[58]
Cu3(TDPAT)	rht-MOF-7	5	77	3.23	García-Holley et al., 2018[15]
		100	77	4.89	
		100	160	4.5	
Sc(BDC)3		1	77	1.5	Perles et al., 2005[59]
Zn4O(NTB)2	SNU-1	1	77	1.9	Young Lee, Yeon Jang and Paik Suh., 2005[60]
Zn2(abtc)(DMF)2	SNU-4	1	77	2.07	Lee et al., 2008[61]
		50	77	3.7	
Cu2(abtc)(DMF)2	SNU-5’	1	77	1.83	Lee et al., 2008[61]
		50	77	5.22	
Cu2(BPnDC)2(4,4’-bpy)	SNU-6	1	77	1.68	Park and Suh., 2008[62]
		70	77	4.87	
Cu2(TCM)	SNU-21S	1	77	1.95	Kim and Suh., 2011[63]
		70	77	4.37	
Zn2(TCPBDA)(H2O)2	SNU-30	61	77	3.27	Park, Cheon and Suh, 2010[62]
Cu2(bdcppi)	SNU-50’	1	77	2.1	Prasad, Hong and Suh, 2010[64]
		1	87	1.39	
		60	77	5.53	
Zn4O(CVB)3	SNU-70	20	77	7	Ahmed et al., 2019[65]
		100	77	10.5	

Zn4O(TCBPA)2	SNU-77H	1	77	1.79	Park H. J. et al., 2011[66]
		90	77	8.1	
Mo3(BTC)2	TUDMOF-1	1	77	1.75	Kramer, Schwarz and Kaskel, 2006[67]
Zr(BPDC)2	UiO-67	5	77	3.23	García-Holley et al., 2018[15]
		100	77	5.86	
		100	160	5.53	
Zr(ACDB)2	UiO-68-Ant	5	77	3.81	García-Holley et al., 2018[15]
		100	77	7.58	
		100	160	7.18	
Zn4O(T2DC)(BTB)4/3	UMCM-2	46	77	6.9	Koh, Wong-Foy and Matzger, 2009[68]
Zn4O(bpdc)1.5(NDC)1.5	UMCM-9	20	77	7.5	Ahmed et al., 2019[65]
		100	77	11.5	
Cu3(BHB)	UTSA-20	1	77	2.9	Guo et al., 2011[69]
		15	77	4.1	
Cu3(bhtc)2	UMCM-150	1	77	2.1	Wong-Foy, Lebel and Matzger, 2007[70]
		45	77	5.7	
Y(BTC)		1	77	1.57	Luo et al., 2008[71]
		10	77	2.1	
Zn(MeIM)2	ZIF-8	55	77	3.01	Zhou et al., 2007[72]
		30	77	3.3	
Co(MeIM)2	ZIF-67	1	77	1.53	Panchariya et al., 2018[73]
Zn(NDC)(bpe)0.5		40	77	2	Chen, Ma, et al., 2006[74]
Zn(peip)		1	77	2.27	Liu, Oh and Soo Lah, 2011b[75]
Zn2(BDC)(tmbdc)(dabco)		1	77	2.08	Chun et al., 2005[76]
Zn2(BDC)2(dabco)		1	77	2.1	Lee et al., 2007[13]
		83.2	77	3.17	Takei et al., 2008[77]
Zn2(btatb)		1	77	2.2	Farha et al., 2008[78]
Zn2(NDC)2(dabco)		1	77	1.7	Chun et al., 2005[76]
Zn2(tftpa)2(dabco)		1	77	1.78	Chun et al., 2005[76]
Zn2(tmbdc)2(4,4'-bpy)		1	77	1.68	Chun et al., 2005[76]

Zn2(tmbdc)2(dabco)		1	77	1.85	Chun et al., 2005[76]
Zn3(bpdc)3(4,4'-bpy)		1	77	1.74	Lee et al., 2005[79]
Zn(5-AT)2	ZTF-1	1	77	1.6	Panda et al., 2011[80]
Zn(Mlai)	IMOF-3	1	77	1.5	Debatin et al., 2010[81]

Table S2: MOF structures with literature CH_4 uptakes

MOF Name	Common Name	Pressure (Bar)	Temperature (K)	Uptake (%wt)	Reference
Al3(TCPT)6	Alsoc-MOF-1	65	270	33.8	Alezi et al., 2015[82]
		65	270	29	
Cd(bpydb)		35	298	5.5	Sharma et al., 2011[83]
Co2(4,4'-bpy)3(NO3)4		30	298	3.56	Kondo et al., 1997[84]
Co2(azpy)3(NO3)4		36	298	2.9	Kondo et al., 2000[85]
Co2(BDC)2(dabco)		35	303	11.4	H. Wang et al., 2008[86]
		75	303	12.28	H. Wang et al., 2008[86]
Co2(dobdc)	Co-MOF-74	35	298	11	Mason, Veenstra and Long, 2014[87]
Cu2(BDC)2(dabco)		35	293	10.8	Seki and Mori, 2002[88]
		35	298	13.2	Seki, 2001[89]
Cu3(BTC)2		35	303	12.7	Senkovska and Kaskel, 2008[90]
Cu3(TDPAT)	Cu-TDPAT	35	298	13.2	Li et al., 2012[91]
Al(OH)(NDC)	DUT-4	35	303	8.8	Senkovska et al., 2009[92]
Al(OH)(bpdc)	DUT-5	35	303	9.8	Senkovska et al., 2009[92]
Co2(NDC)2(dabco)	DUT-8(Co)	60	298	4.5	Klein et al., 2012[93]
Cu2(NDC)2(dabco)	DUT-8(Cu)	60	298	12.8	Klein et al., 2012[93]
Zn2(NDC)2(dabco)	DUT-8(Zn)	60	298	3.7	Klein et al., 2012[93]
Ni5O2(BTB)2	DUT-9	30	298	12	Gedrich et al., 2010[94]
		70	298	17.3	
Zn4O(TCPBDA)3/2	DUT-13	50	298	13.9	Grünker et al., 2011[95]
Co2(bipy)3(BTB)4	DUT-23(Co)	100	298	21.1	Klein et al., 2011[96]
Cu2(BBCDC)	DUT-49	35	298	19.2	Stoeck et al., 2012[97]
Zn6(BTB)4(4,4′-bpy)3	FJI-1	35	273	20.6	Han et al., 2011[19]
		35	298	15.2	
Cu3(BTC)2	HKUST-1	35	298	15.5	Peng, Krungleviciute, et al., 2013[98]
		65	298	17.8	
Zn4O(NH2-bdc)3	IRMOF-3	36.5	298	13	Eddaoudi et al., 2002[99]
Zn4O(C2H4-bdc)3	IRMOF-6	36.5	298	19.4	Eddaoudi et al., 2002[99]
Zn4O(NDC)3	IRMOF-8	35	298	12.2	Feldblyum et al., 2013[100]

Mg2(dobdc)	Mg-MOF-74, CPO-27-Mg	35	298	13.62	Mason, Veenstra and Long, 2014[87]
Al(OH)(bdc)	MIL-53(Al)	35	298	10.6	Bolinois et al, 2017[101]
Cr(OH)(bdc)	MIL-53(Cr)	30	304	8.8	Bourrelly et al., 2005[102]
Cr3OF(BTC)2	MIL-100(Cr)	35	303	10.7	Llewellyn et al., 2008[103]
Fe3OF(BTC)2	MIL-100(Fe)	35	303	8.8	Wiersum et al., 2013[104]
Cr3OF(H2O)2(bdc)3	MIL-101(Cr)	35	303	9.3	Wiersum et al., 2013[104]
Ti8O8(OH)4(bdc)6	MIL-125	35	303	9.7	Wiersum et al., 2013[104]
Mn2(dobdc)	Mn-MOF-74, CPO-27-Mn	35	297	9.6	Wu, Zhou and Yildirim, 2009[105]
Zn4O(bdc)3	MOF-5 or IRMOF-1	36.5	298	15.1	Eddaoudi et al., 2002[99]
Zn 4O(BTB) 2	MOF -177	35	298	13.8	Furukawa et al., 2010[34]
		65	298	19.5	
Zn 4O(BBC) 2	MOF -200	10	298	5.12	Furukawa et al., 2010[34]
		35	298	11.5	
		65	298	17.5	
Zn 4O(BTB)4/3(NDC)	MOF -205	10	298	5.7	Furukawa et al., 2010[34]
		35	298	14.9	
		65	298	20	
Zn 4O(BTE)4/3(bpdc)	MOF -210	35	298	13.2	Furukawa et al., 2010[34]
		65	298	19.3	
Cu 2(bptc)	MOF -505, NOTT -100	35	300	13.3	He, Zhou, et al., 2013[106]
		65	270	16.2	
Ni 2(dobdc)	Ni -MOF -74, CPO -27 -Ni	35	298	12.2	Mason, Veenstra and Long, 2014[87]
Cu 6(BDPP) 3(H 2O) 6	NJU -Bai10	35	290	17.6	Lu et al., 2013[107]
Cu 2(tptc)	NOTT -101	35	300	17	He, Zhou, et al., 2013[106]
		65	300	19.8	
Cu 2(qptc)	NOTT -102	35	300	18.1	He, Zhou, et al., 2013[106]
		65	300	22.2	
Cu 2(2,6 -nddi)	NOTT -103	35	300	17.9	He, Zhou, et al., 2013[106]

		65	300	20.8	
Cu 2(C26 H20 O 8)	NOTT -107	35	298	15.7	He,Zhou et al., 2014[108]
Cu 2(1,4 -nddi)	NOTT -109	35	300	15.1	He,Zhou et al., 2014[108]
		65	300	18	
Cu 3(C66 H36 O12)	NOTT -119	35	298	16.2	Yan, Yang, et al., 2011[44]
Cu 3 (btdi)(H 2O) 3	NU -111	35	298	19.8	Peng, Srinivas, et al., 2013[109]
		65	270	32.9	
Cu 3(TIPTB)	NU -125, NOTT -122	35	298	18.3	Wilmer et al., 2013[110]
		65	298	22	
Cu 3(TIPTPB)(H 2O) 3	NU -140	65	270	29.6	Barin et al., 2014[111]
		65	300	25.4	
Zr 6 O 4(OH) 4(TPT)	NU -800	35	298	15.2	Gomez -Gualdron et al., 2014[112]
		65	270	27.7	
Cu 2(sbtc)	PCN -11	35	298	14.5	X. -S. Wang, Ma, Rauch, et al., 2008[52]
Cu 2(adip)	PCN -14	65	270	33.3	Peng, Srinivas, et al., 2013[109]
		65	298	26.4	
Cu 2(ebdc)	PCN -16	35	300	15.9	He,Zhou et al., 2014[108]
Cu 2(bdi)	PCN -46	35	298	19.4	Zhao et al., 2010[56]
Cu 3(btei)	PCN -61	35	298	16.7	Yuan et al., 2010[57]
Cu 3(ntei)	PCN -66	35	298	16.6	Yuan et al., 2010[57]
Cu 3(ptei)	PCN -68	35	298	17.9	Yuan et al., 2010[57]
Cu 2(bttcd)	PCN -80	35	296	15	Lu et al., 2012[113]
Zn 2 (TCPBDA)	SNU -30	50	194	6.4	Park, Cheon and Suh, 2010[62]
		50	298	4.5	
Zn 2(TCPBDA)(bpta)	SNU -31	50	298	1.5	Park, Cheon and Suh, 2010[62]
Cu 2(bdcppi)	SNU -50	1	195	10.6	Prasad, Hong and Suh, 2010[64]
		61	298	14.5	
Zn 4O(CVB) 3	SNU -70	1	195	3.8	Prasad and Suh, 2012[114]
		45	298	18.3	

Zn 4O(CEB) 3	SNU -71	1	195	4.7	Prasad and Suh, 2012[114]
		45	298	10.8	
Zn 4O(TCBPA) 2	SNU -77H	1	195	8.04	H. J. Park et al., 2011[66]
		35	298	17.8	
		60	298	18.08	
Zr 6 O 4(OH) 4(bdc) 6	UiO -66	35	303	6.7	Wiersum et al., 2013[104]
Zr6O4(OH)4(NH2-bdc)6	UiO-66-NH2	35	303	7.5	Wiersum et al., 2013[104]
Cu3(BHB)	UTSA-20a	35	298	12.5	He,Zhou et al., 2014[108]
		65	298	14.2	
Cu3(TIPAB)	UTSA-34	35	290	11.9	He,Zhou et al., 2014[108]
Zn4O(NDC)3	UTSA-38	35	300	7.5	Das et al., 2011[115]
Cu2(dceni)	UTSA-40	35	300	12	He, Xiang, et al., 2013[116]
Cu2(PDD)(H2O)2	UTSA-75	65	298	20.4	Li et al., 2015[117]
Cu2(PDDP)(H2O)2	UTSA-76	65	298	20.8	Li et al., 2015[117]
Cu2(tptc)(PDDP)(H2O)2	UTSA-77	65	298	20.4	Li et al., 2015[117]
Cu2(DCPAI)(H2O)2	UTSA-80	65	298	19.4	Wen et al., 2014[118]
Cu2(DFMTP)(H2O)2	UTSA-88	65	298	17.1	Chang et al., 2015[119]
Zn(MeIM)2	ZIF-8	36	300	7	Zhou et al., 2007[72]
Cu2(BDPP)(H2O)2	ZJU-5	65	298	20.8	Li et al., 2015[117]
Cu2(FDDI)	ZJU-25	35	300	17.2	He,Zhou et al., 2014[108]
Cu2(cpda)	ZJU-36	35	300	17	He,Zhou et al., 2014[108]
		65	300	22.7	
Cu6(CTIA)2	ZJU-70	35	298	12.7	Duan et al., 2015[120]
		65	270	16.3	
Cu2(BDEDDI)(H2O)2	ZJUN-50	35	298	17.6	Song, Ling, et al., 2015[121]
		65	298	21.5	
Zn2(BDC)2(dabco)		35	303	12.5	Senkovska and Kaskel, 2008[90]
Zn3O(2,7-ndc)2		35	298	7.3	Park et al., 2009[122]
Zn2(dobdc)	Zn-MOF-74, CPO-27-Zn	35	298	9.1	Wu, Zhou and Yildirim, 2009[105]

Table S3: MOF structures with literature CO_2 uptakes

MOF Name	Common Name	Pressure (Bar)	Temperature (K)	Uptake (%wt)	Reference
Al3(TCPT)6	Alsoc-MOF1	40	298	66.7	Alezi et al., 2015[82]
Zn8(ad)4(BPDC)6O.2Me2NH2	Bio-MOF-1	1	313	5.48	An and Rosi, 2010[123]
Co2(ad)2(CO2CH3)2·2DMF	Bio-MOF-11	1	298	15.3	An, Geib and Rosi, 2010[123]
Al4(OH)2(OCH3)4(NH2-bdc)3	CAU-1	1	273	24.1	Si et al., 2011[124]
Cd(DBNBVP)2(ClO4)2		1	273	12.3	Wu and Lin, 2005[125]
Cd2(HFIDP)(H2O)2		1	195	12.7	Hou et al., 2011[126]
Cd6(CPOM)3(H2O)6		1	293	8.5	Tian, J et al., 2010[127]
		1	297	5.6	
		30	297	14	
Cd(ADA)(4,4′-bipy)0.5.(DMF)	Cd-ADA-1	1	298	3.4	Pachfule et al., 2010[128]
Cd(MeIM)2	CdIF-1	1	273	5.6	Tian,Y.-Q et al., 2010[129]
Cd(eIm)2	CdIF-4	1	273	4	Tian,Y.-Q et al., 2010[129]
Cd(nIm)2	CdIF-9	1	273	8.8	Tian,Y.-Q et al., 2010[129]
Co(BDP)		40	313	41.3	Herm et al., 2011[130]
Co(tImb)		1	298	7.2	Chen, S.-S et al., 2011[131]
Co(tImb).DMF.H2O		1	298	11.7	Chen, S.-S et al., 2011[131]
Co2(dobdc)	Co-MOF-74	0.1	296	10.36	Caskey, Wong-Foy and Matzger, 2008[132]
		1	296	23.6	
Zn(BTT)	CPF-6	1	273	16.2	Lin et al., 2012[133]
Cu2(pmdc)2(bpy)	CPL-2	1	298	6.6	García-Ricard and Hernández Maldonado, 2010[134]
Ni3(OH)(bdc)3(tpt)	CPM-33a	1	273	21.2	Zhao et al., 2015[135]
Ni3(OH)(dobdc)3(tpt)	CPM-33b	1	298	12.7	Zhao et al., 2015[135]
		1	273	25.6	
		1	298	19.8	

(CH3)2NH2][In3O(BTC)2(H2O)3]2[In3(BTC)4]·7DMF·23H2O	CPM-5	1	273	13.7	S.-T. Zheng et al., 2010[136]
		1	299	9.6	
Cu(2-pymo)2		0.86	293	3.8	Navarro et al., 2006[137]
Cu(BDC-OH)		2	296	8.9	Xiang et al., 2012[138]
Cu2(pmdc)2(pz)		1	300	6.4	Kitaura et al., 2005[139]
Cu3(BTB)		20	273	61.1	Zheng et al., 2012[140]
Cu3(BTC)2		1	296	18.8	Xiang et al., 2012[138]
Cu4O(OH)2(Me2trzpba)4		1	298	5.8	Lincke et al., 2011[141]
Cu-BTTri		1	298	12.3	Demessence et al., 2009[142]
		40	313	42.8	
Cu3(TDPAT)(H2O)3	Cu-TDPAT	0.1	298	5.8	Li et al., 2012[91]
		1	298	20.6	
Cu3(TPBTM)(H2O)3	Cu-TPBTM	20	298	50.8	Baishu Zheng et al., 2011[143]
Fe3[(Fe4Cl)3(BTT)8(MeOH)4]2	Fe-BTT	1	298	12	Sumida et al., 2010[144]
Fe3O(OH)(BTC)2	Fe-MIL-100	0.9	298	6.6	Mason et al., 2015[145]
Fe(pz)Ni(CN)4		1	298	9.3	Sumida et al 2012[146]
Cu(BTTA)(H2O)	FJI-H14	1	195	35.5	Liang et al., 2017[147]
		1	298	22.2	
Zn(bcphfp)	FMOF-2	1	298	4.5	Fernandez et al., 2010[148]
Cu3(BTC)2	HKUST-1	1	298	15.3	Millward and Yaghi, 2005[149]
		30	298	31.9	
[Zn3(pbdc)2]·HPIP·H3O·5H2O	HPIP@ZnPC -2	0.15	298	4.6	Ling et al., 2013[150]
[Zn3(pbdc)2]·HPYR·H3O·4H2O	HPYR@ZnP C-2	0.15	298	3	Ling et al., 2013[150]
Zn(BHTHT)	IFMC-1	1	195	24.8	Qin et al., 2012[151]
		1	273	15.3	
		1	298	10.6	
Zn(Mlai)	IMOF-3	1	273	7.2	Debatin et al., 2010[81]
In2(OH)2(obb)2		1	298	8.6	Y.-X. Tan et al., 2011[152]
In3O(abtc)1.5(H2O)3(NO3)	socMOF M080	1	273	17.9	Moellmer et al., 2010[153]

In3(BTC)4(choline)		1	273	12.3	Chen et al., 2009[154]
Zn4O(NH2-BDC)2	IRMOF-3	1.1	298	5.1	Millward and Yaghi, 2005[149]
		35	298	45.1	
Zn4O(dobdc)2	IRMOF-6	1.2	298	4.6	Millward and Yaghi, 2005[149]
		40	298	46.6	
Zn4O(NDC)3	IRMOF-8	1	273	12.2	Orefuwa et al., 2013[155]
		30	273	38.6	
		30	298	34	
Zn4O(HPDC)2	IRMOF-11	1.1	298	7.3	Millward and Yaghi, 2005[149]
		35	298	39.3	
Zn4O(TPDC)3	IRMOF-16	1	298	5.4	Bae et al., 2009[156]
Mg2(DH3PhDC)-CH2NH2	IRMOF-74- III-CH2NH2	1	298	12.3	Fracaroli et al., 2014[157]
Fe3O(TCDC)(H2O)3	LIFM-26	1	273	19.2	C.-X Chen et al., 2017[158]
		1	298	12.7	
Zr6O8(TDA)(H2O)8	LIFM-29	1	273	9.9	C.-X. Chen et al., 2016[159]
		1	298	6.13	
Zr6O8(tftpa)(H2O)8	LIFM-30	1	273	10.3	C.-X. Chen et al., 2016[159]
		1	298	4.9	
Zr6O8(NDC)(H2O)8	LIFM-31	1	273	10.3	C.-X. Chen et al., 2016[159]
		1	298	6.5	
Zr6O8(dhbpdc)(H2O)8	LIFM-32	1	273	10.6	C.-X. Chen et al., 2016[159]
		1	298	5.25	
Zr6O8(dabpdc)(H2O)8	LIFM-33	1	273	13.7	C.-X. Chen et al., 2016[159]
		1	298	7.08	
Cu(etz)	MAF-2	1	298	3.6	Zhang and Chen, 2009[160]
		1	273	8.84	
Zn2(btm)2	MAF-23	1	273	12.7	Liao et al., 2012[161]
		1	298	9.9	

Co(dpt24)2	MAF-25	1	195	18.6	Lin, Zhang and Chen, 2010[162]
		1	273	4.83	
		1	283	3	
Co(mdpt24)2	MAF-26	1	195	14.3	Lin, Zhang and Chen, 2010[162]
		1	273	3.75	
		1	283	2.9	
Zn(atz)2	MAF-66	1	273	21.7	Lin et al., 2012[163]
		1	298	16.2	
Mg(TCPBDA)		1	195	20.9	Cheon et al 2009[164]
		1	273	8.3	
		1	298	6.2	
Mg2(dobpdc)		0.15	298	12.1	McDonald et al., 2012[165]
		1	298	14.5	
Mg(3,5-pdc)	Mg-MOF-1	1	298	2.7	Mallick et al., 2010[166]
Mg2(dobdc)	Mg-MOF74, MgCPO-27	0.1	298	20.3	Bao et al., 2011[167]
		1	298	27.5	Dietzel, Besikiotis and Blom, 2009[168]
		36	278	40.8	
Al(OH)(bdc)	MIL-53(Al), USO-1-Al	1	303	9.2	Rallapalli et al., 2011[169]
		25	304	30.6	Bourrelly et al., 2005[102]
Cr(OH)(bdc)	MIL-53(Cr	1	304	8.1	Bourrelly et al., 2005[102]
		25	304	30.8	
Al12O(OH)18(Al2(OH)4)(BTC)6	MIL-96(Al)	10	303	16.2	Loiseau et al., 2006[170]
		20	303	18.6	
Cr3OF(H2O)3(BTC)2	MIL-100(Cr)	50	304	44.2	Llewellyn et al., 2008[103]
Cr3OF(H2O)2(BDC)3	MIL-101(Cr)	1	296	5.8	Chowdhury et al., 2012[171]
		50	304	56.9	Llewellyn et al., 2008[103]
Cr3OF(H2O)2(NTC)1.5	MIL-102(Cr)	30	304	12	Surblé et al., 2006[172]
Al4(OH)8(C10O8H2)	MIL-120	10	303	15.6	Volkringer et al., 2009[173]
mmen-Cu-BTTri		1	298	15.6	McDonald et al., 2011[174]

Mn(bdc)(dpe)		1	195	17.7	Foo et al., 2016[175]
Mn(NDC)(DEF)		1	195	11.7	Hoi, Kobayashi and Myunghyun,. 2006[176]
		1	273	6.2	
Mn(pmdc)		0.9	293	7.3	Beobide et al., 2008[177]
[Mn2(2,6-ndc)2(bpda)2]·5DMF	Mn-bpda	1	195	24.5	Lee et al., 2016[178]
		35	298	21.6	
Zn3(bdc)3	MOF-2	1	298	2.4	Millward and Yaghi, 2005[149]
		30	298	11.97	
Zn4O(bdc)3	MOF-5 or IRMOF-1	1	296	3.94	Millward and Yaghi, 2005[149]
		35	298	48.8	
Zn4O(BTB)2	MOF-177	1	298	6.5	Saha et al., 2010[179]
		50	298	60.8	Furukawa et al., 2010[34]
Zn4O(BBC)2(H2O)3	MOF-200	50	298	73.9	Furukawa et al., 2010[34]
Zn4O(BTB)(NDC)(H2O)3	MOF-205	50	298	62.6	Furukawa et al., 2010[34]
Zn4O(BTE)(BPDC)(H2O)3	MOF-210	50	298	74.2	Furukawa et al., 2010[34]
Al(OH)(bpydc	MOF-253	1	298	6.2	Bloch et al., 2010[177]
Cu2(bptc)(H2O)2(DMF)3	MOF-505	1.1	298	12.6	Millward and Yaghi, 2005[149]
Zn2(BDC)2(4,4’-bpy)	MOF-508	5	303	20.6	Bárcia et al., 2008[180]
Al(ABDC)(OH)	NH2-MIL53(Al)	5	303	8.4	Couck et al., 2009[181]
		13	303	22.8	
Ti(NH2-bdc)2	NH2-MIL125	1	273	15	Kim et al., 2013[63]
		1	298	8.8	
Ni(DBNBVP)2Cl2		1	273	8.1	Wu and Lin, 2006[182]
Ni3(L-TMTA)2(bpy)4		1	298	8.2	Z. Chen et al., 2011[183]
Ni-4Pyc		10	298	26.5	Nandi et al., 2015[184]
Ni2(dobdc)	Ni-MOF-74, CPO-27-N	0.1	296	10.3	Caskey, Wong-Foy and Matzger, 2008[132]
		1	296	20.3	
		22	278	34.4	Dietzel, Besikiotis and Blom, 2009[168]

Cu3(cobai)2(H2O)5	NJU-Bai3	1	273	21.5	Duan et al., 2012[185]
		20	273	49.3	
		20	298	44.3	
[Cu2(H2O)2(obaddi)]·4 H2O·2 DMA	NOTT-125	1	273	28.6	Alsmail et al., 2014[186]
		1	298	15.4	
		20	273	50.3	
		20	298	48.3	
Cu4(TDTM)	NOTT-140	1	293	11.7	C. Tan et al., 2011[45]
		20	293	47.7	
		20	283	46.2	
Me2NH2)1.75[In(bptpc)]1.75(DMF)12	NOTT-202a	1	195	46.8	Yang et al., 2012[187]
Cu3(btdi)(H2O)3	NU-111	30	298	62.8	Peng, Srinivas, et al., 2013[109]
Zr(TBAPy)2	NU-1000	1	298	10.7	Farha et al., 2010[47]
		40	298	67.1	
Cu3(TATB)2 (catenated)	PCN-6	1	273	25.65	Kim et al., 2011[63]
		1	298	15.9	
		30	298	53.9	
Cu3(btei)	PCN-61	35	298	50.8	Yuan et al., 2010[57]
Cu3(ntei)	PCN-66	35	298	53.6	Yuan et al., 2010[57]
Cu3(ptei)	PCN-68	35	298	57.2	Yuan et al., 2010[57]
Cu(NddIP)0.5	PCN-88	1	273	23.8	Li et al., 2013[188]
		1	296	15.6	
Zn(PDAT)	PCN-123	1	295	3.9	J. Park et al., 2012[189]
Zr(TCPP)2	PCN-222, MOF-545	1	298	4.9	Lv et al., 2018[190]
		30	298	37.6	
Pd(2-pymo)2		0.86	293	6.8	Navarro et al., 2006[137]
Pd(F-pymo)2		0.86	293	9.7	Navarro et al., 2007[191]
		1.2	273	13.5	
Sc2(BDC)3		1	303	3	Miller et al., 2009[192]
(Me2NH2)[In(ABDC)2]	SHF-61	20	298	9.6	Carrington et al., 2017[193]

Zn3(NTB)2	SNU-3	1	195	22.9	Suh, Cheon and Lee, 2007[194]
		1	273	6.5	
Zn2(abtc)(DMF)2	SNU-4	1	195	35.5	Lee et al., 2008[61]
		1	273	17.3	
Cu2(abtc)3	SNU-5	1	195	52.9	Lee et al., 2008[61]
		1	273	27.8	
Cu2(BPnDC)2(4,4'-bpy)	SNU-6	1	273	9.9	Park and Suh, 2008[195]
Zn2(BPnDC)2(bpy)	SNU-9	30	298	23	Park and Suh, 2010[196]
Co2(MTB)	SNU-15	1	273	6.5	Cheon and Suh, 2009[197]
Cu2(TCM)	SNU-21S	1	298	10	Kim and Suh, 2011[63]
Zn2(TCPBDA)(H2O)2	SNU-30	1	195	31.6	Park, Cheon and Suh, 2010[62]
		1	273	10.3	
		1	298	4.9	
		50	298	18	
Zn2(TCPBDA)(bpta)	SNU-31	1	195	14.6	Park, Cheon and Suh, 2010[62]
		1	273	5	
		1	298	2.6	
		40	298	8.8	
Cu2(bdcppi)	SNU-50	1	195	47.2	Prasad, Hong and Suh, 2010[64]
		1	273	19.1	
		1	298	13.7	
		46	298	42.9	
Zn4O(CEB)2	SNU-71	1	195	36.7	Prasad and Suh, 2012[114]
		1	298	4.2	
Ni2(CYC-2C-CYC)(bptc)	SNU-M10	1	195	19.5	Choi and Suh, 2009[198]
		1	273	12.7	
		1	298	8.5	
Ni2(CYC-4C-CYC)(bptc)	SNU-M11	1	195	19.5	Choi and Suh, 2009[198]
[Zn4O(bdc)3].(ZnO)0.125	SUMOF-2	1	273	15.9	Yao et al., 2012[199]
Zn4O(NDC)3	SUMOF-3	1	273	13	Yao et al., 2012[199]

Zn4O(bdc)2(bpdc)(H2O)	SUMOF-4	1	273	13.7	Yao et al., 2012[199]
Cu(bpy)2(EDS)	TMOF-1	1	200	22.9	Zhang et al., 2016[200]
		1	273	9	
		1	298	5.8	
		1	308	4.9	
Zn2(obb)2(bpta)	TMU-22	1	203	24.1	Safarifard et al., 2016[201]
Zn2(obb)2(bpfn)	TMU-24	1	203	21.7	Safarifard et al., 2016[201]
Zr6O4(OH)4(bpdc)12	UiO(bpdc)	20	303	42.1	Li et al., 2014[202]
Zn4O(BDC)(BTB)4/3	UMCM-1	1	298	3.8	Yazaydın et al., 2009[203]
		24	298	50.8	Mu, Schoenecker and Walton, 2010[204]
Cu3(BPT)2	UMCM-150	1	298	10.2	Yazaydın et al., 2009[203]
Ni2(BDC)2(DABCO)	USO-2-Ni	1	298	10	Arstad et al., 2008[205]
Ni2(2-amino-BDC)2(DABCO)	USO-2-Ni-A	1	298	14	Arstad et al., 2008[205]
In(OH)(BDC)	USO-3-In-A	1	298	8	Arstad et al., 2008[205]
Al(OH)(Sbpdc)	USTC-253	1	273	14	Jiang et al., 2015[206]
		1	298	8.5	
Al(OH)(Sbpdc)(TFA)	USTC-253- TFA	1	273	21.2	Jiang et al., 2015[206]
		1	298	11.3	
Cu(BDC−OH)(4,4′-bipy)	UTSA-15a	1	296	5.1	Z. Chen, Xiang, Hadi D. Arman, et al., 2011a[207]
Cu3(BHB)	UTSA-20a	1	296	17	Guo et al., 2011[69]
Zn(BDC-OH)(DABCO)0.5	UTSA-25a	1	296	12	Z. Chen, Xiang, Hadi D Arman, et al., 2011b[208]
Zn4(TIPAB)(DMA)4	UTSA-33a	1	273	8.9	He, Zhang, Xiang, Fronczek, et al., 2012[209]
Zn2(bttb)(diPyNI)	YO-MOF	1	273	14.4	Mulfort et al., 2010[210]
		1	298	4.5	
Zn(MeIM)2	ZIF-8	1	298	4.3	Yazaydın et al., 2009[203]
Zn(nIm)(bIm)	ZIF-68	1	298	6.4	Banerjee et al., 2009[211]
Zn(nIm)(cbIm)	ZIF-69	1	298	7.9	Banerjee et al., 2009[211]
Zn(nIm)(Im)	ZIF-70	1	298	4.43	Banerjee et al., 2009[211]
Zn(nbIm)(nIm)	ZIF-78	2	298	9.52	Banerjee et al., 2009[211]

Zn(nIm)(mbIm)	ZIF-79	1.1	298	5.9	Banerjee et al., 2009[211]
Zn(nIm)(cnIm)	ZIF-82	1	298	7.84	Banerjee et al., 2009[211]
Zn(almeIm)	ZIF-93	1	298	6.7	Morris et al., 2010[212]
Zn(cyamIm)	ZIF-96	1	298	8.5	Morris et al., 2010[212]
Cu2(BTADD)(H2O)2	ZJNU-40	1	273	24.9	Song et al., 2014[213]
		1	296	16.3	
[Cu2(qdip)(H2O)2]·3DMF·2EtOH	ZJNU-43	1	273	24.9	Song, Hu, et al., 2015[214]
		1	296	17.2	
[Cu2(qodip)(H2O)2]·3DMF·3MeOH Z	ZJNU-45	1	273	23.5	Song, Hu, et al., 2015[214]
		1	296	16.1	
Zn(BDC-NH2)(dabco)0.5		1	298	8.8	Zhao et al., 2011[215]
Zn(BDC-OH)(dabco)0.5		1	298	11.7	Zhao et al., 2011[215]
Zn(BPZNO2)		1.2	298	18	Mosca et al., 2018[216]
Zn(dtp)		1	195	14	J.-R. Li et al., 2008[217]
Zn(MIai)		1	298	7.9	Debatin et al., 2010[81]
Zn2(2,5-BME-bdc)2(dabco)		1	195	16.8	Henke et al., 2012[218]
Zn2(BDC)2(dabco)		1	294	8.1	Mishra et al., 2012[219]
		25	294	37.3	
Zn2(BME-bdc)2-(bipy)		1	195	23.6	Henke and Fischer, 2011[220]
		1	273	9.2	
		1	298	5.56	
Zn2(BMOE-bdc)2(dabco)		1	195	25.4	Henke et al., 2010[221]
Zn2(BMOP-bdc)2(dabco)		1	195	8.6	Henke et al., 2010[221]
Zn2(bpdc)2(bpe)		1	273	7.3	J. Zhang et al., 2010[222]
		1	298	4.7	
Zn2(DB-bdc)2(dabco)		1	195	9.9	Henke et al., 2012[218]
Zn2(MOE-bdc)2(dabco)		1	195	30.7	Henke et al., 2010[221]
Zn2(NDC)2(diPyNI)		1	298	5.8	Bae et al., 2011[223]
Zn2(ox)(atz)2		1.2	273	16.1	Vaidhyanathan et al., 2009[224]
		1.2	293	14.2	

Zn4(OH)2(BTC)2		1	295	6.7	Z. Zhang et al., 2010[225]
Zn4O(BMOE-bdc)3		1	195	18.1	Henke et al., 2010[221]
Zn4O(BMOP-bdc)3		1	195	11.9	Henke et al., 2010[221]
Zn4O(FMA)3		2	296	3.8	Xiang et al., 2012[138]
Zn4O(MOE-bdc)3		1	195	47	Henke et al., 2010[221]
[Zn4(BDC)4(BPDA)4]·5DMF·3H2O	Zn-bpda	1	298	7.5	Lee et al., 2013[226]
		35	298	13.2	
Zn2(dobdc)	Zn-MOF-74	0.1	296	5.4	Caskey, Wong-Foy and Matzger, 2008[132]
		1	296	19.5	
Zn(5-AT)2	ZTF-1	1	273	19.8	Panda et al., 2011[80]

Table S4: Individual coefficient of determination values for each fold in the 10 runs

	Fold number									
Run	1	2	3	4	5	6	7	8	9	10
1	0.91	0.87	0.87	0.92	0.87	0.87	0.92	0.86	0.90	0.85
2	0.86	0.88	0.89	0.90	0.84	0.86	0.86	0.92	0.84	0.92
3	0.86	0.86	0.93	0.91	0.90	0.83	0.92	0.90	0.87	0.83
4	0.85	0.87	0.89	0.91	0.92	0.82	0.87	0.87	0.89	0.88
5	0.89	0.90	0.93	0.83	0.89	0.88	0.87	0.85	0.84	0.92
6	0.89	0.90	0.82	0.94	0.86	0.89	0.86	0.87	0.89	0.85
7	0.88	0.87	0.87	0.91	0.91	0.89	0.79	0.86	0.90	0.87
8	0.89	0.84	0.92	0.86	0.88	0.88	0.88	0.85	0.86	0.88
9	0.79	0.91	0.87	0.87	0.92	0.90	0.82	0.91	0.90	0.86
10	0.88	0.89	0.83	0.81	0.88	0.88	0.87	0.89	0.91	0.91

Hyperparameters for other machine learning models

Linear Regression

This was fitted using the “fitrlinear” function in MATLAB 2020. All other parameters that are not stated are set to their default values.

Lambda = 0.048818

Learner type = Least Squares

Regularisation = Ridge

Decision Trees

This was fitted using the “fitrtrees” function in MATLAB 2020. All other parameters that are not stated are set at their default values.

Minimum Leaf size = 3

Maximum number of splits = 195

Support Vector Mechanism

This was fitted using the “fitrsvm” function in MATLAB 2020. All other parameters that are not stated are set at their default values.

Box Constraint = 0.11404

Epsilion = 0.18408

Kernel Function = Linear

Standardize data = False

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