Supporting Information for

Potentials of Ultramicroporous Metal Organic Frameworks in CO_2 Clean-up

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Table S1. List of selected triazolate based metal organic frameworks.

S. No.	Compound formula/code	Dense	Potentially Porous	Porous	Adsorption	Remark	Reference
1.	$[Yb(Tz)_3]$ and $[Eu_2(Tz)_5(TzH)_2]$	Yes				First 3D networks of lanthanides with complete nitrogen coordination spheres	Chem. Commun., 2006, 2060–2062.
2	1:$\{[Zn_{2.5}(trz)_2(btc)(H_2O)].2H_2O\}_n$ 2:$[Zn_{2.5}(trz)(Hbtc)_2(H_2O)_2]_n$ 3:$\{[Zn(Htrz)(Hbtc)(H_2O)].2H_2O\}_n$	Yes				The topologies and dimensionality of the complexes depend on the deprotonation extent of the two ligands. 1 was obtained at the initial pH value of 3.6 adjusted by TEA, and both its ligands are completely deprotonated. Containing monodeprotonated trz and doubly deprotonated Hbtc, 2 is isolated at pH 3.4 by slow evaporation of the filtrate. Upon further evaporation, 3 with neutral Htrz and doubly deprotonated Hbtc is produced.	CrystEngComm, 2008, 10, 1140–1143.
3.	1:$Zn(L)(bdc)_{0.5}\cdot 0.25H_2O$ 2:$Zn(L)(bdc)_{0.5}\cdot 0.17H_2O$ HL = 1,2,4-triazol-3-amine, H2bdc = terephthalic acid	Yes			The solvent-accessible volume calculated using the Platon program is ca. 1116.3 Å^3 and 012.6 Å^3, equal to 27.5% and 32.5% of the cell volume for 1 and 2. But do not take CO_2 or N_2	The formation of these MOFs is controlled by different speeds of crystallization. Operation of controlling the speed of crystallization may play a profound role in determining the aggregation fashions of Zn(II) ions and L− ligands, resulting in the various layers, viz. a 4·82 net vs. a 4·6·12 net.	Dalton Trans., 2013, 42, 13802.
4.	1: $[Cu_3(\mu_3\text{-}O)(\mu_3\text{-}trz)_3]_2[OH]_2.15H_2O$ 2: $Cu[Cu_3(\mu_3\text{-}O)(\mu_3\text{-}trz)_3Cl_3]$ 3: $[Cu_2(\mu_3\text{-}trz)(\mu_3\text{-}Cl)_2]$		Yes			Taking the van der Waals radii into account, the aperture may only admit the passage of a sphere with a 4.5 Å diameter in 1. If this highly open structure is viewed from the [-1,0,1] axis, a larger channel can be seen with cross dimensions of ca. 11.1x5.9 Å. 3 is of interest as it exhibits unique 2D inorganic layers which are different from those of basic copper halide skeletons such as square dimers, cubane tetramers, zigzag chains, double stranded ladders, hexagonal grid chains, it has mixed valence copper atoms and it presents the first example of 1,2,4-triazoles as organic	Crystal Growth & Design, 2006, 6, 1393-1398.

					components in the field of inorganic organic hybrid copper halides.	
5.	1:ZnCl(AmTRZ) 2:$Zn(HCO_2)$(AmTRZ) 3:$Zn_5(OH)_2(AmTRZ)_6(NO_3)_2.6H_2O$ 4:$Zn_5(OH)$(AmTRZH)-$(AmTRZ)_6(HCO_2)_3.5H_2O$	Yes			Isostructural compounds 1 and 2 display a two-dimensional layer structure.3 is a dense three-dimensional Framework. 4 is built from porous Zn-AmTRZ layers containing 12- and 8-membered rings, which are connected to each other by dinuclear Zn tetrahedra building units. Water and format anions occupy the void inside the framework. 4 has channels which are 3.21x3.22Å^2 and 8.83x8.83Å^2 taking the van der Waals radii into account.	Crystal Growth & Design, 2007, 7, 7.
6.	1·(H_2O):$[Zn_3(AmTAZ)_3S](NO3)\cdot(H_2O)$ 2·2(EtOH):$Zn_7(AmTAZ)_8(CO_3)_2(OH)_2\cdot 2(EtOH)$		Yes		1·(H2O) is constructed from triangular Zn_3S units that are bridged through AmTAZ ligands into a cationic three-dimensional (3D) network with nitrate and water molecules residing in the cavities. 2·2(EtOH) shows a complex 3D network constructed from seven crystallographically unique zinc centers bridged by AmTAZ, carbonate, and hydroxide anions.	Crystal Growth & Design, 2009, 9, 3609–3614
7.	1:$[Co(atz)(L1)_{0.5}]\cdot$DMF 2:$[Co(atz)(L2)_{0.5}]\cdot$DMF Hatz = 3-amino-1,2,4-triazole, L1 = 4,4′-biphenyldicarboxylate, L2 = 3,3′-biphenyldicarboxylate		Yes	N_2 77K: Langmuir surface areas of 902 and 737 m^2/g, BET surface areas of 683 and 552 m^2/g for 1 and 2. CO_2, CH_4, H_2 adsorptions done and selectivities studied.	Isomeric 1 and 2 based on positional isomeric biphenyldicarboxylate ligands exhibit distinct temperature-dependent CO2 sorption behaviors. They contain naked amino groups and possess the same topology net. The square aperture diameter for each channel is 4.7 × 4.8 Å^2 along the [010] direction for 1 and [101] direction for 2 (excluding vWaals radii. The likely reason for the distinct adsorption behaviors should be related to the stronger interaction of CO_2 with amino groups.	Cryst. Growth Des. 2014, 14, 2003−2008.
8.	1:$[Co_{2.5}(btc)$-$(atz)_2(Hatz)(DMF)]\cdot 2DMF$ (1) 2:$[Co_{2.5}(btc)(Hbtc)_{0.5}(atz)(CH_3CN)(H_2O)]\cdot H_2O$		Yes	N_2 77K: Langmuir surface areas of 609 and 471 m^{2}g^{-1}, BET surface areas of 465 and 356 m^{2}g^{-1} for 1 and 2. The enhanced CO2 uptakes of 1 and 2 should be attributed to their free $-NH_2$ groups, the exposed Co^{2+} sites	Both contain suitable pore sizes and highly polar channel systems functionalized by amino groups, open metal sites, carbonyl or free carboxylic acid sites and uncoordinated triazolate nitrogen atoms on the pore surfaces, exhibiting multipoint interactions between CO_2 molecules and frameworks, resulting in high CO_2 uptake and selectivity for CO_2 over N_2. Two types of pores in 1 ~4.1 × 4.7 and 6.8 × 8.1 Å^2 (excluding van der Waals radii of the atoms) respectively. 1 has 45.6% solvent void accessible	Dalton Trans., 2013, 42, 13990.

				volume. 2 has channels of 3.5 × 5.3 and 5.0 × 5.8 Å^2 and 32.2% of solvent accessible volume.	
9.	MAF-2[Cu(etz)]$_n$ Hetz = 3,5-diethyl-1,2,4-triazole	Yes	Solvent sorption	By virtue of the kinetically controlled flexibility and hydrophobic pore surface, MAF-2 can adsorb large amounts of small organic molecules but excludes H_2O. MAF-2 can also separate benzene and cyclohexane efficiently, as its flexible scaffold can distort to a certain degree so that benzene can diffuse through the distorted apertures but cyclohexane cannot.	J. AM. CHEM. SOC. 2008, 130, 6010–6017.
10.	$[Cu_3(\mu 3\text{-}OH)(\mu 2\text{-}O)(dmtrz)_2(HCOO)(\mu 2\text{-}H_2O)(H_2O)_3].H2O$	Yes	CO_2 273K BET and langmuir surface area was calculated to be ca.105 m^2/g and 147 m^2/g	3D structure with 1D channels along the c axis. The pore size is calculated to be ca. 6.9 Å (taking van der Waals radii in to consideration) and the solvent-accessible volume is estimated to be ca. 46.2%.	CrystEngComm, 2013, 15, 3484–3489.
11.	MET1: $(Mg(C_2N_3H_2)_2$, MET2: $(Mn(C_2N_3H_2)_2$, MET3: $(Fe(C_2N_3H_2)_2$, MET4: $(Co(C_2N_3H_2)_2$, MET5: $(Cu(C_2N_3H_2)_2$, MET6: $(Zn(C_2N_3H_2)_2$,	Yes	Pore size, and SA table in paper	All the metal ions are octahedrally coordinated to the nitrogen atoms of triazolate such that five metal centers are joined through bridging triazolate ions to form super-tetrahedral units that lie at the vertexes of a diamond-type structure. The variation in the size of metal ions across the series provides for precise control of pore apertures to a fraction of an Angstrom in the range 4.5 to 6.1 Å.	Chem. Eur. J. 2012, 18, 10595 – 10601.
12.	C_6H_6@MAF-42-lp,=$[Cu_4(btm)_2]$ $.C_6H_6$ O53, O74 and O100 are MAF42 oxidized to 53, 74 and 100% H_2btm=bis(5-methyl-1,2,4-triazolate-3-yl)methane)	Yes	CH_4 and CO_2 adsorption has been studied	3D porous framework having large 1D rhombic channels (void 37.8%, cross-section size 4.8x7.1–6.0x10.8 Å^2) with disordered benzene molecules filled inside. The oxidation degree has been related to the adsorption behavior of the MOFs	NATURE COMMUN. DOI: 10.1038/ncomms 7350.
13.	MAC-4: $\{[Zn_5(dmtrz)_3(IPA)_3(OH)]\cdot DMF\cdot H_2O\}_n$ (Hdmtrz = 3,5-dimethyl-1H-1,2,4-triazole, H_2IPA = isophthalic acid) MAC-4-OH: $\{[Zn_5(dmtrz)_3(OH\text{-}IPA)_3(OH)]\cdot DMF\cdot 5H_2O\}_n$ (OH-	Yes	N_2 77K : MAC-4 has a BET and Langmuir surface area of 796 and 1151 m^2/g. MAC-4-OH has a BET and Langmuir surface area of 339 and 496 m^2/g. CO_2 adsorption done.	MAC-4-OH is an iso-reticular framework of MAC-4 with channels functionalized by hydroxyl groups. MAC-4-OH shows a significant enhancement for CO_2 uptake compared with that of MAC-4 due to the existence of electrostatic attractive interactions, though its surface area is lower than that of MAC-4. The Qst at zero coverage of activated MAC-4-OH is ca 31 kJ/mol, which is much higher that of MAC-4	Dalton Trans., 2012, 41, 4007–4011.

	H_2IPA = 5-hydroxyisophthalic acid)			(21 kJ/mol), indicating stronger binding ability of activated MAC-4-OH to the CO_2 molecules.	
14.	1:$\{[NH_2(CH3)_2][Zn(atz)(ox)].H_2O\}_n$ (Hatz = 5-amino-1H-tetrazole, H_2ox = oxalic acid)	Yes	Selective for CO_2 over CH_4 and N_2. CO_2 195K: The BET and Langmuir surface areas were calculated to be 125 and 165 m^2/g.	Complex 1 reveals an anionic porous framework with disordered $[NH_2(CH_3)_2]^+$ cations scattering in its channels, which provides the favorable condition for encapsulation of metal cations via exchange process. All the amino groups of atz^- ligands point to the center of the channel, which is conducive to the interaction between the framework and guest molecules/ions in the channels.	RSC Adv., 2015, 5, 24655–24660.
15.	MTAF-1: $(Zn_5(\mu3\text{-}O)_2(C_9N_3H_5O_2)_5(H^+)_4(H_2O)_{17}(C_3H_7NO)_{10})$	Yes	N_2 77K: BET surface area of 2020 m^2/g (P/P_0 = 0.01−0.15), corresponding to a Langmuir surface area of 2300 m^2/g (P/P0 = 0.9). Ar at 87 K reveals similar surface area values.	MTAF-1 represents the first example of a double-walled MOF based upon a unitary organic linker, and this kind of double walled arrangement has prevented the formation of interpenetration and can enhance the robustness of the framework. It has rectangular channels of 11.583 Å × 9.947 Å (atom-to-atom distance) along a or b axis and square channels of 9.984 Å × 9.984 Å along the c axis.	Inorg. Chem. 2012, 51, 4423−4425.
16.	1:$\{[Zn_2(HBDC)_2(dmtrz)_2].guest\}_n$ H_2BDC = 1,4-benzenedicarboxylate acid, Hdmtrz = 3,5-dimethyl-1H, 1, 2, 4-triazole	Yes	N2 77K: BET surface area of ca. 552 m^2/g, Langmuir surface area of ca. 807.8 m^2/g, and the pore size of ca. 6.7 A° (HK method).	The MOF has 1D channels along c axis, of 7.0 x7.0 A° taking van der Waals radii into calculation. CO2 and vapor sorption studied. It shows selective adsorption of linear and monobranched hexane isomers over a dibranched one.	Chem. Commun., 2011, 47, 7197–7199.
17.	1:$[Zn(FA)(datrz)_2]_n$ (H_2FA = fumaric acid, Hdatrz = 3,5-diamino-1,2,4-triazole)	Yes	N2 77K : BET and Langmuir surface areas are 721 m^2/g and 498 m^2/g.	The solvent accessible volume in is 38.9%. At zero coverage, the CO_2 adsorption enthalpy for compound 1 is 23.98 $kJmol^{-1}$.	Z. Anorg. Allg. Chem. 2015, 1556–1559
18.	1:$[Zn_4(TRZ)_4(TTBDC)_2]_n$ 2:$[Zn_2(TRZ)_2(DOBDC)]_n$ (TRZ = 1,2,4-triazole, TTBDC = trans,trans-1,3-butadiene-1,4-dicarboxylic acid, DOBDC = 2,5-dihydroxyterephthalic acid).	Yes	N_2 77K: The BET and Langmuir surface areas are 255.5 cm^3/g and 402.5 cm^3/g for 1, 288.7 cm^3/g and 448.1 cm^3/g for 2.	PLATON calculations show that pillar-layered MOF 1 and 2 have 53.0% and 47.2% potential guest-accessible volumes, respectively. Both MOFs show not only remarkable H_2 and CO_2 uptake capacity, but also high CO_2 over CH_4 selectivity. In 2, OH groups act as lewis base sites for better uptake.	Inorganic Chemistry Commun. 2015, 62, 107–110.
19.	(SNNU-21):$\{[(CH_3)_2NH_2]_2[Cd_5(DATRZ)_4(BDC)_4]\}_n$ (SNNU-22): $\{Cd_4(ATRZ)_2(BDC)_3(DMF)(H_2O)\}_n$ (SNNU-23):	Yes	BET surface areas derived from the N_2 sorption isotherms are 190.1, 222.9 and 624.7 m^2/g for SNNU-21, -22 and -23. H_2, CH_4, CO_2,	All of these rod MOFs show not only remarkable CO_2 uptake capacity, but also high CO_2 over CH_4 and C_2-hydrocarbons over CH_4 selectivity under ambient conditions. SNNU-21 has two types of 1-D channels exist along the a-axis direction with the dimensions	Dalton Trans., 2017, 46, 836–844.

	$\{[(CH_3)_2NH_2]_2[Zn_5(TRZ)_4(BDC)_4]\}_n$ (TRZ = 1,2,4-triazole, ATRZ = 3-amino-1,2,4-triazole and DATRZ = 3,5-diamino-1,2,4-triazole, BDC = 1,4-benzenedicarboxylic acid).			C_2H_2 adsorption studied.	of about 6.0 Å × 7.0 Å and 7.5 Å × 10.5 Å with DMF cations in the pore. SNNU-22 has channels of 4.0 Å × 5.0 Å and 6.0 Å × 10.0 Å. SNNU-23 has two types of channels with dimensions of about 3.5 Å × 11 Å and 6.0 Å × 12 Å extend along the a-axis, and one type of channel (3.0 Å × 6.5 Å) exists along the b-axis direction.	
20.	1:[Zn(AmTAZ)(CH_3COO)] 2:$[Zn_4(AmTAZ)_4(SO_4)(OH)(C_2O_4)_{0.5}].2H_2O$ 3: [Cd(AmTAZ)Br 4:[Cd(AmTAZH) SO_4]	Yes		Not truly ultra-microporous	1 is 2D. 2 has 3D framework with three kinds of 1D channel; hexagonal prismatic channel (11.5x8.0A°), quadrangular prismatic channels (6.9x9.6A°) and a second quadrangular prismatic channel (7.1x7.1A°). 3 crystallizes in a chiral space group P212121, giving a homochiral 3D framework with 2 types of helical channels (left- and right-handed). 3-amino-1,2,4-triazole molecules in 4 behave as neutral m2-2,4-bridges to connect the 2D $CdSO_4$ sheets into a 3D framework.	Journal of Solid State Chemistry, 2008, 181, 2078–2086.
21.	1: $\{[Zn_7(trz)_6(1,3\text{-}bdc)_4(H_2O)_2]\cdot 2H_2O\}_n$ 2:$\{[Zn_7(trz)_6(hip)_4(H_2O)_2]\cdot 8H2O\}_n$ 3:$[Zn_4(trz)_4(Hnip)_2(nip)]_n$ 4:$[Zn_5(trz)_2(Hbtc)_4(H_2O)_4]_n$ H_2hip : 5-hydroxyisophthalic acid H_2nip: 5-nitroisophthalic acid	Yes			All 3D. 1 displays intersecting ring channels as viewed from b and c directions. Even after interpenetration, it presents rhombic-shaped channels along the b-axis, and the channel size is ~4.8 × 5.1 $Å^2$. If 1 is viewed from the c-axis, a larger channel can be seen with cross dimensions of about 5.6×6.3 $Å^2$. 2 is isostructural to 1 and the channel size is ~ 4.6 × 5.0 $Å^2$ along the b-axis, and the channel size is about 5.1 × 5.3 $Å^2$ viewed from the c-axis.	Crystal Growth & Design, 2009, 9, 105.
22.	$\{[Cu_3(dmtrz)_2(OX)_2\text{-}(H_2O)_2].8.5H_2O\}_n$		Yes	N_2 77K: BET surface area: 676.4 m^2/g. Pore volume of 0.212 cm^3/g. The Horvath–Kawazoe (HK) model indicates a pore diameter of 4.31A	It shows single-crystal-to-single-crystal transformation during a reversible dehydration and rehydration process accompanied by color change from blue to violet to blue. The hydrogen adsorption of anhydrous 1a was evaluated at 77 K and 87 K. The H_2 sorption isotherm shows type-I behaviour without hysteresis and noticeable change in properties upon repeated cycles. At 1 atm, anhydrous 1a showed a gravimetric H_2 uptake of 1.48 and 1.26 wt% at 77 and 87 K, respectively, which corresponds to a H_2 storage capacity of 19.2 and 16.3 g/L.	CrystEngComm, 2011, 13, 768–770.
23.	$Zr(OH)_2(C_2O_4)$	No	Water adsorption	It has a void volume of 8.9%, which is quite	The homometallic 3D framework displays channels along the c axis with a square	Cryst. Growth Des., 13, 11, 5100-5106

				small. Guest free phase shows reversible uptake of water but no gas uptake.	cross-section with side dimensions of 6.492(2) Å (Zr−Zr separation) decorated by the hydroxo units (O•••O separation, 3.382(4) Å). Here, hydroxyl moieties are terminally bound to metal and point towards channel.	
24.	barium titanyl oxalate (BTO): $BaTi(O)(C_2O_4)_2.5H_2O$	Yes			The chemical formula is more accurately described as $Ba_2Ti_2O_2(C_2O_4)_4.10H_2O$ in order to account for the number of unique atoms in the structure. Seven of the ten water molecules are associated with barium atoms, and the remaining three waters occupy interstitial sites in the structure and are not coordinated to either titanium or barium atoms. The compound readily loses water beginning at room temperature, depending on drying conditions and/or relative humidity; hence in the past the compound has been referred to most often as the tetrahydrate, $BaTi(O)(C_20_4)_2.4H_20$.	Chem. Mater., 1992, 4, 1208-1216.
25.	$[Ti_2O_3(H_2O)_2](C_2O_4)\cdot H_2O$	Yes			This is the first report of a single Ti(IV) oxalate. The structure consists of inorganic corrugated layers of corner-sharing TiO_6 octahedra, which forms infinite –Ti–O–Ti– connections, linked together by the oxalate anions and rest co-ordination sites occupied by water giving a nonporous framework.	Solid State Sciences, 2003, 5, 175–182.
26.	$NH_4[Ti(C_2O_4)_2\cdot 2H_2O$	Yes			3D structure of the eight-coordinated polymeric titanium(III) complex contains a counter-balancing NH_4^+ cations in the pore making the framework non-porous in nature.	Inorganica Chimica Acta, 1993, 203, 219-222.
27.	1. $[Eu(NTA)(H_2O)_2]\cdot H_2O$ 1a. $[Eu(NTA)(H_2O)_2]$ 2. $[Tb(NTA)(H_2O)]$ 3. $[Ho(NTA)(H_2O)]$ 4. $[Ho(NTA)(H_2O)]$ 5. $[Tm(NTA)(H_2O)]$ Where, NTA = nitrilotriacetate			No adsorption data available.	1 is an irregular 2D lattice motif with alternative L- and R-type single-chain helixes while 1a is 3D structure. But, both 2 and 3 are 2D double layer structures. Again, 4 and 5 display 3D frameworks, which have 1D channel fabricated through interweaving left/right-hand triple-stranded helixes.	*Crystal Growth & Design*, 2010, **10**, 775-781.
28.	$(C_8H_4CeO_{18}Zr)_n .nH_2O$				It is a 3D structure with pore along two crystallographic axes. Each Ce^{4+} & Zr^{4+} occupied by four oxalates in μ^2 chelating fashion and two water molecules to give neutral framework.	*CSD Communication(Private Communication)*, 2007, CCDC 227146.
29.	$[Sm_2(fumarate)_3(H_2O)4]\cdot 3H_2O$	Yes			The layered pillared Sm-fumarate layer is wavy and this makes the 3D framework less open. Despite the rigidity of	*Dalton Trans., 2006, 765-768.*

				fumarate, MOF upon dehydration (loses ~15% mass) shrinks reversibly.	
30.	MIL-53(Al)-FA: Al(OH)(fumarate)·3.5H_2O	Yes	The porosity of the activated Al fumarate was determined by N_2 porosimetry at 77 K. The experimental BET area of 1080 m^2g^{-1}. For pure dry CO_2, the breakthrough capacity is around 75% of the equilibrium saturation capacity. Under 14% RH, an uptake of 1.4 mmol/g was observed, which is 17% less than predicted from the CO_2 equilibrium isotherm, indicating the influence of water on CO_2 adsorption.	It has square-shaped 1-D channels with dimensions 5.7 x 6.0 Å^2. The Al-hydroxy-fumarate is quite rigid and its dehydrated form shows a notable structural change only at 250MPa (2500bar) and above. It is very stable due to the inorganic SBU- hydroxyl bridged Al- chains. Despite of having hydrophilic channels material is quite stable to water (type-IV isotherm for water sorption).	*Angew. Chem. Int. Ed., 2015, 54, 3664 –3668.* *RSC Adv., 2014, 4, 24073-24082.* *Ind. Eng. Chem. Res., 2016, 55, 2134−2143.*
31.	MIL-88A: $Fe^{III}_3O(CH_3OH)_3\{O_2C\text{-}C_2H_2\text{-}CO_2^-\}_3\cdot(CH_3CO_2^-)\cdot(CH_3OH)_{4.5}$	Yes	Interestingly, despite the presence of acetate ions in the channels, MIL-88 takes up about 4.5mmol/g of CO_2 selectively over N_2 as ascertained from a dynamic breakthrough study.	MIL-88A exhibits a 3D structure built up from trimers of iron(III) octahedra linked to fumarate di-anions to create a 3D framework with a cage-structure with 6Å windows. This structure consists of both 1D pore channel along the c axis, which is filled with methanol and cages, which are filled with acetate groups. After removal of methanol it creates potential voids.	*Angew. Chem. Int. Ed., 2004, 43, 6286 –6289.*
32.	MIL-88B: $Fe_2NiO(OOC–C_6H_4–COO)_3\cdot$ 3DMF	Yes	From N_2 porosimetry at 77K, calculated BET surface area 1120, 549, 465, 355 and 30 m^2g^{-1} for bipyridine, pyridine, pyrazine, DMF and water phase respectively. CO_2 adsorption capacity of the all phases increase with the increase in porosity of the samples. Bipyridine phase shows the highest capacity, 101 cc g^{-1} STP of CO_2.	MIL-88B has terminally bound DMF, which can easily be replaced by terminal ligands like H_2O, pyridine, pyrazine, 4,4'-bipyridine. This helps retain the breathing effect. Among all the phases, MIL-88B with terminal bipyridine shows highest surface area.	*Dalton Trans., 2013, 42, 550–557.*

33.	MOF-801: Powder form is denoted as MOF-801-P and single crystal form is denoted as MOF-801-SC.		Yes	BET and Langmuir surface area for MOF-801-SC are 690 and 770 m^2 g^{-1} respectively whereas those for MOF-801-P are 990 and 1070 m^2 g^{-1}. CO_2 Uptakes at 0.15 and 1 bar & 298K are 0.75 and 2.22 mmol g^{-1}. CO_2/N_2 Selectivity at 1 bar and 298K is 78.	There are two crystallographically independent tetrahedral cavities, with slightly different sizes of 5.6 Å and 4.8 Å diameter in the core framework. The diameter of the octahedral cavity is 7.4 Å.	*J. Am. Chem. Soc. 2014, **136**, 4369.*
34.	IRMOF-1: $Zn_4O(FMA)_3$		Yes	The Langmuir & BET surface areas: 1618 and 1120 m^2g^{-1}, respectively. It can take 69 wt% CO_2 at 300 K & 28 bar. At 1 bar it takes approx. 8.5 wt% of CO_2, HOA: 29 kJ/mol.	The Zn-fumarate has a 3D primitive cubic (α-Po) structure with intersecting pores of ~6.8 x 6.8 A°. The structure is built from octahedral Zn_4O units, bridged by fumarate.	*Inorg. Chem., 2009, **48**, 4649-4651.*
35.	UiO-66(Zr-Terepthalate):		Yes	BET surface area: 1105 m^2g^{-1}, CO_2 Uptake at 1 bar & 298K: 1.8 mmol/g, CO_2/N_2 Selectivity at 1 bar and 298K: 27 and HOA: 25 kJ/mol.	UiO-66 is one of the few known water-stable MOFs that are readily amenable to direct ligand substitution. In this work, UiO-66 has been synthesized with amino-, nitro-, methoxy-, and naphthyl-substituted ligands to impart polar, basic, and hydrophobic characteristics.	*Langmuir, 2012, 28, 15606−15613.*
	$UiO\text{-}66\text{-}NH_2$			BET surface area: 1112 m^2g^{-1}, CO_2 Uptake at 1 bar & 298K: 2.97 mmol/g, CO_2/N_2 Selectivity at 1 bar and 298K: 58 and HOA: 28 kJ/mol.	Its channels are functionalized by amine groups. It shows a significant enhancement for CO_2 uptake compared with that of non-functionalized UIO-66 due to the existence of electrostatic attractive interactions between amine group present and CO_2.	
36.	UiO-66-EA		Yes	Langmuir surface area: 567 m^2g^{-1}, CO_2 Uptake at 1 bar & 298K: 1.69 mmol/g, CO_2/N_2 Selectivity at 1 bar and 298K: 365 and HOA: 66 kJ/mol.	CO_2 uptake is less due to the bulky nature of the aliphatic amine groups. High HOA value for UiO-66-EA at low coverage is indicative of a chemisorption interaction and that is why high CO_2/N_2 Selectivity is found for this material.	*J. Mater. Chem. A, 2015, 3, 21849–21855.*
37.	$[Ln_2(fum)_2(ox)]$ Where, Ln = Eu and Tb	Yes		Adsorption studies not done.	These are amorphous due to the loss of coordination water and probable collapse of the open frameworks.	*Inorg. Chem., 2007, **46**, 1337 1342.*
38.	UTSA-16: $[KCo_3(C_6H_4O_7)(C_6H_5O_7)(H_2O)_2]$		Yes	It has high uptake (160 cm^3 cm^{-3}) of CO_2 at 296 K & 1 bar pressure. The CO_2/N_2 selectivity is 314	This is an open framework with diamondoid cage of dimension 3.3 Å x 5.4 Å. It is an Ultra microporous material.	*Nat. Commun., 2012, 3, 954-963.*

			at 100 kPa and 296 K.		
39.	NOTT-300: $[Al_2(OH)_2(L)](H_2O)_6$ (L = biphenyl-3,3′,5,5′-tetracarboxylate)	Yes	No uptake of H_2 and N_2 at 77 K and at 87 K respectively. Saturated CO_2 uptake at 273 K and 7.0 bar = 8.7 mmol g^{-1}, Zero-loading HOA: 27–30 kJ mol^{-1}, selectivities for CO_2 (CO_2/CH_4= 100; CO_2/N_2= 180; CO_2/H_2 >105)	It consists of corner-sharing $[AlO_4(OH)_2]$ octahedra linked through two mutually cis-μ_2-OH groups forming infinite chains. Four such chains are cross-linked to give rise to square-shaped channels of size ~6.5 × 6.5 Å. The pore is functionalized with free hydroxyl groups in four different directions which are actually favorable CO_2 adsorption sites.	*Nature Chemistry, 2012, **4**, 887-894.*
40.	$[Co^{II}Co^{III}(OH)Cl_2(bbta)]$ Where, H_2bbta = 1H,5H-benzo(1,2-d:4,5-d0)bistriazole)	Yes	From a volumetric point-of-view, CO_2 uptake: 9.1 mmol cm^{-3} at 298 K and 1 bar, CO2 capture capacity: 4.1 mmol cm^{-3} from simulated flue gases (CO_2 pressure 0.10–0.15 bar at 313 K) at relative humidity (82%), Zero-loading HOA = 130-140 kJ mol^{-1}, at 298 K CO_2/N_2 selectivity: 262,	The study shows the potential of monodentate hydroxide to act as a good candidate for CO_2 affinity.	*Energy Environ. Sci., 2015, 8, 1011–1016.*
41.	MFM-300(V^{III}): $[V^{III}_2(OH)_2(L)]$, Where, LH_4=biphenyl-3,3′,5,5′-tetracarboxylic acid}	Yes	Very less uptake of N_2, CO_2 uptake: 6 mmol g^{-1} at 1 bar and 298K, at low coverage isosteric heat of adsorption (Q_{st}) = 27.5–28 kJ mol^{-1},	This is a hydroxyl functionalized MOF. The pore size is ~6.7 x 6.7Å for MFM-300(V^{III}).	*Nat. Commun., 2017, **8**, 14212.*
42.	Mg/DOBDC Co/DOBDC Ni/DOBDC Zn/DOBDC	Yes	BET surface area: 1495, 1080, 1070 and 816 m^2 g^{-1} for Mg/DOBDC, Co/DOBDC, Ni/DOBDC and Zn/DOBDC; CO_2 uptake at 296 K & 1 atm: 35.2, 30.6, 25.6 and 24.4 wt% for Mg/DOBDC, Co/DOBDC, Ni/DOBDC and Zn/DOBDC; HOA: 47 kJ/mol for Mg/DOBDC & 41 and 37 kJ mol^{-1} for Ni/ DOBDC and Co/DOBDC respectively.	This study shows the systematic evaluation of the effects of metal identity on surface area and CO_2 uptake owing to the strong head-on interaction of the polarized oxygens of the CO_2 with the open metal site.	*J. Am. Chem. Soc. 2008, 130, 10870–10871.*

43.	SGU-29: $Na_2CuSi_5O_{12}$	Yes	From N_2 at 77K adsorption BET surface area: 457 m^2 g^{-1}. CO_2 uptake at 1000, 100, and 0.4 mbar and 298 K are 156, 126, and 26 cm^3 cm^{-3} , respectively; HOA for CO_2 = 51 kJ/mol.	The channel in SGU-29 has a window size of 4.5 × 7.3 Å. It has H_2O-specific and CO_2-specific adsorption sites but does not have H_2O/CO_2-sharing sites. Therefore, it readily adsorbs both H_2O and CO_2 from the humid flue gases and atmosphere, without interfering with the adsorption of CO_2.	*Science, 2015, 350, 302.*
44.	Cu-BTC	Yes	At all pressure range, the experimental sample loaded with 4 wt % water adsorbs more CO_2 (~700 mg g^{-1}) than the dry sample (~500 mg g^{-1}) agrees well to simulation study. Again, a fully hydrated Cu-BTC adsorbs very less CO_2 (200 mg g^{-1}) at all pressures, which is due to the fully occupied pores with water molecules.	This study shows enhancement of CO_2 Adsorption in Metal-Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. This result was first discovered using molecular simulation and then verified experimentally, showing the power of molecular modeling.	*Chem. Mater., 2009, 21, 1425–1430.*
45.	[Ni(II)$_2$Ni(III)(μ3-OH)(LP)$_3$(L2)$_{1.5}$] Where, LP = linear Pyridine carboxylate, L2= linear di-carboxylate)	Yes	These possess surface areas in excess of 2000 m^2 g^{-1} (from 77 K N_2 adsorption)	All the frameworks have cavities in the range of ultra-micro pore sized windows along with some micro pore-sized ones.	*Nat. Commun. 2012, 3, 642.*
46.	1. SIFSIX-2-Cu 2. SIFSIX-2-Cu-i 3. SIFSIX-3-Zn	Yes	1. BET surface area (N_2 sorption) 3,140 m^2 g^{-1}; pore size 13.05 A°; CO_2 uptake at 298 K & 1 bar pressure: 1.84 mmol g^{-1}; Q_{st} for CO_2 at low loading: 22 kJ mol^{-1}; Selectivity (IAST) at 1 bar: CO_2/N_2 = 13.7, CO_2/CH_4 = 5.3; 2. BET surface area (N_2 sorption) 735 m^2 g^{-1}; pore size 5.15 A°; CO_2 uptake at 298 K & 1 bar pressure: 5.41 mmol g^{-1}; Q_{st} for CO_2 at low loading: 31.9 kJ mol^{-1}, Selectivity	Crystal engineering or reticular chemistry strategy controls pore functionality and size in a series of MOMs with coordinately saturated metal centres and periodically arrayed hexafluorosilicate (SiF62−) anions and enables a ‘sweet spot’ of kinetics and thermodynamics that offers high volumetric uptake at low CO2 partial pressure (less than 0.15 bar).	*Nature, 2013,* ***495****, 80.*

			(IAST) at 1 bar: CO_2/N_2 = 140, CO_2/CH_4 = 33, CO_2/H_2 = 240; 3. BET surface area (N_2 sorption) 250 m^2 g^{-1}; pore size e 3.84 A°; Q_{st} for CO_2 at low loading: 45 kJ mol^{-1}; Selectivity (IAST) at 1 bar: CO_2/N_2 = 1,818, CO_2/CH_4 = 231, CO_2/H_2 = >1,800;		
47.	**(1)** $[\{[CuSiF_6(4,4'\text{-Bipyridine})_2]\cdot 8H_2O\}]$ **(2)** $[\{[Zn(4,4'\text{-Bipyridine})_2\ (SiF_6)\}_n]$	Yes	The specific surface area of compound **(1)** (volumetric Ar sorption at 87.5 K)= 1337 m^2 g^{-1}; At 36 atm and 298 K the density of CH_4 adsorbed in **(1)** is 0.21 g ml^{-1}.	Both compound **(1) & (2)** are similar in structure. Both form non-interpenetrated 3D network and both consists of 8 X 8 Å^2 along *c*-axis and 6 X 2 Å^2 along *a* and *b*-axes. Compound **(2)** was made in DMF-dioxane mixed solvent and if synthetic medium is water then it gives interpenetrated $[\{[Zn(4,4'\text{-Bipyridine})_2(H2O)_n\}(SiF_6)_n]$.	*Angew. Chem. Int. Ed., 2000, 39, 2081-2084.*
48.	Mg_2(DHFMA) Where, DHFMA = dihydroxyfumaric acid.	Yes	Due to smaller length of DHFMA Mg(DHFMA) Becomes a truly microporous MOF.	One in every six atoms in DHFMA is an open metal site, whereas one in every nine atoms in DOBDC is an open metal site. So when these isostructural MOFs are compared the CO2 interacts via a direct head-on mode in the DOBDC (M...O=C=O = 2.33 Å) while it acts a bridging molecule between two adjacent metal sites in the case of DHFMA (M...O=C=O = ~2.6 Å). Such a unique binding mode results in a much enhanced binding energy of CO_2 in Mg_2(DHFMA), i.e., 50.1 kJ/mol, which is 20% (8.8 kJ/mol) stronger than that in Mg2(DOBDC).	*J. Phys. Chem. C, 2017, 121, 1171−1181.*
49.	**(1)** NOTT-101/ OEt **(2)** Cu-BTTri **(3)** Ni-4PyC (IISERP-MOF1) **(4)** VEXTUO **(5)** Mg-MOF-74	Yes	CO_2 working capacity (pure component experimental data at 303 K & 1 bar): 3.8, 3.7, 3.4, 3.1 and 2.6 mol kg^{-1} for compound **(1)** to **(5)** respectively; CO_2/H_2 selectivity (mixture simulation data at 313 K & 20 bar): 60, 20, 279, 48 and 365; Compound **(3) i.e Ni-Pyc (IISERP-**	All the MOFs are single ligand based MOFs and that is why it minimizes the chance of co-precipitation of impurity and results in a large scale production. 4-pyridine carboxylic acid (4-PyC) is a short ditopic linker (~4.95 Å) and the presence of the ring in Pyc makes Ni-Pyc (IISERP-MOF1) significantly rigid. It has a cubic framework with ultra-micropore (3.5 and 4.8 Å pores). IISERP-MOF1 was synthesized in THF/H_2O/MeOH mixed solvent system.	*Sci. Adv., 2016; 2: e1600909* *&* *Sci. Adv., 2015, 1, e1500421.*

		MOF1) has BET surface area of 945 m^2 g^{-1} (77K N2) and exhibits a saturation CO_2 uptake of 11 mmol g^{-1} (195 K) and adsorbs 3.6 mmol g^{-1} at 303K at 1 bar, respectively.		
50.	**IISERP-MOF2:** $Ni_9(\mu\text{-}H_2O)_4(H_2O)_2(C_6NH_4O_2)_{18}$	Yes	BET surface area (N_2 77 K adsorption) 470 m^2 g^{-1} and a Langmuir surface area of 700 m^2 g^{-1}; CO2 uptake at 1 bar & 303 K = 4.2 mmol g^{-1}; Saturation uptake: ~7 mmol g^{-1}; At 1 bar and 313 K CO_2 selectivity (s(CO_2/N_2) = 1853; IISERP-MOF2 shows a CO_2/N_2 separation of 3.97 mmol g^{-1}as determined from a dynamic flow breakthrough separation; HOA for CO_2 = 33 kJ mol^{-1}.	Pyc ligand with Ni- salt in DMF/CH_3CN mixed solvent forms IISERP-MOF2 a different phase of Ni-Pyc. NiPyC has the lowest parasitic energy among all the MOFs (PE (kJ/kg of CO_2)): IISERP-MOF2 = 655, Mg-MOF-74 = 727, monoethanolamine = 1000.	*J. Am. Chem. Soc., 2017, 139, 1734.*

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Table S2. Costs involved in the synthesis of selected MOFs.

Cost for large quantity of metal salt required for production of a range of MOFs		
Metal salt	Price (£/Kg)	MOFs
Copper(II) hydroxide	0.65	CuBTC (HKUST-1, Basolite C-300) MOF-14
Zinc carbonate hydroxide	0.48	ZIF8 (Basolite Z1200), MOF-177, MOF-5, Zn-MOF-74, Various ZIFs
Aluminium chloride hexahydrate	0.40	MIL-53
Zirconium hydroxide	0.80	UIO-66(Zr)
Cost for large quantity of organic linker required for production of a range of MOFs		
Organic linker	Price (£/Kg)	MOFs
2-methyl imidazole	7.15	ZIF8 (Basolite Z1200),
Trimesic acid	24.75	Cu-BTC (HKUST-1, Basolite C-300), Fe-BTC (Basolite F-300), MIL-100
2,5-dihydroxy terephthalic acid	350.00	MOF-74 (CPO-27)
Terephthalic acid	1.50	UIO-66 MIL-101 MIL-53 (Basolite A100)
Imidazole	~4.00	Various ZIFs

Above table S2 is adopted from Materials 2017, 10, 1428; doi:10.3390/ma10121428.

Table S3. Costs of production selected MOFs.

Cost of the starting materials for production of some MOFs	
Adsorbent	**Cost (US $/Kg)**
CuBTC (HKUST-1)	20.08
CoCo ($Co_3[Co(CN)_6]_2$)	35.14
MOF-5 (IRMOF-1)	2.93
Zn/DOBDC (Zn-MOF-74)	1.90
Ni/DOBDC (Ni-MOF-74)	6.48
Mg/DOBDC (Mg-MOF-74)	1.19
Co/DOBDC (Co-MOF-74)	13.33
MIL-100	15.64
MIL-101	4.57
Silica gel	1.00

Costs listed are based on the purchase of one metric ton or greater quantity.
Above table is adopted from Liu et al., Chem. Soc. Rev., 2012, **41**, 2308–2322.