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Synthesis and characterization of three amino-functionalized metal-organic frameworks based on 2-Aminoterephthalic ligand

Ying Yang,[a] Rijia Lin,[a] Lei Ge,[a*] Lei Hou,[b] Paul Bernhardt,[c] Thomas Rufford,[a] Shaobin Wang,[d] Victor Rudolph,[a] Yaoyu Wang,[b] Zhonghua Zhu[a*]

[a] *School of Chemical Engineering, The University of Queensland, Brisbane 4072 Australia*

[b] *College of Chemistry & Materials Science, Northwest University, Xi'an 710069, China*

[c] *School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane 4072 Australia*

[d] *Department of Chemical Engineering, Curtin University, GPO Box U1987, Perth, WA 6845, Australia*

SUPPORTING INFORMATION

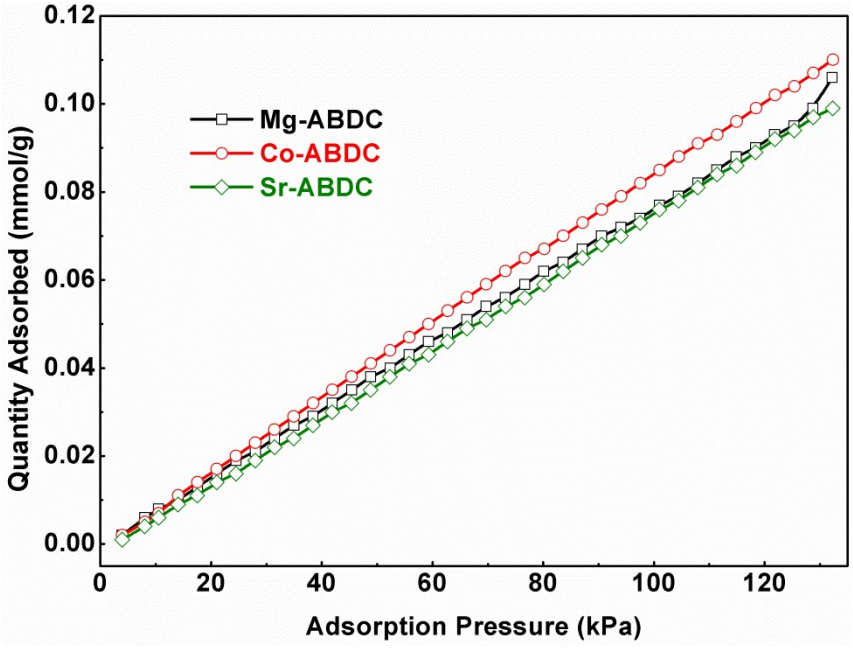

Fig. S1 N_2 adsorption at 25 °C on M-ABDC (M = Mg, Co, Sr)

Table S1 Langmuir constants of CO_2 and N_2 adsorption at 0 °C and selectivity of CO_2/N_2 on M-ABDC[a]

Samples	CO_2		N_2		Selectivity of CO_2/N_2
	q_{m1} (mmol/g)	b_1 (kPa^{-1})	q_{m2} (mmol/g)	b_1 (kPa^{-1})	
Mg-ABDC	2.022	0.0151	17.24	4.47E-06	396
Co-ABDC	1.536	0.0179	13.14	6.41E-06	326
Sr-ABDC	285.53	4.66E-06	51.84	1.44E-06	18

[a] Langmuir equation: $q = \frac{q_m bp}{1 + bp}$; The adsorption equilibrium selectivity: $S_{CO_2/N_2} = \frac{x_1}{x_2} \times \frac{y_1}{y_2} \approx \frac{q_{m1} b_1}{q_{m2} b_2}$

CO_2/N_2 selectivity prediction via IAST

This method was following the procedures in the reporting references.[1, 2] The experimental adsorption data for pure CO_2 and N_2 (measured at 0 °C) were fitted using a Langmuir-Freundlich (L-F) model:

$$q_i = \frac{a \times b \times p_i^{1/n}}{1 + b \times p_i^{1/n}}$$

Where q_i adsorbed amounts at pressure and p_i.

The adsorption selectivities for binary mixtures of CO_2/N_2 were calculated using the Ideal Adsorption Solution Theory (IAST), which was reported by Myers and Prausnitz.[1] And the selectivity was defined by:

$$S_{i/j} = \frac{x_i \times y_j}{x_j \times y_i}$$

Where x_i is the mole fraction of component i in the adsorbed phase and y_i is the mole fraction of component i in the bulk.

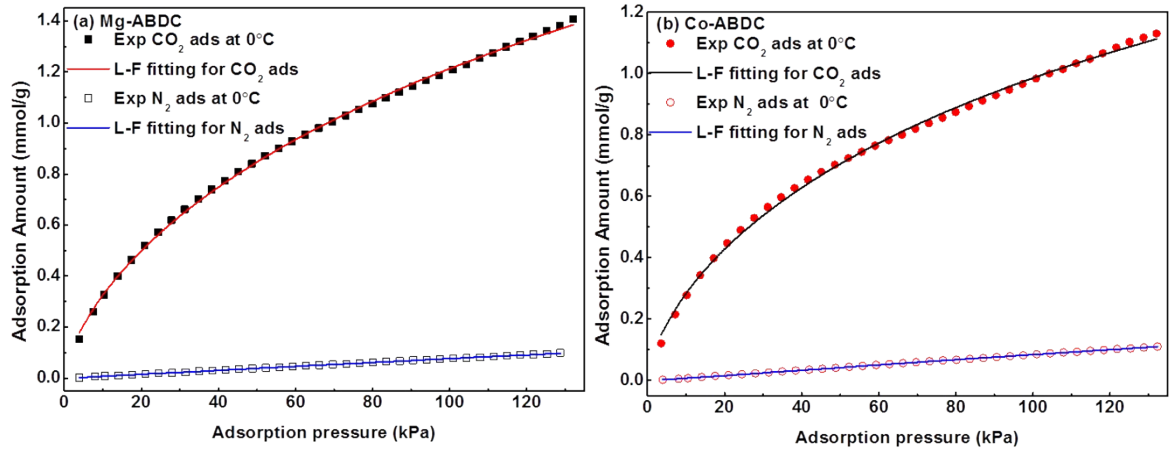

Fig. S2 CO_2 and N_2 adsorption isotherms at 0 °C and fitting by L-F model

Table S2 Fitting parameter of CO_2 and N_2 adsorption data by L-F model

L-F model fitting parameter		a	b	n	Chi^2	R^2
Mg-ABDC	CO_2 ads	4.33649	0.01709	1.47436	0.0001	0.99919
	N_2 ads	0.84485	0.00073	0.93764	2.0336E-7	0.99977
Co-ABDC	CO_2 ads	3.04922	0.02229	1.50271	0.00016	0.99795

	N_2 ads	0.68623	0.00087	0.90620	1.3745E-7	0.99988

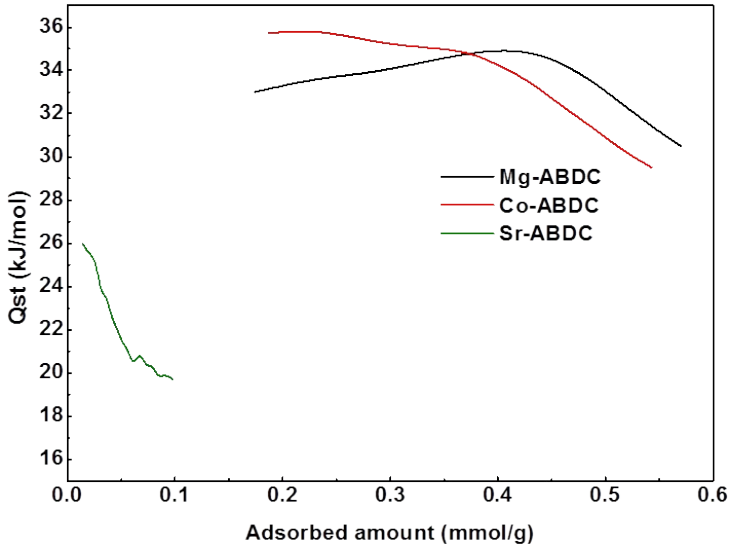

Fig. S3 Isosteric heats of CO_2 adsorption calculated by Clausius-Clapeyron equation based on adsorption isotherms at 0 °C and 25 °C

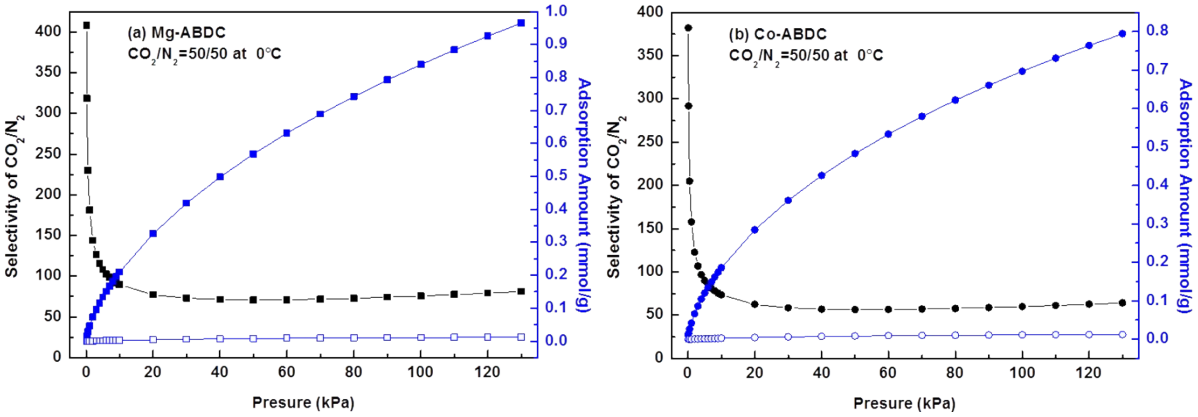

Fig. S4 IAST adsorption isotherms of CO_2+N_2 mixture at 50/50 and selectivities of Mg-ABDC and Co-ABDC

Table S3 Comparison of the adsorption capacity and selectivity with some reported MOFs containing LBSs or/and OMSs

Material	Features	BET surface area (cm^2/g)	CO_2 adsorbed amount (mmol/g)	Adsorption conditions	Selectivity of CO_2/N_2	References
Mg-ABDC	LBSs and OMSs	63	1.4	1.0 bar&298 K	>70[a]	This work
Co-ABDC	LBSs and OMSs	71	1.1	1.0 bar&298 K	>55[a]	This work
IRMOF-3	LBSs	2160	1.2	1.1 bar&298 K		[3]
Uio-66(Zr)-NH_2	LBSs	1112	1.8	1.0 bar&303 K		[4]
[CuL_4]	LBSs	810	4.95	1.0 bar&298 K		[5]
NH_2-MIL-53(Al)	LBSs and breathing		7.2	24 bar&283 K	12[c]	[6]
CAU-1	LBSs	1268	7.2	1 bar&273 K	101[b]	[7]
Cu-BTC	OMSs	1571	12.7	15 bar&298 K	5.1[b]	[8]
Cu-BTC (hydrated 4 wt%)	OMSs	1492(Langmuir)	11.36	4.8 bar&298 K	28[a]	[9]
Cu-TDPAT	LBSs and OMSs	1938	5.89	1.0 bar&298 K	~79[a]	[10]
CuBTTri	OMSs	345	1.27	1.0 bar&298 K	25[c]	[11]
mmen-CuBTTri	LBS	870	2.38	1.0 bar&298 K	327[a]	[12]
Cu_3(btei) [PCN-61]	OMSs	3350	21.4	20 bar&298 K	20[a]	[13]
Cu_3(tpbtm)	OMSs	3160	23.5	20 bar&298 K	33[a]	[13]
Ni_2(dhtp)	OMSs	1218	1.1	1.0 bar&298 K	7[c]	[14]
ZTF-1	LBS	355.3	5.6	1.0 bar&273 K	10[c]	[15]
Cd-ANIC-1	LBS	329.3	4.72	1.0 bar&273 K		[16]
Co-ANIC-1	LBS	274.0	4.22	1.0 bar&273 K		[16]

Selectivity calculation: a, from IAST; b, from slopes of adsorption isotherms at low pressure; c, $S=q_1/q_2$ (where component 1 is more adsorbed).

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