



Supplementary Materials

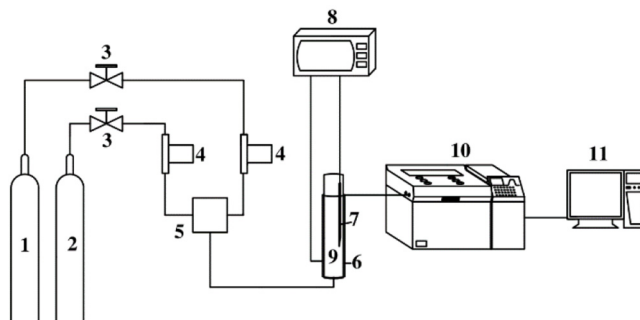


Fig. S1. CO₂ dynamic adsorption unit. (1-argon cylinder; 2-CO₂ cylinder; 3-gas pressure relief valve; 4-mass flow controller; 5-gas mixer; 6-heating mantle; 7-temperature probe; 8-temperature controller; 9-reactor; 10-gas chromatography; 11-gas chromatography work station)

Table S1. Textural Properties of Mg-MOF-74 and Mg-MOF-nNH₂

Samples	Textural properties			
	BET surface area (m ² /g)	Average pore size (nm)	Total pore volume (cm ³ /g)	Micropore volume (cm ³ /g)
Mg-MOF-74	1122.47	2.00	0.57	0.43
Mg-MOF-1/10NH ₂	1056.34	2.31	0.61	0.41
Mg-MOF-1/8NH ₂	924.19	2.32	0.54	0.46
Mg-MOF-1/6NH ₂	692.16	2.45	0.42	0.27
Mg-MOF-1/4NH ₂	515.36	3.57	0.46	0.21

Table S2. Parameters Values of Lagergen's Pseudo-first-order Kinetics Model and Ho's Pseudo-second-order Kinetics Model of Mg-MOF-1/8NH₂

Temperature/K	pseudo-first-order kinetics			pseudo-second-order kinetics			Avrami			
	q _e mmol/g	k ₁ min ⁻¹	R ²	q _e mmol/g	k ₂ min ⁻¹	R ²	q _e mmol/g	k _a min ⁻¹	n	R ²
303K	4.04	0.08	0.998	5.33	0.01	0.996	4.00	0.08	1.02	0.999
313K	3.06	0.09	0.996	3.95	0.02	0.998	3.15	0.08	0.92	0.999
323K	2.37	0.18	0.969	2.72	0.08	0.991	2.47	0.17	0.75	0.983

Table S3. Parameters Values of Langmuir, Freundlich Isotherms Models of Mg-MOF-1/8NH₂

Temperature/K	Langmuir			Freundlich		
	q _m mmol/g	K _L min ⁻¹	R ²	K _f	1/n	R ²
303K	6.16	0.017	0.971	0.32	0.55	0.964
313K	4.51	0.020	0.943	0.31	0.51	0.935
323K	4.02	0.021	0.959	0.25	0.52	0.952

Table S4. Comparison of Mg-MOF-74 and Mg-MOF-1/8NH₂ CO₂ Adsorption Capacity

Adsorbents	303K C ₀ = 100%	313K C ₀ = 100%	323K C ₀ = 100%
Mg-MOF-74	3.57mmol/g	2.53mmol/g	1.83 mmol/g
Mg-MOF-1/8NH ₂	3.90 mmol/g	3.00 mmol/g	2.64 mmol/g

Table S5. The Parameters of Thermodynamics

Adsorbents	CO ₂ thermodynamic parameters				
	ΔG(kJ/mol)			ΔH (kJ/mol)	ΔS (J/mol)
	303K	313K	323K		
Mg-MOF-1/8NH ₂	-10.22	-10.27	-10.32	-8.64	5.2

Table S6. The Parameters of Equivalent Heat of Adsorption

q _a (mmol/g)	1	1.3	1.6	1.9	2.2	2.5
R ²	0.998	0.997	0.993	0.991	0.989	0.989
slope	-1635.8	-1916.6	-2204.1	-2561.9	-3026.5	-3611.4
Q _{st}	27.20	31.87	36.65	42.60	50.32	60.05

Table S7. Fitted Parameters of the Deactivation Model of Mg-MOF-1/8NH₂ at Different Temperatures

T	k ₀ M/Q	k ₀ (cm ³ min ⁻¹ g ⁻¹)	k _d (min ⁻¹)	R ²
303K	2.77	1.11 × 10 ²	0.37	0.992
313K	3.26	1.30 × 10 ²	0.48	0.995
323K	1.89	0.76 × 10 ²	0.49	0.982

Table S8. Fitted Parameters of the Deactivation Model of Mg-MOF-1/8NH₂ at Different Temperatures

T	k ₀ M/Q	k ₀ (cm ³ min ⁻¹ g ⁻¹)	k _d (min ⁻¹)	R ²
303K	3.78	1.51 × 10 ²	0.74	0.998
313K	2.21	0.88 × 10 ²	0.52	0.985
323K	1.81	0.72 × 10 ²	0.57	0.962

Table S9. Fitted Parameters of the Deactivation Model of Mg-MOF-74 at Different Concentrations

C ₀	k ₀ M/Q	k ₀ (cm ³ min ⁻¹ g ⁻¹)	k _d (min ⁻¹)	R ²	q(mmol/g)
10%	3.78	1.512 × 10 ²	0.74	0.998	1.08
20%	4.06	1.624 × 10 ²	0.863	0.999	1.49
30%	6.11	2.444 × 10 ²	1.49	0.996	1.72
50%	2.55	1.020 × 10 ²	1.02	0.988	2.21

Table S10. Fitted Parameters of the Deactivation Model of Mg-MOF-1/8NH₂ at Different Concentrations

C ₀	k ₀ M/Q	k ₀ (cm ³ min ⁻¹ g ⁻¹)	k _d (min ⁻¹)	R ²	q(mmol/g)
10%	2.81	1.124 × 10 ²	0.38	0.959	1.27
20%	2.76	1.104 × 10 ²	0.45	0.914	1.82
30%	1.88	0.752 × 10 ²	0.54	0.988	2.11
50%	1.94	0.776 × 10 ²	0.63	0.992	3.31

Table S11. CO₂ Adsorption of Other Material Capacity

Adsorbents	Adsorption conditions		CO ₂ adsorption (mmol/g)	Ref
	Pressure (bar)	Adsorption temperature (K)		
Mg-MOF-1/8NH ₂	1	303	3.9	this work
Mg-MOF-74	1	303	3.57	this work
AC Norit RB1	1	294.2	2.456	[1]
anthracite-based AC	1	303	1.38	[2]
Zeolite 13X	1	298	4.66	[3]
NaM	1	298	2.95	[4]
N-rich porous carbon	1	298	2.3	[5]
Mesoporous alumina	1	298	1.2	[6]
MIL-125	1	298	2.18	[7]
MIL-101(Cr)	1	298	1.22	[8]
UPC-106	1	298	2.42	[9]
MOF-177	1	298	0.77	[10]
Fe-BTT	1	298	3.07	[11]
HKUST-1	1	298	4.16	[12]

References

- Vaart R, Huiskes C, Bosch H, et al. Single and mixed gas adsorption equilibria of carbon dioxide/methane on activated carbon. *Adsorption* 2000;6:311-323.
- Maroto-Valer MM, Tang Z, Zhang Y. CO₂ capture by activated and impregnated anthracites. *Fuel Process Technol.* 2005;86:1487-1502.
- Cavenati S, Grande CA, Rodrigues, et al. Adsorption equilibrium of methane, carbon dioxide, and nitrogen on zeolite 13X at high pressures. *J. Chem. Eng. Data* 2004;49:1095-1101.
- ChouHary VR, Mayadevi S, Singh AP. Sorption isotherms of methane, ethane, ethene and carbon dioxide on NaX, NaY and Na-mordenite zeolites. *J. Chem. Soc.* 1995;91:2935-2944.
- Chao C, Kim J, Ahn W S. Efficient carbon dioxide capture over a nitrogen-rich carbon having a hierarchical micro-mesopore structure. *Fuel* 2012;95:360-364.
- Chen C, Ahn WS. CO₂ capture using mesoporous alumina prepared by a sol-gel process. *Chem. Eng. J.* 2011;166:646-651.
- Kim SN, Kim J, Kim HY, et al. Adsorption/catalytic properties of MIL-125 and NH₂-MIL-125. *Catal. Today* 2013;204:85-93.
- Chen C, Feng NJ, Guo QR, et al. Surface engineering of a chromium metal-organic framework with bifunctional ionic liquids for selective CO₂ adsorption: Synergistic effect between multiple active sites. *J. Colloid. Interface. Sci.* 2018;521:91-101.
- Fan W, Wang X, Liu X, et al. Regulating C₂H₂ and CO₂ Storage and separation through pore environment modification in a microporous Ni-MOF. *ACS Sust. Chem. Eng.* 2018;7:2134-2140.
- Millward A R, Yaghi O M. Metal-organic frameworks with exceptionally high capacity for storage of carbon dioxide at room temperature. *J. Am. Chem. Soc.* 2005;127:17998-17999.
- Hon LC, Babarao R, Hill MR. A route to drastic increase of CO₂ uptake in Zr metal organic framework UiO-66. *Chem. Commun.* 2013;49:3634-3636.
- Chong C, Li B, Zhou L, et al. Synthesis of hierarchically structured hybrid materials by controlled self-assembly of metal-organic framework with mesoporous silica for CO₂ adsorption. *ACS Appl. Mater. Inter.* 2017;9:23060-23071.