BEILSTEIN JOURNAL OF NANOTECHNOLOGY

Supporting Information

for

Facile synthesis of Fe-based metal–organic frameworks from Fe_2O_3 nanoparticles and their application for CO_2/N_2 separation

Van Nhieu Le, Hoai Duc Tran, Minh Tien Nguyen, Hai Bang Truong, Toan Minh Pham and Jinsoo Kim

Beilstein J. Nanotechnol. **2024,** *15,* 897–908. doi:10.3762/bjnano.15.74

Additional experimental data

Preparation of the reference MIL-100(Fe) sample

The reaction mixture was prepared with a molar composition of 1.0 Fe: 0.67 H_3BTC: 1.2 HNO_3: 2.0 HF: 280 H_2O in a 100 mL Teflon-lined autoclave. It was stirred for 20 min at ambient temperature. Subsequently, the mixture was tightly sealed and incubated at 160 °C for 24 h in an electric oven. Afterward, it was cooled down to room temperature. The MIL-100(Fe) was then retrieved from the orange slurry after centrifugation and subjected to multiple washes with dimethylformamide and ethanol to eliminate any residual reactants from the product mixture. Finally, the MIL-100(Fe) was left to dry overnight at 70 °C.

Table S1: The characteristic parameters alongside correlation coefficients from fitting the Langmuir–Freundlich (L–F) model.

Samples	The obtained parameters from fitting CO_2			
	q_{sat} (mmol·g^{-1})	a (kPa^{-1})	n	R^2
M-100Fe@Fe_2O_3#0.90	3.59748	0.00225	0.96613	0.9999
M-100Fe@Fe_2O_3#1.35	4.47178	0.0035	0.91115	0.9999
M-100Fe@Fe_2O_3#1.80	5.75658	0.00417	0.87543	0.9998
M-100Fe@Fe_2O_3#2.25	6.31350	0.00446	0.8521	0.9998
MIL-100(Fe)	5.29325	0.00873	0.86948	0.9998

Samples	The obtained parameters from fitting N_2			
	q_{sat} (mmol·g^{-1})	a (kPa^{-1})	n	R^2
M-100Fe@Fe_2O_3#0.90	0.48828	0.00143	1.02837	0.9998
M-100Fe@Fe_2O_3#1.35	0.97068	0.00123	0.94648	0.9999
M-100Fe@Fe_2O_3#1.80	1.28516	0.00119	0.94557	0.9999
M-100Fe@Fe_2O_3#2.25	1.60773	0.00111	0.91890	0.9999
MIL-100(Fe)	0.65055	0.00372	0.97849	0.9998

The Langmuir–Freundlich (L–F) model is described as the following equation [1,2]:

$$q = q_{\mathrm{sat}} \frac{ap^n}{1+ap^n} \quad (1)$$

Where q (mmol·g^{-1}) stands for the uptake amount; q_{sat} (mmol·g^{-1}) stands for the saturation uptake capacity on the adsorptive sites; p (kPa) is the pressure of bulk gas at equilibrium with the adsorbed phase; a (kPa^{-1}) is the affinity coefficient of the sites; n is the coefficient of the L–F model.

The CO_2/N_2 selectivity was calculated using the formula as below [3]:

$$S_{CO_2/N_2} = \frac{q_{CO2}/p_{CO2}}{q_{N2}/p_{N2}} \quad (2)$$

Where q_{CO2} and q_{N2} are loading amounts of CO_2 and N_2 in mmol g^{-1} estimated by IAST, respectively. p_{CO2} and P_{N2} are the partial pressure of CO_2 and N_2 in kPa, respectively.

The Clausius–Clayperon equation is described as the following equation [1,4]:

$$lnP = -\frac{Q_{st}}{RT} + C \quad (3)$$

Herein, P is the pressure in kPa, R is the ideal gas constant in J mol^{-1} K^{-1}, T is the absolute temperature in K, and C is the constant in the dimensionless unit.

Table S2: Compared CO_2 uptake capacity on various adsorbents at 1 bar.

Adsorbents	Adsorption capacity (mmol·g^{-1})	Temperature (K)	References
ZSM-5	1.50	303	[5]
MCM-41	0.79	298	[6]
Mesoporous alumina	1.18	298	[7]
SBA-15	0.47		
γ-Alumina	0.68		
Zeolite-13X	1.70	298	[8]
ZIF-8	0.83		
ZIF-70	1.43	298	[9]
UIO-66	1.79	298	[10]
d-UiO-6-2.0HCl	1.42	298	[11]
UiO-66_FA_mod	1.44	298	[12]
MF-MOF-801	1.37	298	[13]
MF-MOF-804	1.00		
MW-MIL-100(Fe)	1.50 (1981 $m^2 \cdot g^{-1\#}$; 250 °C♣)	298	[14]
MIL-100(Fe)	1.29 (1107 $m^2 \cdot g^{-1\#}$; 120 °C♣)	298	[15]
MIL-100(Fe)	0.92 (1083 $m^2 \cdot g^{-1\#}$; 150 °C♣)	298	[16]
MIL-100(Fe)	1.77 (1825.4 $m^2 \cdot g^{-1\#}$; 150 °C♣)	298	This work
M-100Fe@Fe_2O_3#1.80	1.11 (1365.4 $m^2 \cdot g^{-1\#}$; 150 °C♣)		

[#] BET surface area; ♣Activation temperature before measuring CO_2 adsorption capacity over the absorbents

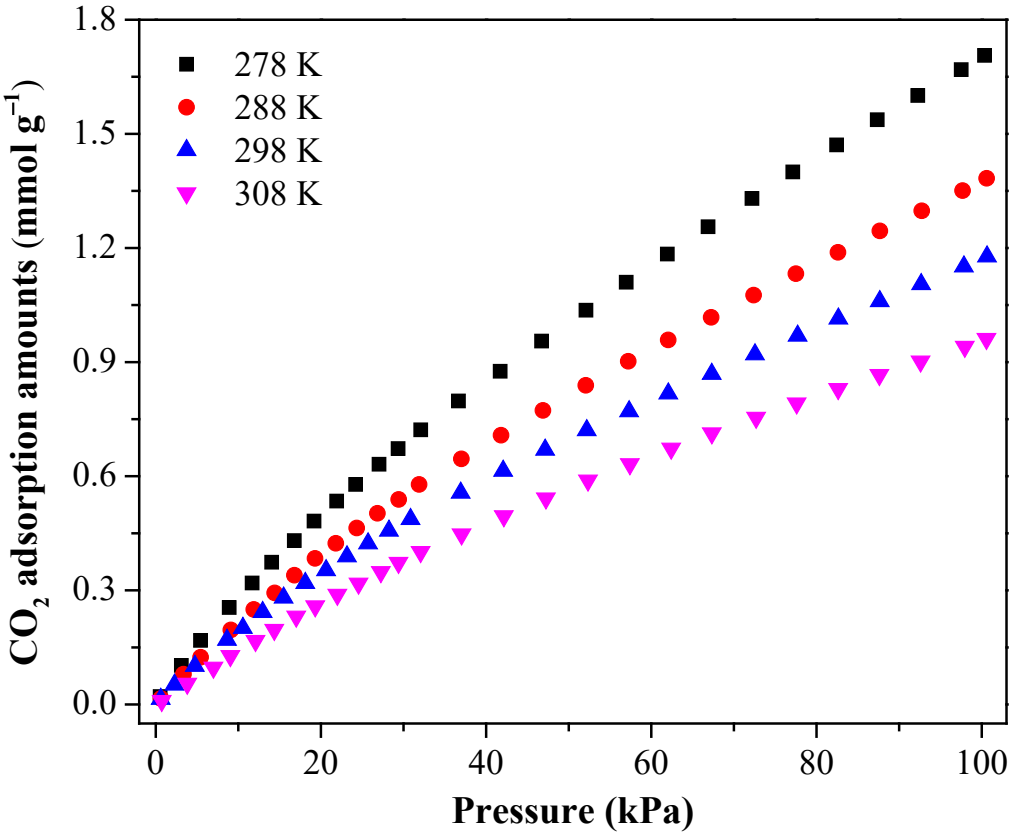

Figure S1: CO_2 isotherms at several different temperatures on M-100(Fe)@Fe_2O_3#1.80 sample.

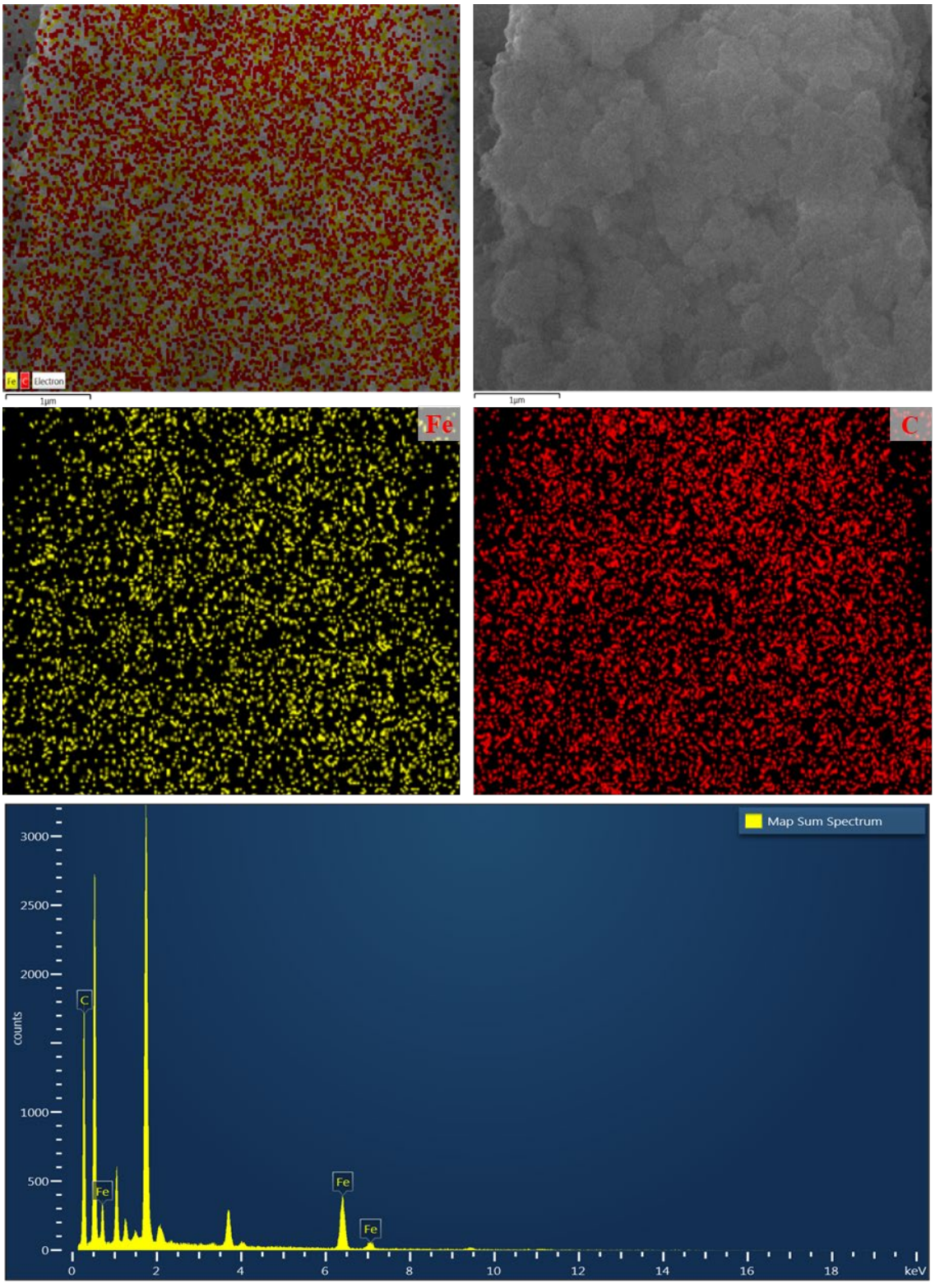

Figure S2: EDX mapping of elemental Fe and C on the M-100Fe@Fe2O3#1.80 sample

References

1. Le, V. N.; Nguyen, V. C.; Nguyen, H. T.; Tran, H. D.; Tu, T. N.; Kim, W.-S.; Kim, J. *Microporous Mesoporous Mater.* **2023,** *360*, 112716.

2. Le, V. N.; Vo, T. K.; Yoo, K. S.; Kim, J. *Sep. Purif. Technol.* **2021,** *274*, 119079.

3. Le, V. N.; Vo, T. K.; Lee, J. H.; Kim, J. C.; Kim, T.-H.; Oh, K. H.; Bae, Y.-S.; Kwak, S. K.; Kim, J. *Chem. Eng. J.* **2021,** *404*, 126492.

4. Peng, J.; Xian, S.; Xiao, J.; Huang, Y.; Xia, Q.; Wang, H.; Li, Z. *Chem. Eng. J.* **2015,** *270*, 282-289.

5. Li, Y.; Yi, H.; Tang, X.; Li, F.; Yuan, Q. *Chem. Eng. J.* **2013,** *229*, 50-56.

6. Chanapattharapol, K. C.; Krachuamram, S.; Youngme, S. *Microporous Mesoporous Mater.* **2017,** *245*, 8-15.

7. Chen, C.; Ahn, W.-S. *Chem. Eng. J.* **2011,** *166*, 646-651.

8. McEwen, J.; Hayman, J.-D.; Ozgur Yazaydin, A. *Chem. Phys.* **2013,** *412*, 72-76.

9. Banerjee, R.; Furukawa, H.; Britt, D.; Knobler, C.; O'Keeffe, M.; Yaghi, O. M. *J. Am. Chem. Soc.* **2009,** *131*, 3875-3877.

10. Hu, Z.; Khurana, M.; Seah, Y. H.; Zhang, M.; Guo, Z.; Zhao, D. *Chem. Eng. Sci.* **2015,** *124*, 61-69.

11. Liang, W.; Coghlan, C. J.; Ragon, F.; Rubio-Martinez, M.; D'Alessandro, D. M.; Babarao, R. *Dalton Trans.* **2016,** *45*, 4496-4500.

12. Koutsianos, A.; Kazimierska, E.; Barron, A. R.; Taddei, M.; Andreoli, E. *Dalton Trans.* **2019,** *48*, 3349-3359.

13. Wang, Y.; Li, L.; Yan, L.; Cao, L.; Dai, P.; Gu, X.; Zhao, X. *Chin. Chem. Lett.* **2018,** *29*, 849-853.

14. Le, V. N.; Kwon, H. T.; Vo, T. K.; Kim, J.-H.; Kim, W.-S.; Kim, J. *Mater. Chem. Phys.* **2020,** *253*, 123278.

15. Mutyala, S.; Yakout, S. M.; Ibrahim, S. S.; Jonnalagadda, M.; Mitta, H. *New J. Chem.* **2019,** *43*, 9725-9731.

16. Ben-Mansour, R.; Qasem, N. A. A.; Habib, M. A. *Int. J. Energy Environ. Eng.* **2018,** *9*, 169-185.