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Electronic Supporting Information (ESI)

Preparation of an interpenetrating bimetal metal-organic framework via metal metathesis used for promoting gas adsorption†

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Experimental Section

1. Raw materials

Scandium nitrate hydrate ($Sc(NO_3)_3 \cdot xH_2O$, 99%), chromic chloride hexahydrate ($CrCl_3 \cdot 6H_2O$, 99%) and biphenyl dicarboxylic acid (BPDC-H_2, 98%) were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. N, N-dimethylformamide (DMF, 99%), acetone (CH_3COCH_3, 99%) and hydrochloric acid (HCl, 36%) provided by Sinopharm Chemical Reagent Co., Ltd. The above reagents were used directly without further purification.

2. Fitting of pure component isotherms

The single-component CO_2, N_2O and C_2H_2 and adsorption isotherms of MIL-126(Sc) and MIL-126(Cr/Sc) were fitted using the dual-site Langmuir-Freundlich (DSLF) model, and R^2 was greater than 0.9999.

$$q = q_1 \frac{b_1 P^{1/n_1}}{1 + b_1 P^{1/n_1}} + q_2 \frac{b_2 P^{1/n_2}}{1 + b_2 P^{1/n_2}} \quad (1)$$

Where q is the equilibrium adsorbed amount of an adsorbent (mmol/g); q_1 and q_2 are the saturation uptakes of site 1 and site 2 (mmol/g); b_1 and b_2 are the affinity coefficients of site 1 and site 2 (1/bar); n_1 and n_2 are the corresponding deviations from an ideal homogeneous surface.

3. Qst calculation

The Qst of MIL-126(Sc) and MIL-126(Cr/Sc) with CO_2, N_2O and C_2H_2 were calculated using the C_2H_2 and CO_2 single-component adsorption isotherms at 273 K and 298 K via the Clausius-Clapeyron equation.

$$In\frac{p_2}{p_1} = \frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \quad (2)$$

In the above equation, *P* represents the pressure, the unit is bar, *T* is the temperature in K, and *R* is the gas constant (8.314).

Supporting Table and Figures

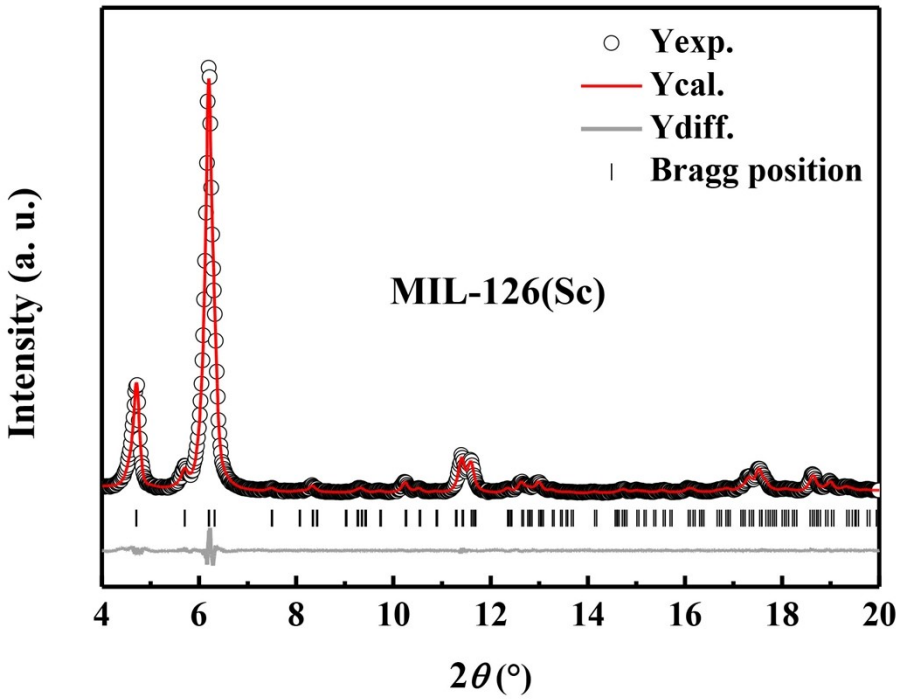


Fig. S1 Rietveld-refined XRD pattern of MIL-126(Sc) (Rwp = 4.73%, Rp = 3.56%, GOF = 1.06, a =b=21.91Å, c = 36.35 Å, α = β = 90°, γ =90°). The black circles and red lines represent experimental data and calculated values, respectively.

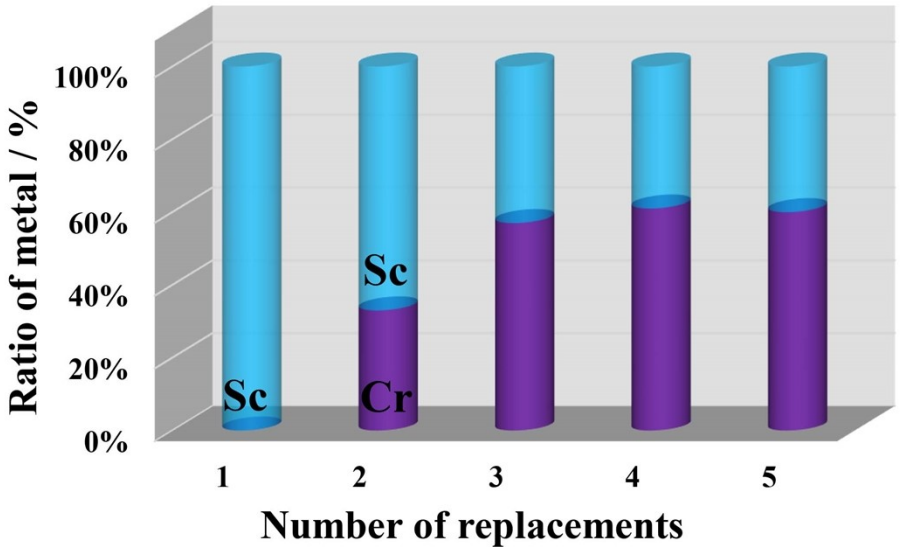


Fig. S2 Change of metal ratio (n/n_{total} %) in MIL-126 for different exchange times under standard conditions. The exchange time is 3 h for one exchange process. Obviously, the exchange ratio of Cr(III) increased rapidly in the first 3 times and then showed no obvious change.

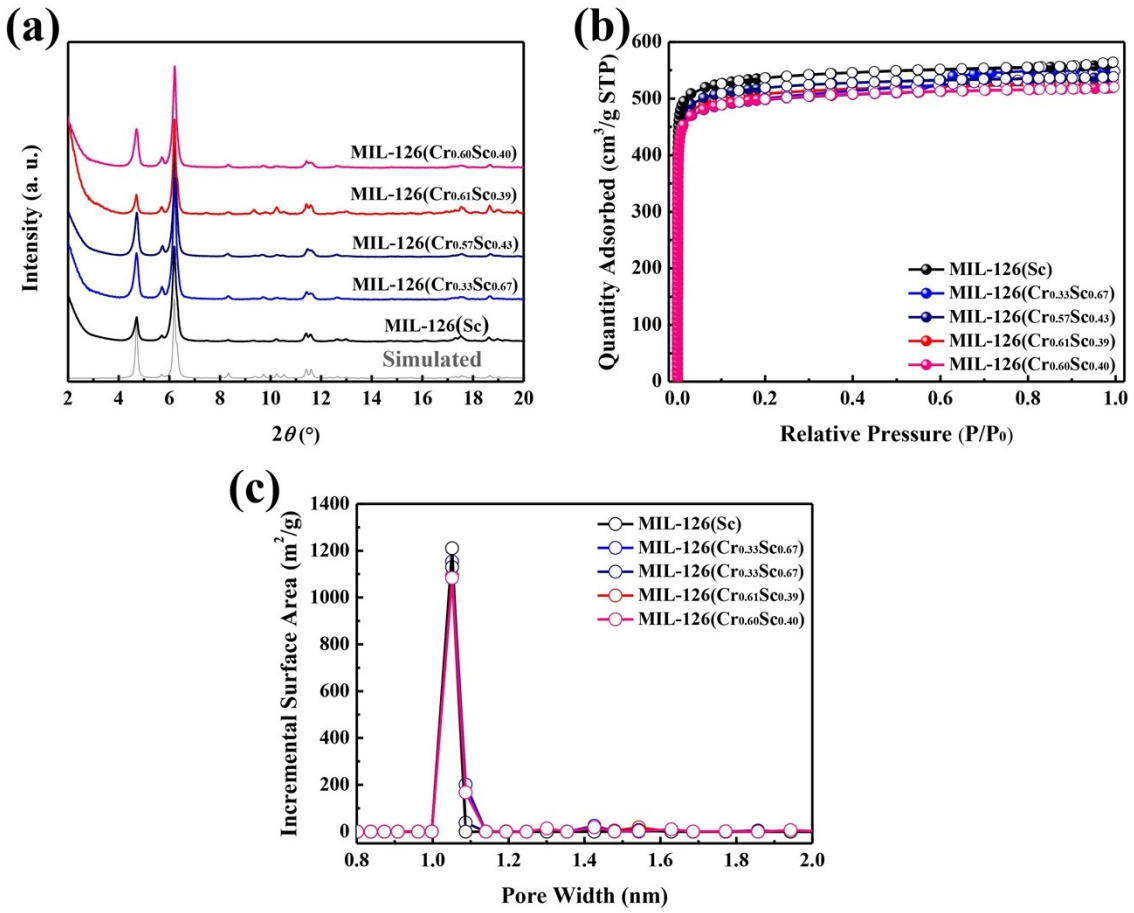


Fig. S3 PXRD (a), N_2 adsorption-desorption isotherms at 77 K (b) and pore size distribution (c) of MIL-126(Sc) and the modified materials.

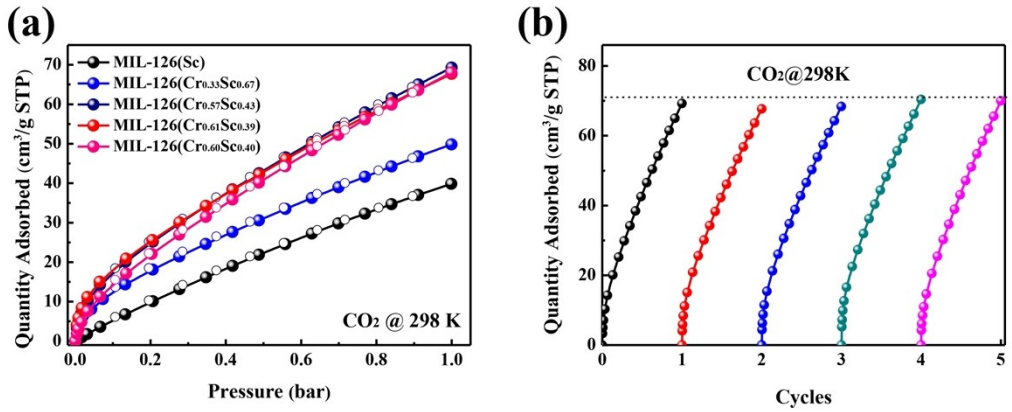


Fig. S4 (a) CO_2 adsorption-desorption isotherms at 298 K of MIL-126(Sc) and the modified materials. (b) CO_2 adsorption recycles of MIL-126(Cr/Sc) at 298 K and 1 bar. Note: MIL-126($Cr_{0.61}Sc_{0.39}$) is marked as MIL-126(Cr/Sc) for clarity in this work.

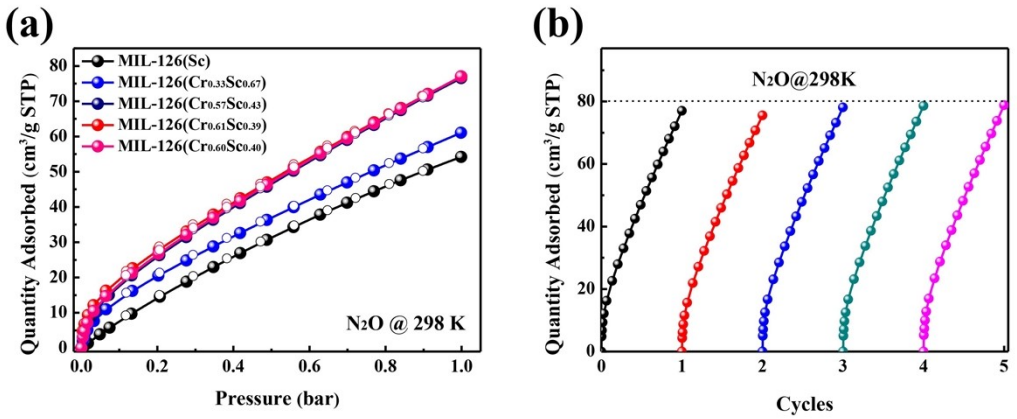


Fig. S5 (a) N_2O adsorption-desorption isotherms at 298 K of MIL-126(Sc) and the modified materials. (b) N_2O adsorption recycles of MIL-126(Cr/Sc) at 298 K and 1 bar.

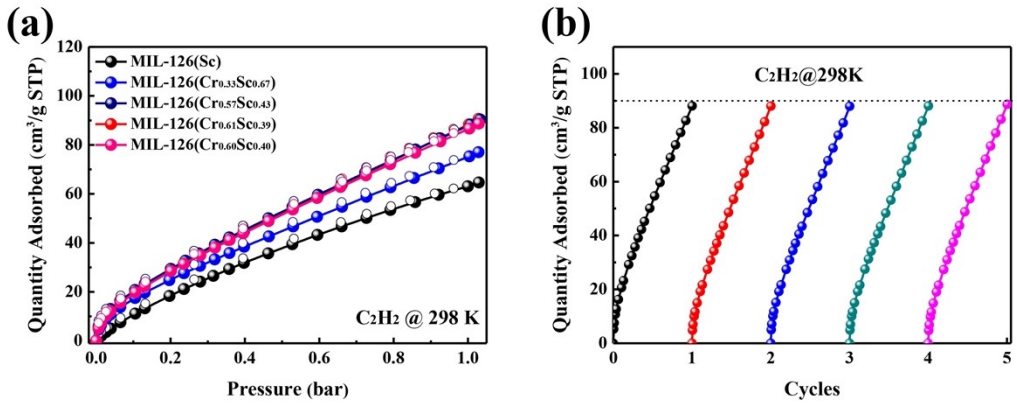


Fig. S6 (a) C_2H_2 adsorption-desorption isotherms at 298 K of MIL-126(Sc) and the modified materials. (b) C_2H_2 adsorption recycles of MIL-126(Cr/Sc) at 298 K and 1 bar.

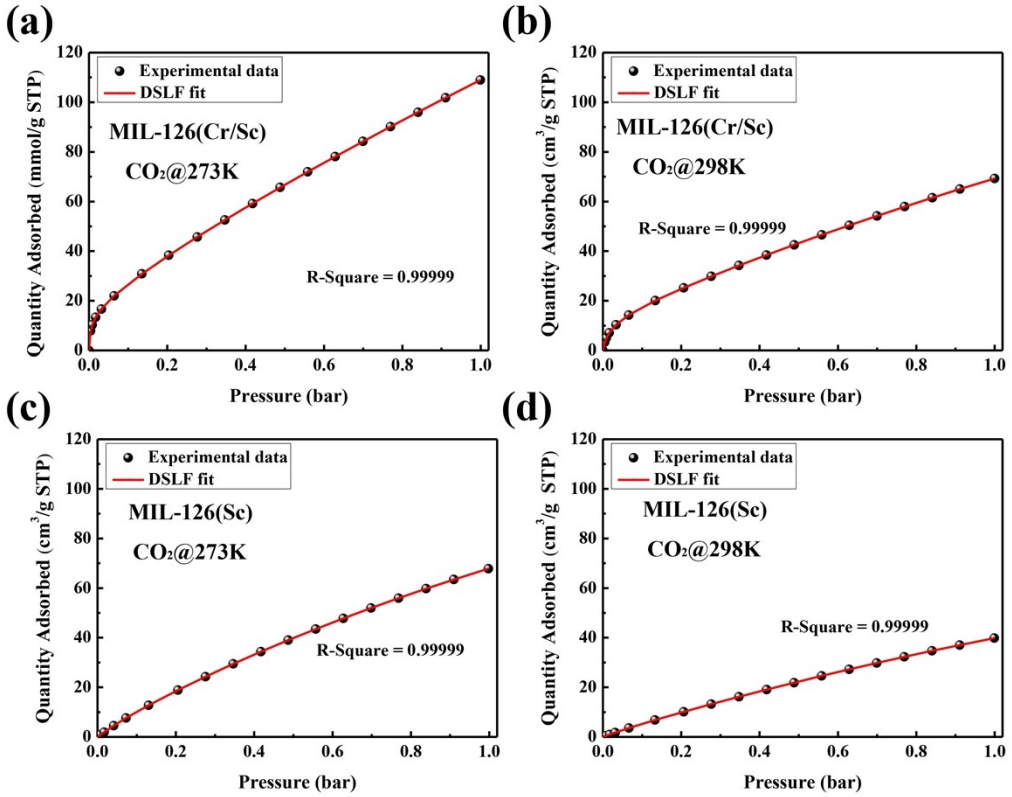


Fig. S7 DSLF fit of CO_2 adsorption isotherms in MIL-126(Sc) and MIL-126(Cr/Sc).

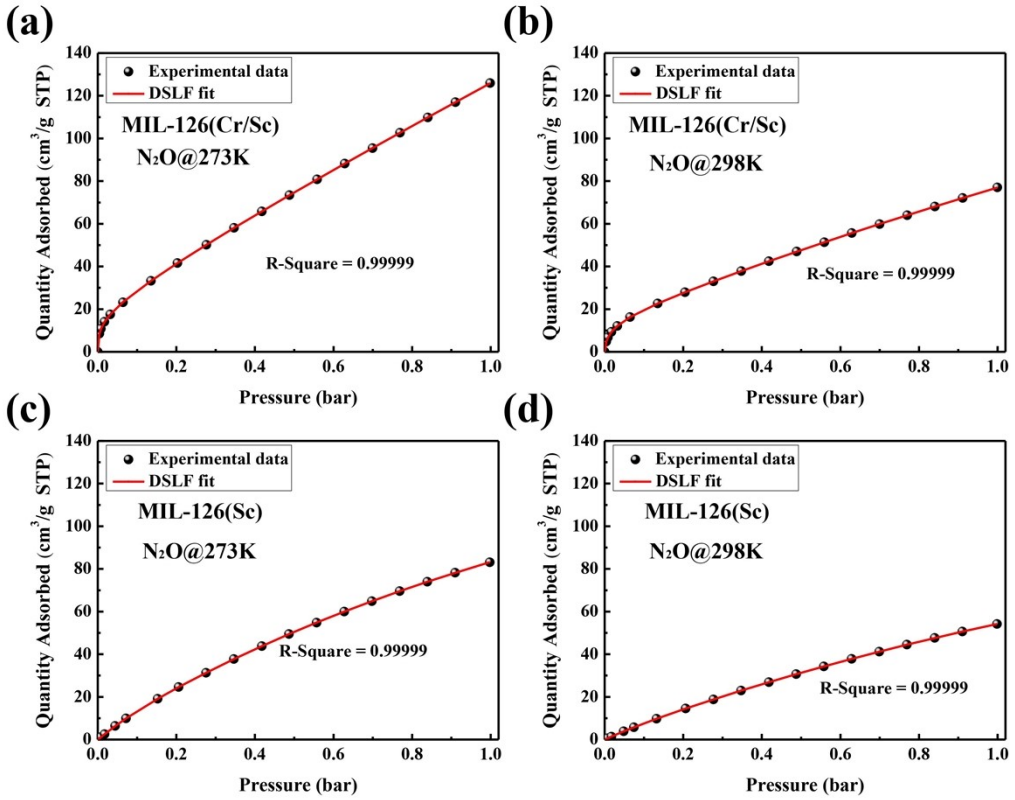


Fig. S8 DSLF fit of N_2O adsorption isotherms in MIL-126(Sc) and MIL-126(Cr/Sc).

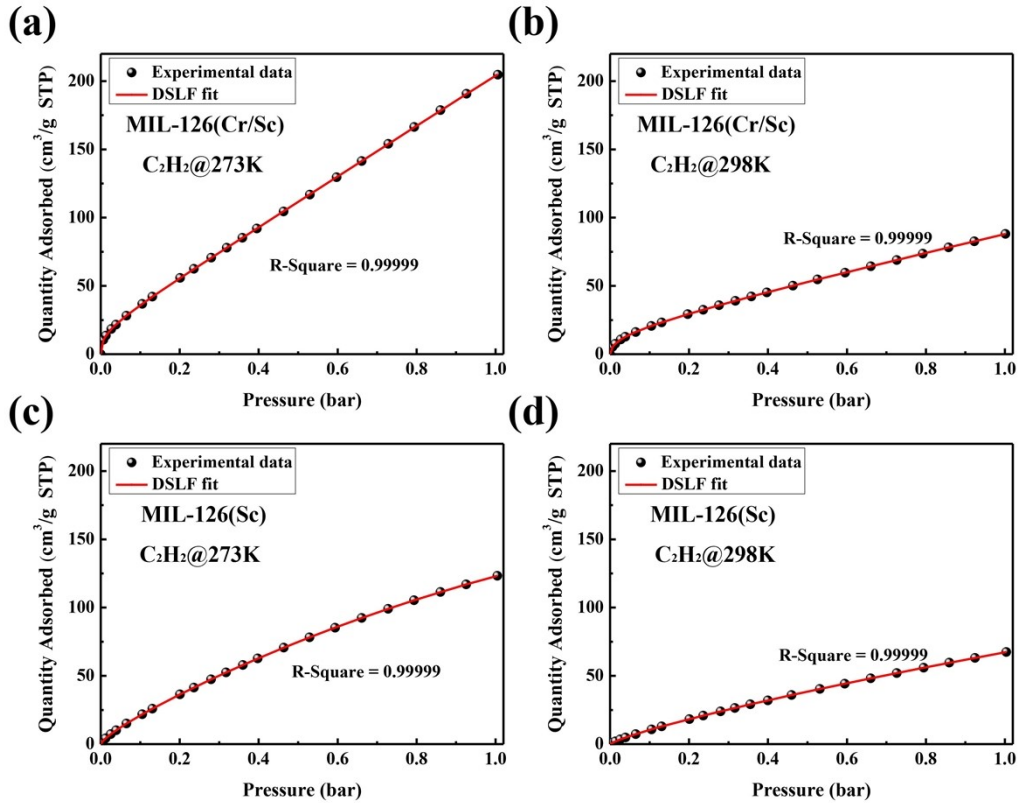


Fig. S9 DSLF fit of C_2H_2 adsorption isotherms in MIL-126(Sc) and MIL-126(Cr/Sc).

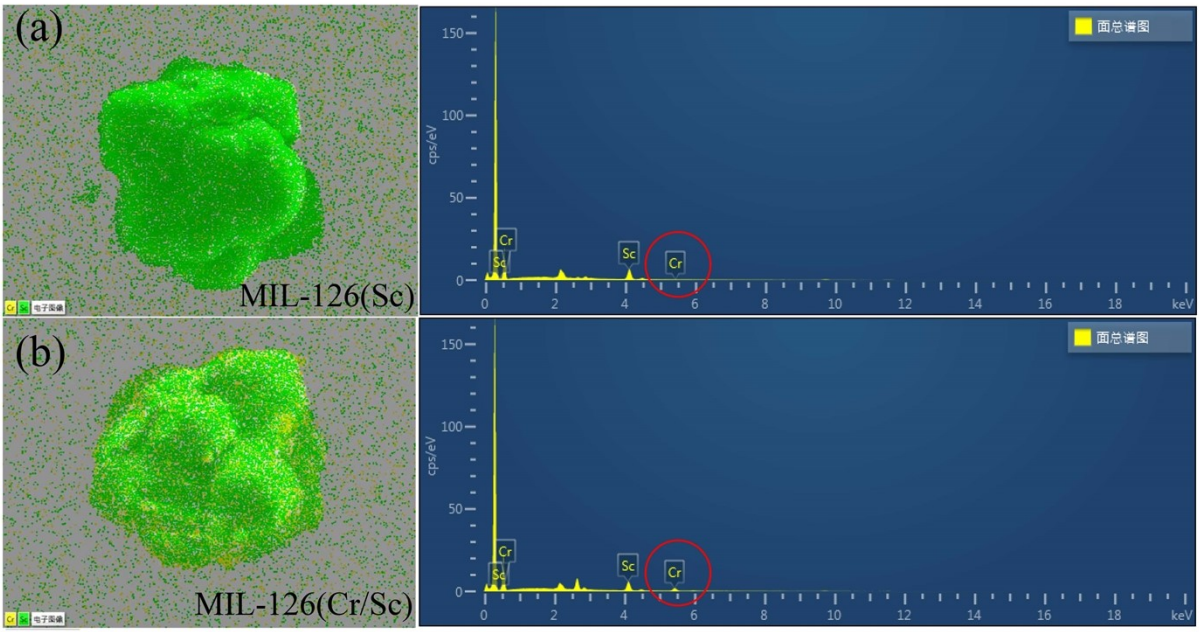


Fig. S10 Elemental mapping images and element analysis for MIL-126(Sc) and MIL-126(Cr/Sc) by EDX.

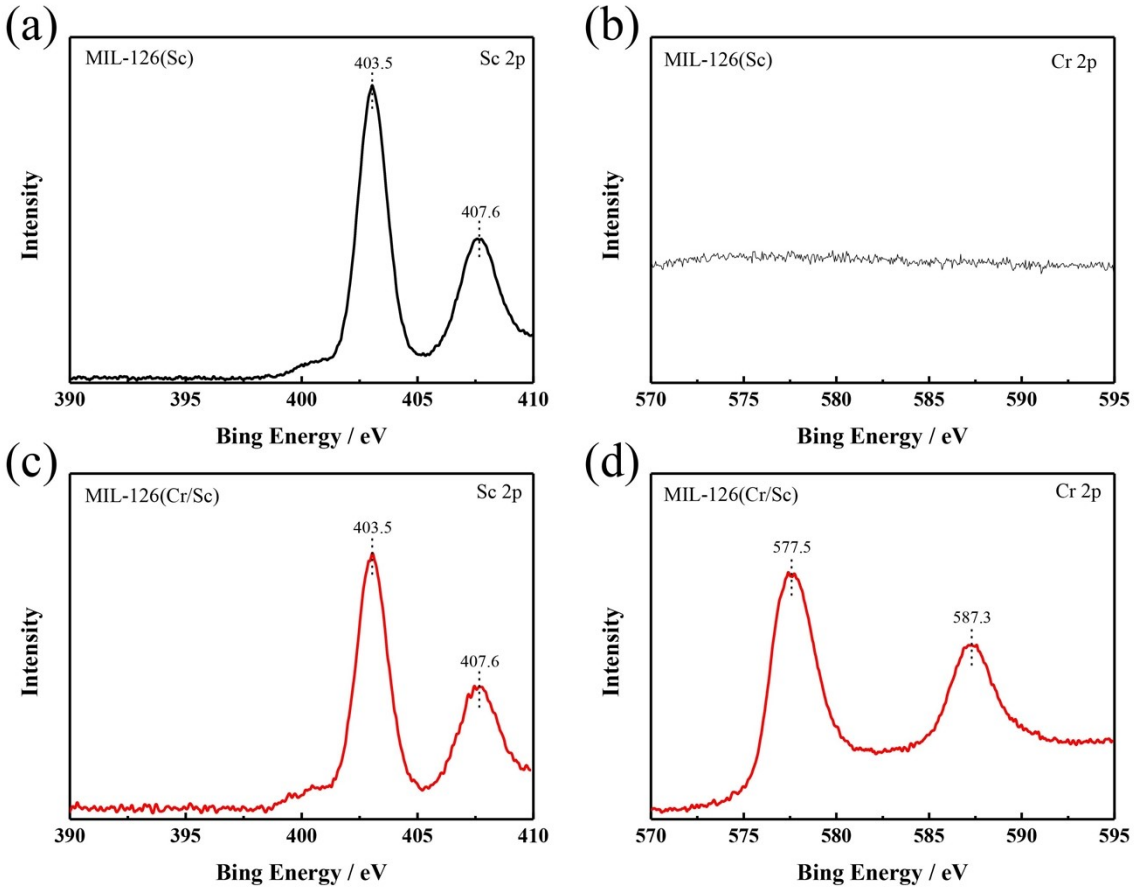


Fig. S11 Local XPS spectra of MIL-126(Sc) and MIL-126(Cr/Sc): Sc 2p and Cr 2p spectra.

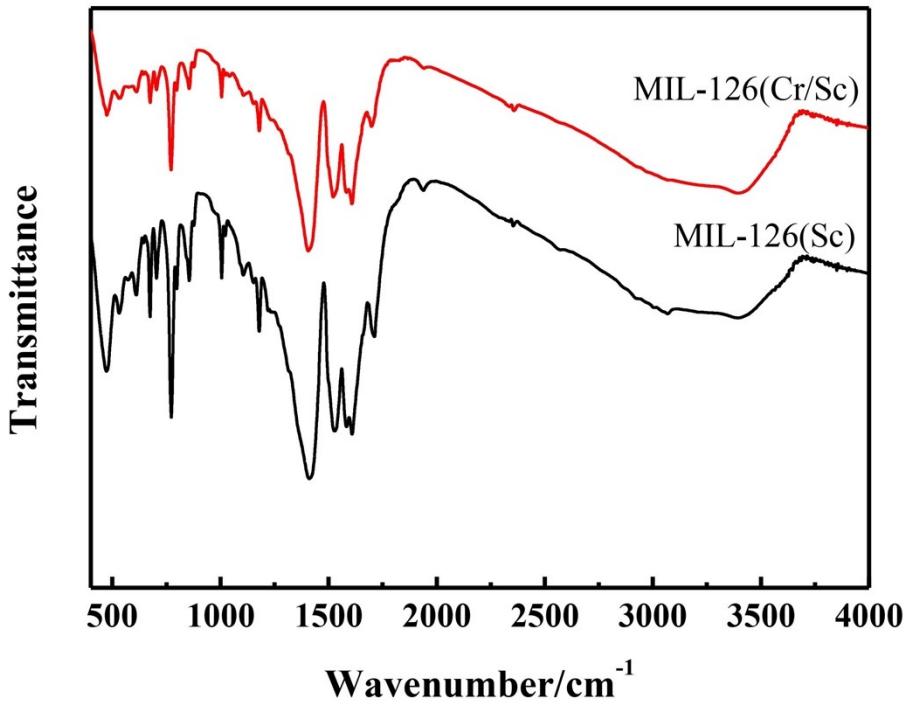
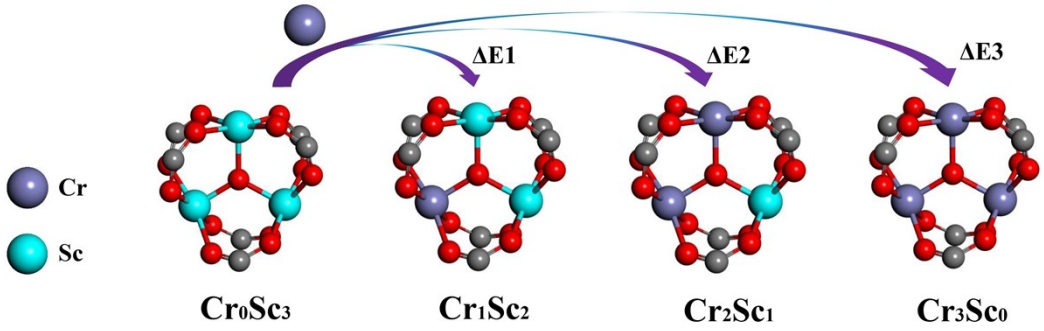


Fig. S12 FTIR spectra of MIL-126(Sc) and MIL-126(Cr/Sc).



	E_0 /eV	E_{cr_atom}/eV	E_{Sc_atom}/eV	ΔE/eV
Cr_0Sc_3	-165.40			
Cr_1Sc_2	-163.32	-0.88	-1.82	1.14
Cr_2Sc_1	-161.65	-0.88	-1.82	1.88
Cr_3Sc_0	-160.30	-0.88	-1.82	2.28

Fig. S13 Formation energy of Cr_nSc_{3-n} (n = 1,2,3). The formation energy value was determined by DFT calculation based on the formula: $\Delta E = E_0(Cr_nSc_{3-n}) + n*E_{Sc\_atom} - n*E_{Cr\_atom} - E_0(Cr_0Sc_3)$.

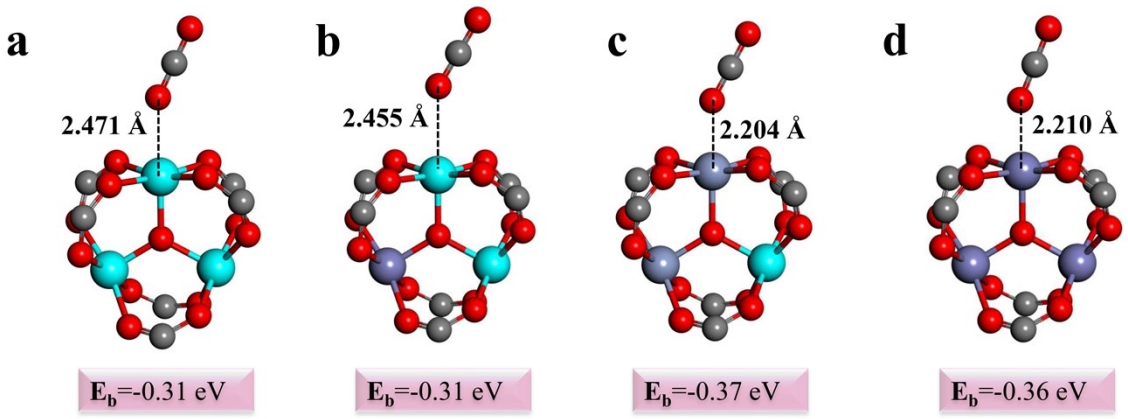


Fig. S14 The DFT-calculated adsorption configurations of CO_2 on the open metal sites in MIL-126 with different Cr content using a cluster model (Cr: light purple; Sc: cyan; C: grey; O: red).

Table S1. DSLF fit parameters for CO_2 in MIL-126(Cr/Sc) and MIL-126(Sc).

Adsorbents	T. T.[a]	q_1	b_1	n_1	q_2	b_2	n_2
MIL-126(Cr/Sc)	273	1.76E1	1.98E1	1.61	3.01E3	3.16E-2	1.12
MIL-126(Cr/Sc)	298	2.71E2	2.42E-1	0.91	1.75E1	1.35E1	1.30
MIL-126(Sc)	273	2.26E2	0.39E-1	0.94	4.72E0	1.58E1	0.91
MIL-126(Sc)	298	1.20E1	0.39E-1	0.81	6.79E0	5.37E0	1.04

Table S2. DSLF fit parameters for N_2O in MIL-126(Cr/Sc) and MIL-126(Sc).

Adsorbents	Gas	q_1	b_1	n_1	q_2	b_2	n_2
MIL-126(Cr/Sc)	273	2.15E1	9.55E0	1.93	2.56E5	4.15E-4	1.08
MIL-126(Cr/Sc)	298	2.02E1	8.93E0	1.59	4.54E2	1.49E-1	0.95
MIL-126(Sc)	273	1.16E1	1.08E1	0.94	2.01E2	5.63E-1	0.87
MIL-126(Sc)	298	1.55E2	4.42E-1	0.85	7.48E0	7.74E0	0.97

Table S3. DSLF fit parameters for C_2H_2 in MIL-126(Cr/Sc) and MIL-126(Sc).

Adsorbents	Gas	q_1	b_1	n_1	q_2	b_2	n_2
MIL-126(Cr/Sc)	273	3.82E4	1.66E-3	2.70	1.55E3	1.00E-2	0.80
MIL-126(Cr/Sc)	298	2.07E1	5.59E0	1.71	1.31E5	5.37E-4	1.05
MIL-126(Sc)	273	9.94E1	1.22E0	1.30	1.75E2	6.40E-1	0.70
MIL-126(Sc)	298	4.14E0	8.94E0	1.13	6.16E2	1.14E-1	1.07

[a]: “T. T.” stands for test temperature, the unit is “K”.

Table S4. Summary of the adsorption uptake (298 K, 1bar), selectivity and heat of adsorption data for top-performing C_2H_2-selective materials.

Adsorbents	$C_2H_2(cm^3g^{-1})$	Qst ($kJmol^{-1}$) [a]	Ref.
MOF-OH	68	17	1
MOF-NH_2	60	16	1
ATC-Cu	112	79	2
FeNi-M'MOF	96	27	3
JCM-1	75	37	4
DICRO-4-Ni-i	43	37	5
HOF-3a	47	19	6
CuI@UiO-66-$(COOH)_2$	51	74	7
ZJU-74a	86	45	8
Zn2(bpy)(btec)	55	29	9
NKMOF-1-Ni	61	60	10
UTSA-74a	107.4	31	11
FJU-36a	56	33	12
SIFSIX-21-Ni	91	38	13
MUF-17	67	49	14
Zn-MOF-74	122[b]	31	10
CAU-10	90	27	15
UTSA-300a	69	57	16
Cu@FAU	79.5	50	17
1a	79.5	28.2	18
FJU-90a	180	25	19
MIL-126(Cr/Sc)	**88**	**37**	**This work**

[a] Qst at Zero Coverage for C_2H_2. [b] obtained at 295 K.

Table S5. Comparison of thermal stability of Cr-based tricyclic MOFs.

Adsorbents	BET (m^2g^{-1})	Thermal stability (℃)	Ref.
MIL-126(Cr/Sc)	1354	450	**This work**
Cr-SXU-1	4036	420	20
TYUT-96Cr	632	375	21
PCN-333(Cr)	2548	300	22
PCN-426(Cr)	3155	300	23
MIL-100(Cr)	1950	300	21
MIL-101(Cr)-NDC	2100	300	24
MIL-101(Cr)	4100	275	25

Table S6. Summary of some top-performing MOFs for CO_2 adsorption at 1 bar or 1 atm as noted.

Sample	S_A BET (cm^3/g)	CO_2 uptake (cm^3/g) 273 K	CO_2 uptake (cm^3/g) 298 K	Q_{st} (kJ/mol)	Ref.
ZJU-12	2316	237	131	28	26
CPM-231	1140	232	152	20	27
Mg-MOF-74	1495	229	180	47	28
Cu(TDPTA)	1938	227	131	42	29
MFM-188	2568	216	121	21	30
Cu-tpbtm	3160	217	119	26	31
CPM-200-Fe/Mg	1459	208	127	34	32
NOTT-125	2471	204	93	25	33
SIFSIX-1-Cu	1468	183	118	27	34
CPM-733-dps	1883	238	124	27	35
CPM-733	1328	171	87	24	35
ZSM-5	420	/	33	/	36
13X	488	/	38	/	37
AC	/	/	49	/	38
UIO-66	1525	/	40	25	39
MOF-5	2304	/	47	34	40
MIL-100(Cr)	2153	/	52	/	41
MIL-126(Cr/Sc)	**1354**	**109**	**69**	**40**	**This work**

Table S7. Summary of some top-performing MOFs for N_2O adsorption at 1 bar or 1 atm as noted.

Sample	S_A BET (cm^3/g)	N_2O uptake (cm^3/g) 273 K	N_2O uptake (cm^3/g) 298 K	Q_{st} (kJ/mol)	Ref.
MOF-5	839	/	20.40	/	42
Ni-MOF	447	77	63.00	26	43
ZIF-7	312	/	56.01	/	44
UIO-66	1390	/	96.60	/	45
ZIF-8	1630	/	31.10	/	45
HKUST-1	1850	/	87.60	/	45
MIL-100Cr	2118	184.5	129.40	80	45
ELM-11	621	100.8	89.60	32	46
ELM-12	706	78.4	67.20	36	46
MIL-53Al	1519	56	60.48	25	46
MIL-100Fe-300	2227	140	105.27	37	47
MIL-126(Cr/Sc)	**1354**	**125**	**77**	**31**	**This work**

Table S8. Adsorption energies of MIL-126(Sc) and MIL-126(Cr/Sc) for the selected gas molecules.

	Adsorption energy (eV)	
Gas molecules	MIL-126(Sc)	MIL-126(Cr/Sc)
CO_2	-0.31	-0.37
C_2H_2	-0.37	-0.58
N_2O	-0.28	-0.39

Table S9. Theoretical calculated concentration of unsaturated metal sites

	Chemical[a] Composition	Relative Molecular Mass	Unsaturated metal Sites[b] (mmol/g)
MIL-126(Sc) [48]	$Sc_3O[BPDC]_3X$	913.14	2.19
MIL-126(Cr/Sc)	$Cr_{1.83}Sc_{1.17}O[BPDC]_3X$	**925.95**	**2.16**

[a]: Coordination water molecule and water in pores were ignored. [b]: Concentration of unsaturated metal sites was calculated based on the relative molecular mass and the percentage of unsaturated metal sites values reported in previous work. X=OH^- or Cl^-, here, Cl^- was used for the calculation of the relative molecular mass.

References

1 W. Gong, H. Cui, Y. Xie, Y. Li, X. Tang, Y. Liu, Y. Cui and B. Chen, Efficient C_2H_2/CO_2 Separation in Ultramicroporous Metal-Organic Frameworks with Record C_2H_2 Storage Density, *J. Am. Chem. Soc.,* 2021, **143**, 14869-14876.

2 Z. Niu, X. Cui, T. Pham, G. Verma, P. C. Lan, C. Shan, H. Xing, K. A. Forrest, S. Suepaul, B. Space, A. Nafady, A. M. Al-Enizi and S. Ma, A MOF-based Ultra-Strong Acetylene Nano-trap for Highly Efficient C_2H_2/CO_2 Separation, *Angew. Chem. Int. Ed.,* 2021, **60**, 5283-5288.

3 J. Gao, X. Qian, R.-B. Lin, R. Krishna, H. Wu, W. Zhou and B. Chen, Mixed Metal-Organic Framework with Multiple Binding Sites for Efficient C_2H_2/CO_2 Separation, *Angew. Chem. Int. Ed.,* 2020, **59**, 4396-4400.

4 J. Lee, C. Y. Chuah, J. Kim, Y. Kim, N. Ko, Y. Seo, K. Kim, T. H. Bae and E. Lee, Separation of Acetylene from Carbon Dioxide and Ethylene by a Water-Stable Microporous Metal-Organic Framework with Aligned Imidazolium Groups inside the Channels, *Angew. Chem. Int. Ed.,* 2018, **57**, 7869-7873.

5 H. S. Scott, M. Shivanna, A. Bajpai, D. G. Madden, K.-J. Chen, T. Pham, K. A. Forrest, A. Hogan, B. Space, J. J. Perry and M. J. Zaworotko, Highly Selective Separation of C_2H_2 from CO_2 by a New Dichromate-Based Hybrid Ultramicroporous Material, *ACS Appl. Mat. Interfaces,* 2017, **9**, 33395-33400.

6 P. Li, Y. He, Y. Zhao, L. Weng, H. Wang, R. Krishna, H. Wu, W. Zhou, M. O'Keeffe, Y. Han and B. Chen, A Rod-Packing Microporous Hydrogen-Bonded Organic Framework for Highly Selective Separation of C_2H_2/CO_2 at Room Temperature, *Angew. Chem. Int. Ed.,* 2015, **54**, 574-577.

7 L. Zhang, K. Jiang, L. Yang, L. Li, E. Hu, L. Yang, K. Shao, H. Xing, Y. Cui, Y. Yang, B. Li, B. Chen and G. Qian, Benchmark C_2H_2/CO_2 Separation in an Ultra-Microporous Metal-Organic Framework via Copper(I)-Alkynyl Chemistry, *Angew. Chem. Int. Ed.,* 2021, **60**, 15995-16002.

8 J. Pei, K. Shao, J.-X. Wang, H.-M. Wen, Y. Yang, Y. Cui, R. Krishna, B. Li and G. Qian, A Chemically Stable Hofmann-Type Metal-Organic Framework with Sandwich-Like Binding Sites for Benchmark Acetylene Capture, *Adv. Mater.,* 2020, **32**.

9 Y. Chen, Y. Du, Y. Wang, R. Krishna, L. Li, J. Yang, J. Li and B. Mu, A stable metal-organic framework with well-matched pore cavity for efficient acetylene separation, *AlChE J.,* 2021, **67**.

10 Y.-L. Peng, T. Pham, P. Li, T. Wang, Y. Chen, K.-J. Chen, K. A. Forrest, B. Space, P. Cheng, M. J. Zaworotko and Z. Zhang, Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene, *Angew. Chem. Int. Ed.,* 2018, **57**, 10971-10975.

11 F. Luo, C. Yan, L. Dang, R. Krishna, W. Zhou, H. Wu, X. Dong, Y. Han, T.-L. Hu, M. O'Keeffe, L. Wang, M. Luo, R.-B. Lin and B. Chen, UTSA-74: A MOF-74 Isomer with Two Accessible Binding Sites per Metal Center for Highly Selective Gas Separation, *J. Am. Chem. Soc.,* 2016, **138**, 5678-5684.

12 L. Liu, Z. Yao, Y. Ye, L. Chen, Q. Lin, Y. Yang, Z. Zhang and S. Xiang, Robustness, Selective Gas Separation, and Nitrobenzene Sensing on Two Isomers of Cadmium Metal-Organic Frameworks Containing Various Metal-O-Metal Chains, *Inorg. Chem.,* 2018, **57**, 12961-12968.

13 N. Kumar, S. Mukherjee, N. C. Harvey-Reid, A. A. Bezrukov, K. Tan, V. Martins, M. Vandichel, T. Pham, L. M. van Wyk, K. Oyekan, A. Kumar, K. A. Forrest, K. M. Patil, L. J. Barbour, B. Space, Y. Huang, P. E. Kruger and

M. J. Zaworotko, Breaking the trade-off between selectivity and adsorption capacity for gas separation, *Chem,* 2021, **7**, 3085-3098.

14 O. T. Qazvini, R. Babarao and S. G. Telfer, Multipurpose Metal-Organic Framework for the Adsorption of Acetylene: Ethylene Purification and Carbon Dioxide Removal, *Chem. Mater.,* 2019, **31**, 4919-4926.

15 J. Pei, H.-M. Wen, X.-W. Gu, Q.-L. Qian, Y. Yang, Y. Cui, B. Li, B. Chen and G. Qian, Dense Packing of Acetylene in a Stable and Low-Cost Metal-Organic Framework for Efficient C_2H_2/CO_2 Separation, *Angew. Chem. Int. Ed.,* 2021, **60**, 25068-25074

16 R.-B. Lin, L. Li, H. Wu, H. Arman, B. Li, R.-G. Lin, W. Zhou and B. Chen, Optimized Separation of Acetylene from Carbon Dioxide and Ethylene in a Microporous Material, *J. Am. Chem. Soc.,* 2017, **139**, 8022-8028.

17 S. Liu, X. Han, Y. Chai, G. Wu, W. Li, J. Li, I. da Silva, P. Manuel, Y. Cheng, L. L. Daemen, A. J. Ramirez-Cuesta, W. Shi, N. Guan, S. Yang and L. Li, Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite, *Angew. Chem. Int. Ed.,* 2021, **60**, 6526-6532.

18 W.-J. Shi, Y.-Z. Li, J. Chen, R.-H. Su, L. Hou, Y.-Y. Wang and Z. Zhu, A new metal-organic framework based on rare Zn4F4 cores for efficient separation of C_2H_2, *Chem. Commun.,* 2021, **57**, 12788-12791.

19 Y. Ye, Z. Ma, R.-B. Lin, R. Krishna, W. Zhou, Q. Lin, Z. Zhang, S. Xiang and B. Chen, Pore Space Partition within a Metal-Organic Framework for Highly Efficient C_2H_2/CO_2 Separation, *J. Am. Chem. Soc.,* 2019, **141**, 4130-4136.

20 J.-H. Wang, Y. Zhang, M. Li, S. Yan, D. Li and X.-M. Zhang, Solvent-Assisted Metal Metathesis: A Highly Efficient and Versatile Route towards Synthetically Demanding Chromium Metal-Organic Frameworks, *Angew. Chem. Int. Ed.,* 2017, **56**, 6478-6482.

21 F. Zhang, H. Shang, L. Wang, Y. Wang, J. Yang, Y. Xia, H. Li, L. Li and J. Li, Construction of a Porous Metal-Organic Framework with a High Density of Open Cr Sites for Record N_2/O_2 Separation, *Adv. Mater.,* 2021, **33**.

22 X. Lian, D. Feng, Y.-P. Chen, T.-F. Liu, X. Wang and H.-C. Zhou, The preparation of an ultrastable mesoporous

Cr(III)-MOF via reductive labilization, *Chem. Sci.,* 2015, **6**, 7044-7048.

23 T.-F. Liu, L. Zou, D. Feng, Y.-P. Chen, S. Fordham, X. Wang, Y. Liu and H.-C. Zhou, Stepwise Synthesis of Robust Metal-Organic Frameworks via Postsynthetic Metathesis and Oxidation of Metal Nodes in a Single-Crystal to Single-Crystal Transformation, *J. Am. Chem. Soc.,* 2014, **136**, 7813-7816.

24 A. Sonnauer, F. Hoffmann, M. Froeba, L. Kienle, V. Duppel, M. Thommes, C. Serre, G. Ferey and N. Stock, Giant Pores in a Chromium 2,6-Naphthalenedicarboxylate Open-Framework Structure with MIL-101 Topology, *Angew. Chem. Int. Ed.,* 2009, **48**, 3791-3794.

25 G. Ferey, C. Mellot-Draznieks, C. Serre, F. Millange, J. Dutour, S. Surble and I. Margiolaki, A chromium terephthalate-based solid with unusually large pore volumes and surface area, *Science,* 2005, **309**, 2040-2042.

26 X. Duan, Y. Cui, Y. Yang and G. Qian, A novel methoxy-decorated metal-organic framework exhibiting high acetylene and carbon dioxide storage capacities, *CrystEngComm,* 2017, **19**, 1464-1469.

27 Q.-G. Zhai, X. Bu, C. Mao, X. Zhao, L. Daemen, Y. Cheng, A. J. Ramirez-Cuesta and P. Feng, An ultra-tunable platform for molecular engineering of high-performance crystalline porous materials, *Nat. Commun.,* 2016, **7**.

28 S. R. Caskey, A. G. Wong-Foy and A. J. Matzger, Dramatic tuning of carbon dioxide uptake via metal substitution in a coordination polymer with cylindrical pores, *J. Am. Chem. Soc.,* 2008, **130**, 10870-10871.

29 B. Li, Z. Zhang, Y. Li, K. Yao, Y. Zhu, Z. Deng, F. Yang, X. Zhou, G. Li, H. Wu, N. Nijem, Y. J. Chabal, Z. Lai, Y. Han, Z. Shi, S. Feng and J. Li, Enhanced Binding Affinity, Remarkable Selectivity, and High Capacity of CO_2 by Dual Functionalization of a rht-Type Metal-Organic Framework, *Angew. Chem. Int. Ed.,* 2012, **51**, 1412-1415.

30 F. Moreau, I. da Silva, N. H. Al Smail, T. L. Easun, M. Savage, H. G. W. Godfrey, S. F. Parker, P. Manuel, S. Yang and M. Schroeder, Unravelling exceptional acetylene and carbon dioxide adsorption within a tetra-amide functionalized metal-organic framework, *Nat. Commun.,* 2017, **8**.

31 B. Zheng, J. Bai, J. Duan, L. Wojtas and M. J. Zaworotko, Enhanced CO_2 Binding Affinity of a High-Uptake rht-

Type Metal-Organic Framework Decorated with Acylamide Groups, *J. Am. Chem. Soc.,* 2011, **133**, 748-751.

32 Q.-G. Zhai, X. Bu, C. Mao, X. Zhao and P. Feng, Systematic and Dramatic Tuning on Gas Sorption Performance in Heterometallic Metal-Organic Frameworks, *J. Am. Chem. Soc.,* 2016, **138**, 2524-2527.

33 N. H. Alsmail, M. Suyetin, Y. Yan, R. Cabot, C. P. Krap, J. Lu, T. L. Easun, E. Bichoutskaia, W. Lewis, A. J. Blake and M. Schroeder, Analysis of High and Selective Uptake of CO_2 in an Oxamide-Containing $\{Cu_2(OOCR)_4\}$-Based Metal-Organic Framework, *Chem. Eur. J.,* 2014, **20**, 7317-7324.

34 S. D. Burd, S. Ma, J. A. Perman, B. J. Sikora, R. Q. Snurr, P. K. Thallapally, J. Tian, L. Wojtas and M. J. Zaworotko, Highly Selective Carbon Dioxide Uptake by $Cu(bpy\text{-}n)_2(SiF_6)$ (bpy-1=4,4-Bipyridine; bpy-2=1,2-Bis(4-pyridyl)ethene), *J. Am. Chem. Soc.,* 2012, **134**, 3663-3666.

35 Y. Wang, X. Jia, H. Yang, Y. Wang, X. Chen, A. N. Hong, J. Li, X. Bu and P. Feng, A Strategy for Constructing Pore-Space-Partitioned MOFs with High Uptake Capacity for C_2 Hydrocarbons and CO_2, *Angew. Chem. Int. Ed.,* 2020, **59**, 19027-19030.

36 Y. Li, H. Yi, X. Tang, F. Li and Q. Yuan, Adsorption separation of CO_2/CH_4 gas mixture on the commercial zeolites at atmospheric pressure, *Chem. Eng. J.,* 2013, **229**, 50-56.

37 J. McEwen, J.-D. Hayman and A. O. Yazaydin, A comparative study of CO_2, CH_4 and N_2 adsorption in ZIF-8, Zeolite-13X and BPL activated carbon, *Chem. Phys.,* 2013, **412**, 72-76.

38 R.-L. Tseng, F.-C. Wu and R.-S. Juang, Adsorption of CO_2 at atmospheric pressure on activated carbons prepared from melamine-modified phenol-formaldehyde resins, *Sep. Purif. Technol.,* 2015, **140**, 53-60.

39 Z. Hu, M. Khurana, Y. H. Seah, M. Zhang, Z. Guo and D. Zhao, Ionized Zr-MOFs for highly efficient post-combustion CO_2 capture, *Chem. Eng. Sci.,* 2015, **124**, 61-69.

40 Z. Zhao, Z. Li and Y. S. Lin, Adsorption and Diffusion of Carbon Dioxide on Metal-Organic Framework (MOF-5), *Ind. Eng. Chem. Res.,* 2009, **48**, 10015-10020.

41 L. Li, J. Yang, J. Li, Y. Chen and J. Li, Separation of CO_2/CH_4 and CH_4/N_2 mixtures by M/DOBDC: A detailed dynamic comparison with MIL-100(Cr) and activated carbon, *Microporous Mesoporous Mater.,* 2014, **198**, 236-246.

42 D. Saha, Z. Bao, F. Jia and S. Deng, Adsorption of CO_2, CH_4, N_2O, and N_2 on MOF-5, MOF-177, and Zeolite 5A, *Environ. Sci. Technol.,* 2010, **44**, 1820-1826.

43 X. Zhang, W. Chen, W. Shi and P. Cheng, Highly selective sorption of CO_2 and N_2O and strong gas- framework interactions in a nickel(II) organic material, *J. Mater. Chem. A,* 2016, **4**, 16198-16204.

44 J.-R. Li, R. J. Kuppler and H.-C. Zhou, Selective gas adsorption and separation in metal-organic frameworks, *Chem. Soc. Rev.,* 2009, **38**, 1477-1504.

45 L. Wang, F. Zhang, C. Wang, Y. Li, J. Yang, L. Li and J. Li, Ethylenediamine-functionalized metal organic frameworks MIL-100(Cr) for efficient CO_2/N_2O separation, *Sep. Purif. Technol.,* 2020, **235**.

46 L. Wang, Y. Li, Y. Wang, J. Yang, L. Li and J. Li, Research on CO_2-N_2O separation using flexible metal organic frameworks, *Sep. Purif. Technol.,* 2020, **251**.

47 L. Wang, F. Zhang, J. Yang, L. Li and J. Li, The efficient separation of N_2O/CO_2 using unsaturated Fe^{2+} sites in MIL-100Fe, *Chem. Commun.,* 2021, **57**, 6636-6639.

48 R. J. Marshall, C. T. Lennon, A. Tao, H. M. Senn, C. Wilson, D. Fairen-Jimenez and R. S. Forgan, Controlling interpenetration through linker conformation in the modulated synthesis of Sc metal-organic frameworks, *J. Mater. Chem. A,* 2018, **6**, 1181-1187.