Incorporation of bifunctional aminopyridine into a NbO-type MOF for markedly enhanced adsorption of C₂H₂ and CO₂ over CH₄

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Fig. S1 The electronic photograph of the as-synthesized ZJNU-98.



Fig. S2 Comparison of the experimental and simulated PXRD patterns of ZJNU-98.



Fig. S3 TGA curve of the as-synthesized ZJNU-98 under nitrogen atmosphere.



Fig. S4 Comparison of FTIR spectra of the ligand H_4L and its corresponding as-synthesized MOF ZJNU-98.



 $S_{\text{BET}} = \frac{1}{(3.20114 \times 10^{-7} + 0.00183)}/(22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18} = 2378 \text{ m}^2 \text{ g}^{-1}}{S_{\text{Langmuir}}} = \frac{(1/0.00167)}{(22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18})} = 2607 \text{ m}^2 \text{ g}^{-1}}$ BET constant $C = 1 + 0.00183/(3.20114 \times 10^{-7}) = 5717$

$$(P/P_o)_{n_m} = \frac{1}{\sqrt{C+1}} = 0.01305$$

Fig. S5 The consistency plot (a), BET surface area plot (b), and Langmuir surface area plot (c) for ZJNU-98.



Fig. S6 Comparison of the pure-component isotherm data for (a) C_2H_2 , (b) CO_2 , and (c) CH_4 in **ZJNU-98** with the fitted isotherms at 278 K, 288 K, and 298 K.



Fig. S7 Comparison of the experimental and simulated PXRD patterns of (a) NOTT-101, (b) ZJU-5, and (c) ZJNU-34.



Fig. S8 Comparison of (a) N_2 isotherms at 77 K and (b) DFT-derived PSD of ZJNU-98, ZJNU-34, ZJU-5 and NOTT-101.



 $S_{\text{BET}} = \frac{1}{(3.08152 \times 10^{-7} + 0.00157)} / 22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18} = 2772 \text{ m}^2 \text{ g}^{-1}}{S_{\text{Langmuir}}} = \frac{(1/0.00147)}{22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18}} = 2961 \text{ m}^2 \text{ g}^{-1}}$ BET constant $C = 1 + 0.00157 / 3.08152 \times 10^{-7} = 5096$

$$(P/P_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.01381$$

Fig. S9 The consistency plot (a), BET surface area plot (b), and Langmuir surface area plot (c) for **NOTT-101**.



 $S_{\text{BET}} = \frac{1}{(4.44046 \times 10^{-7} + 0.00163)} \times 22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18} = 2670 \text{ m}^2 \text{ g}^{-1}}{S_{\text{Langmuir}}} = \frac{(1}{0.00149}) \times 22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18} = 2922 \text{ m}^2 \text{ g}^{-1}}{\text{BET constant } C = 1 + 0.00163 \times 4.44046 \times 10^{-7} = 3672}$

$$(p/p_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.016235$$

Fig. S10 The consistency plot (a), BET surface area plot (b), and Langmuir surface area plot (c) for **ZJU-5**.



 $S_{\text{BET}} = \frac{1}{(3.69671 \times 10^{-7} + 0.00177)} + \frac{22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18}}{S_{\text{Langmuir}}} = \frac{1}{(1/0.00161)} + \frac{22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18}}{2704 \text{ m}^2 \text{ g}^{-1}}$ BET constant $C = 1 + 0.00177/3.69671 \times 10^{-7} = 4789$

$$(p/p_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.01424$$

Fig. S11 The consistency plot (a), BET surface area plot (b), and Langmuir surface area plot (c) for **ZJNU-34**.



Fig. S12 (a) C_2H_2 , (b) CO_2 , and (c) CH_4 adsorption-desorption isotherms of **ZJNU-34** at four different temperatures of 298 K, 295 K, 288 K, and 278 K. The solid and open symbols represent adsorption and desorption, respectively.



Fig. S13 (a) C_2H_2 , (b) CO_2 , and (c) CH_4 adsorption-desorption isotherms of **ZJU-5** at four different temperatures of 298 K, 295 K, 288 K, and 278 K. The solid and open symbols represent adsorption and desorption, respectively.



Fig. S14 (a) C_2H_2 , (b) CO_2 , and (c) CH_4 adsorption-desorption isotherms of **NOTT-101** at four different temperatures of 298 K, 295 K, 288 K, and 278 K. The solid and open symbols represent adsorption and desorption, respectively.



Fig. S15 Comparison of the pure-component isotherm data for (a) C_2H_2 , (b) CO_2 , and (c) CH_4 in **ZJNU-34** with the fitted isotherms at 278 K, 288 K, and 298 K.



Fig. S16 Comparison of the pure-component isotherm data for (a) C_2H_2 , (b) CO_2 , and (c) CH_4 in **ZJU-5** with the fitted isotherms at 278 K, 288 K, and 298 K.



Fig. S17 Comparison of the pure-component isotherm data for (a) C_2H_2 , (b) CO_2 , and (c) CH_4 in **NOTT-101** with the fitted isotherms at 278 K, 288 K, and 298 K.



Fig. S18 IAST selectivities for the equimolar (a) C_2H_2/CH_4 and (b) CO_2/CH_4 gas mixtures in **ZJNU-34** at three different temperatures of 278 K, 288 K, and 298 K.



Fig. S19 IAST selectivities for the equimolar (a) C_2H_2/CH_4 and (b) CO_2/CH_4 gas mixtures in **ZJU-5** at three different temperatures of 278 K, 288 K, and 298 K.



Fig. S20 IAST selectivities for the equimolar (a) C_2H_2/CH_4 and (b) CO_2/CH_4 gas mixtures in **NOTT-101** at three different temperatures of 278 K, 288 K, and 298 K.



Fig. S21 Comparison of C_2H_2 , CO_2 and CH_4 isotherms of **ZJNU-98**, ZJNU-34, ZJU-5 and NOTT-101 at three different temperatures of (a) 298 K, (b) 288 K and (c) 278 K. The solid and open symbols represent adsorption and desorption, respectively.





170.0 ppm 165.0 155.0 150.0 160.0 145.0 140.0 135.0 130.0 125.0 120.0

Fig. S22 ¹H and ¹³C NMR spectra.

MOFs	ZJNU-98		
Empirical formula	$C_{21}H_{14}Cu_2N_2O_{10}$		
Formula weight	581.44		
λ (Å)	0.71073		
Crystal system	Trigonal		
Space group	<i>R-3m</i>		
	a = 18.7125(10) Å		
	b = 18.7125(10) Å		
Unit call dimensions	c = 38.299(3) Å		
Onit cen annensions	$\alpha = 90^{\circ}$		
	$\beta = 90^{\circ}$		
	$\gamma = 120^{\circ}$		
$V(\text{\AA}^3)$	11614.0(15)		
Ζ	9		
$D_{\rm c} ({\rm g cm^{-3}})$	0.747		
$\mu (\mathrm{mm}^{-1})$	0.850		
F(000)	2628		
θ range for data collection (°)	2.177 to 27.402		
	$-23 \le h \le 24$		
Limiting indices	$-22 \le k \le 24$		
	$-46 \le l \le 49$		
Reflections collected / unique	34905 / 3199		
R _{int}	0.0314		
Max. and min. transmission	0.919 and 0.894		
Refinement method	Full-matrix least-squares on F^2		
Data/restraints/parameters	3199 / 0 / 106		
Goodness-of-fit on F^2	0.865		
Final Dindiana [I. 2-(D]	$R_1 = 0.0443$		
Final <i>R</i> indices $[I > 2\sigma(I)]$	$wR_2 = 0.1694$		
D in diagonal (all data)	$R_1 = 0.0487$		
A muices (an data)	$wR_2 = 0.1861$		
Largest diff. peak and hole ($e^{A^{-3}}$)	0.870 and -0.378		
CCDC	1898821		

 Table S1 Crystal data and structure refinement for ZJNU-98.

Guest	$q_{\rm sat}$ (mmol g ⁻¹)	b_0 (kPa) ^{-v}	E (kJ mol ⁻¹)	v	R^2
C_2H_2	24.28222	1.07526×10 ⁻⁵	18.791	0.70027	0.9998
CO ₂	25.28245	2.25809×10 ⁻⁷	22.507	1	0.99993
CH ₄	13.4719	1.09446×10 ⁻⁶	15.979	1	0.99999

Table S2 Langmuir-Freundlich parameters for adsorption of C₂H₂, CO₂, and CH₄ in **ZJNU-98**.

 Table S3 Langmuir-Freundlich parameters for adsorption of C₂H₂, CO₂, and CH₄ in

 ZJNU-34.

Guest	$q_{ m sat}$	b_0	Ε	v	
Guest	$(\text{mmol } g^{-1})$	$(kPa)^{-\nu}$	(kJ mol ⁻¹)		
C_2H_2	27.75156	1.17624×10 ⁻⁵	18.208	0.6891	
CO ₂	23.47517	2.52642×10 ⁻⁷	22.378	1	
CH ₄	12.92465	1.42418×10 ⁻⁶	15.577	1	

 Table S4 Langmuir-Freundlich parameters for adsorption of C₂H₂, CO₂, and CH₄ in

 ZJU-5.

Guest	$q_{ m sat}$	b_0	E	v	R^2	
	(mmol g^{-1})	$(kPa)^{-\nu}$	$(kJ mol^{-1})$			
C_2H_2	40.70198	1.52745×10 ⁻⁵	16.496	0.65541	0.99978	
CO ₂	26.88883	2.16142×10 ⁻⁷	22.123	1	0.99991	
CH ₄	15.30125	1.81459×10 ⁻⁶	14.268	1	0.99984	

 Table S5 Langmuir-Freundlich parameters for adsorption of C₂H₂, CO₂, and CH₄ in

 NOTT-101.

Guest	$q_{\rm sat}$	b_0		ν	
	(mmol g ⁻)	(kPa)	(kJ mol ⁻)		
C_2H_2	59.19957	1.48802×10^{-5}	15.787	0.61397	
CO ₂	22.75234	2.18689×10 ⁻⁷	22.416	1	
CH ₄	13.39522	3.93239×10 ⁻⁶	12.786	1	

MOFs SLanemuir			0	C ₂ H ₂ uptake ^a		(CO ₂ uptake ^a		CH. uptako ⁴		C ₂ H ₂ /CH ₄ ^a		CO ₂ /CH ₄ ^a					
	V_p	$_{\rm p}$ $D_{\rm c}$		$(cm^3 g^{-1})$			$(cm^3 g^{-1})$,	_п4 иртаке		L	AST selectivi	ty	IAS	T selectivi	ity	
	$(m^2 g^{-1})$	$(cm^{3}g^{-1})$	(g cm ⁻³)	298 K	288 K	278 K	298 K	288 K	278 K	298 K	288 K	278 K	298 K	288 K	278 K	298 K	288 K	278 K
NOTT-101	2772/2961	1.0579	0.6838	176.6	212.3	258.1	85.0	109.1	141.2	20.8	23.7	29.0	26.7	30.3	35.3	4.80	5.56	6.55
ZJU-5	2670/2922	1.0385	0.679	184.4	222.3	263.9	89.1	116.6	150.6	19.7	24.1	29.1	26.9	29.6	33.4	5.18	5.88	6.71
ZJNU-34	2459/2704	0.9687	0.7064	193.8	232.8	268.6	96.2	125.8	159.9	21.7	27.1	32.9	28.6	32.2	37.4	5.28	5.92	6.75
ZJNU-98	2378/2607	0.9324	0.7017	194.3	229.7	264.1	99.2	128.2	165.5	20.8	25.6	31.8	30.5	34.1	39.2	5.70	6.36	7.21

Table S6 Summary of gas adsorption properties of ZJNU-98, ZJNU-34, ZJU-5, and NOTT-101.

 $S_{\text{BET}}/S_{\text{Langmuir}} = \text{BET}$ and Langmuir specific surface areas; $V_{\text{p}} = \text{experimental pore volume}$; $D_{\text{c}} = \text{calculated framework density without solvent}$ molecules and the terminal water molecules; ^{*a*} at 1 atm

C₂H₂ uptake^a CO₂ uptake^a C_2H_2/CH_4 CO₂/CH₄ $S_{\rm BET}$ MOFs Ref. $(m^2 g^{-1})$ $(cm^3 g^{-1})$ $(cm^3 g^{-1})$ selectivity^a selectivity^a 1 NKMOF-1-Ni 382 61.0 51.1 6409.1 NA 2 PMOF-3 74.5 1378 117.3 156.5 5.1 3 Ni-TIPA 404.6 56.8 39.0 112.2 NA 4 Cu-TDPAH 2171 155.7 116 18 82 5 82^b Cu-TDPAT 1938 177.7 NA NA 55.6^b 24.2^{b} 6 UTSA-15 553 31 34 7 Mn(INA)2 236 59.7 NA 51 NA 8 ZJNU-54 2134 211 120 45.0 6.1 9 ZJU-195 1721.9 214.2 105.0 43.4 NA 10 UTSA-57 206.5 32 37 43.1 20.0 11 FJI-Y3 952 118 41.5 NA NA 12 FJI-C1 1726.3 93.8 41.2 39.3 5.89 13 UPC-21 1725.1 139.5 NA 38.1 NA 14 ZJNU-56 1655 189 122 35.7 7.0 M'MOF-20 34.9^{b} 6.8^b 15 42 21 10 16 MFM-130 2173 85.9 59 34.7^{b} NA 17 ZJNU-69 1655 171.7 104.1 34.5 7.14 18 ZJNU-93 1952 164.0 96.2 34.4 5.2 19 ZJNU-81 2720 184.2 99.0 32.4 5.46 20 ZJNU-59 2043 199.5 31.9 109.4 6.021 ZJNU-89 1618 181.3 103.0 30.7 5.8 19 ZJNU-82 2231 195.4 95.4 30.1 5.37 22 ZJNU-76 179.2 29.7 5.43 1996 95.8 21 ZJNU-88 1693 166.099.2 28.9 5.4 23 ZJNU-77 2432 120.2 78.128.6 5.7

Table S7 Summary of selective C_2H_2/CH_4 and CO_2/CH_4 adsorption properties of some typical MOFs reported so far.

ZJNU-78	1311	122.0	82.0	28.4	5.9	23
UTSA-5	462	59.8	38.4	28.4 ^b	10.2^{b}	24
ZJNU-75	2063	188.6	99.2	28.2	5.44	22
ZJNU-70	1748	184.5	115.5	28.0	6.71	17
ZJNU-71	1860	200.4	115.6	27.6	5.73	17
ZJNU-71	1860	200.4	115.6	27.6	5.73	25
ZJU-199	987	128	62.4	27.3	NA	26
ZJNU-83	2015	196.7	102.7	26.5	4.95	19
UTSA-72	173	27.8	21.7	26.5	9.3	27
ZJNU-58	2487	157.1	81.6	25.7	5.5	20
ZJNU-91	2404	172.5	94.8	25.0	4.92	28
ZJNU-74	2243	180.0	88.1	24.9	4.80	22
ZJNU-92	2845	155.1	79.2	24.5	4.85	28
BUT-35	358	71.6	NA	23.5 ^b	NA	29
BUT-70B	695	87.1	31.3	23.3	NA	30
PCM-48	300	25.54	21	23.3	6.1	31
MFM-127	1557	208^c	66.5	21.2 ^c	3.33	32
UTSA-222	703	85.3	42.7	19	NA	33
UTSA-33	660	83.6	NA	18	NA	34
FJU-36	409.0	52.2	35.5	17.7	NA	35
Zn ₅ (BTA) ₆ (TDA) ₂	414	44	37	15.5	9.1	36
UTSA-36	495	56.8	NA	13.8 ^b	NA	37
QMOF-1	140	41.5	24.6	13.5	6.4	38
ZJU-30	228	52.6	NA	9.58 ^b	NA	39
UPC-33	933.8	44.3	31.8	7.78	8.09	40
UTSA-10	1090	43.0	NA	6.2	NA	41
MFM-126	1004	124 ^c	103.7	NA	11.7	32
SNNU-95	206.6	15.1	14.7	NA	NA	42

 S_{BET} = BET specific surface area; ^{*a*} at ambient conditions; ^{*b*} adsorption selectivity based on Henry's Law constants; ^{*c*} 273 K, 1 bar; NA = not available

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