Supporting Information

A microporous Bismuth-based MOF for efficient separation of acetylene from carbon dioxide

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Fitting of Pure Component Isotherms

Dual-site Langmuir-Freundlich model was used to predict binary mixture adsorption from the experimental pure-gas isotherms.

$$q = q_{A,\ sat}\frac{b_A p^{c_A}}{1 + b_A p^{c_A}} + q_{B,sat}\frac{b_B p^{c_B}}{1 + b_B p^{c_B}}$$

with T-dependent parameters b_A and b_B.

$$b_A = b_{A0} exp(\frac{E_A}{RT})$$
$$b_B = b_{B0} exp(\frac{E_B}{RT})$$

Where p is the pressure of the bulk gas at equilibrium with the adsorbed phase (kPa), q is the adsorbed amount per mass of adsorbent (mmol g^{-1}), $q_{A,sat}$, $q_{B,sat}$ are the saturation capacities (mmol g^{-1}), b_A, b_B are the affinity coefficient.

Calculation for C_2H_2/CO_2 Adsorption Selectivities

The ideal adsorbed solution theory (IAST) was used to estimate the composition of the adsorbed phase from the data of single component isotherms and predict the selectivity of binary mixtures C_2H_2/CO_2. IAST calculations for equimolar C_2H_2/CO_2 mixtures adsorption at 278 and 298 K, respectively were performed by

$$S_{ads} = \frac{q_1/q_2}{p_1/p_2}$$

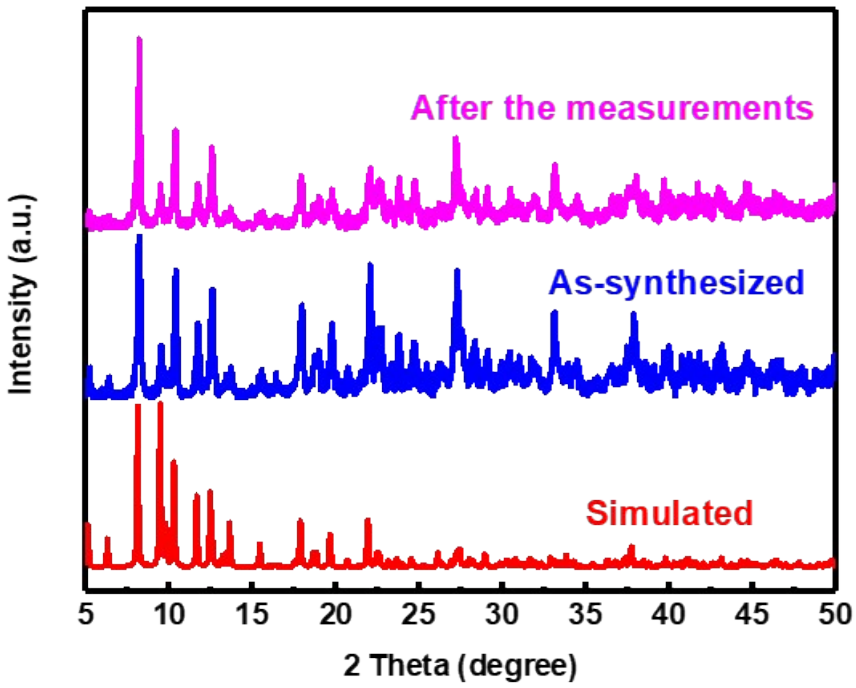


Figure S1. The PXRD patterns of Bi-BTC.

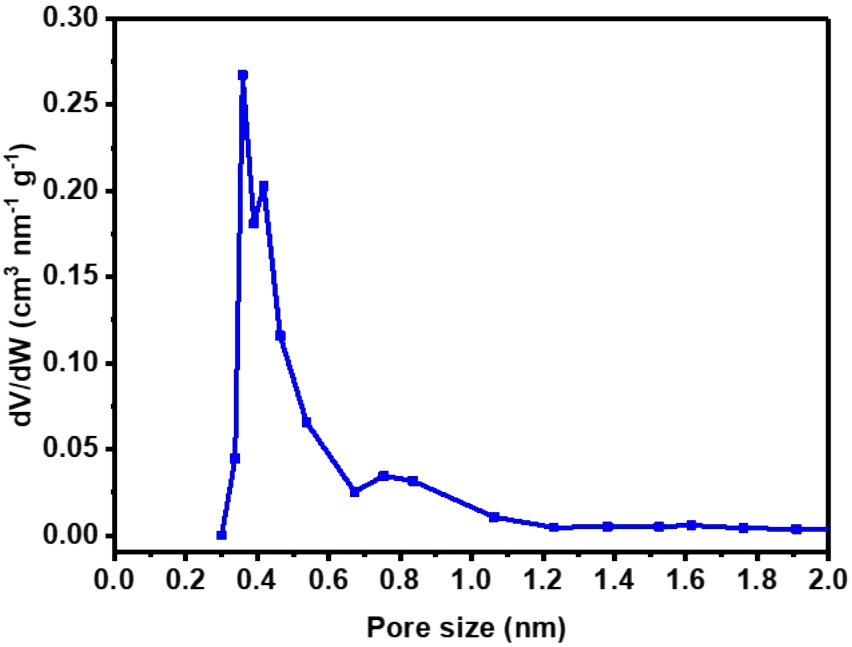


Figure S2. Pore size distribution of Bi-BTC.

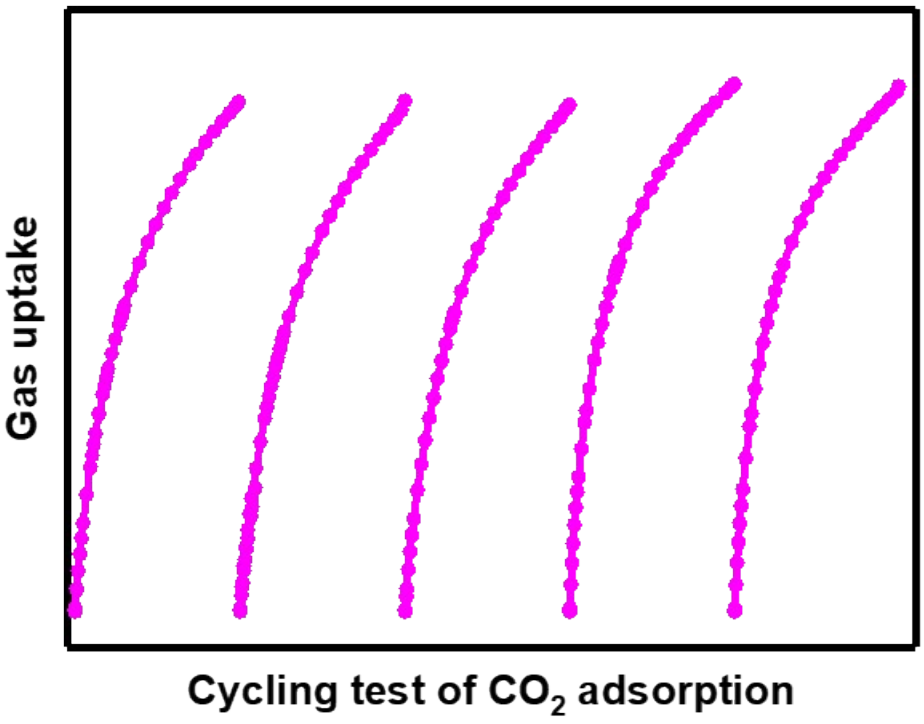
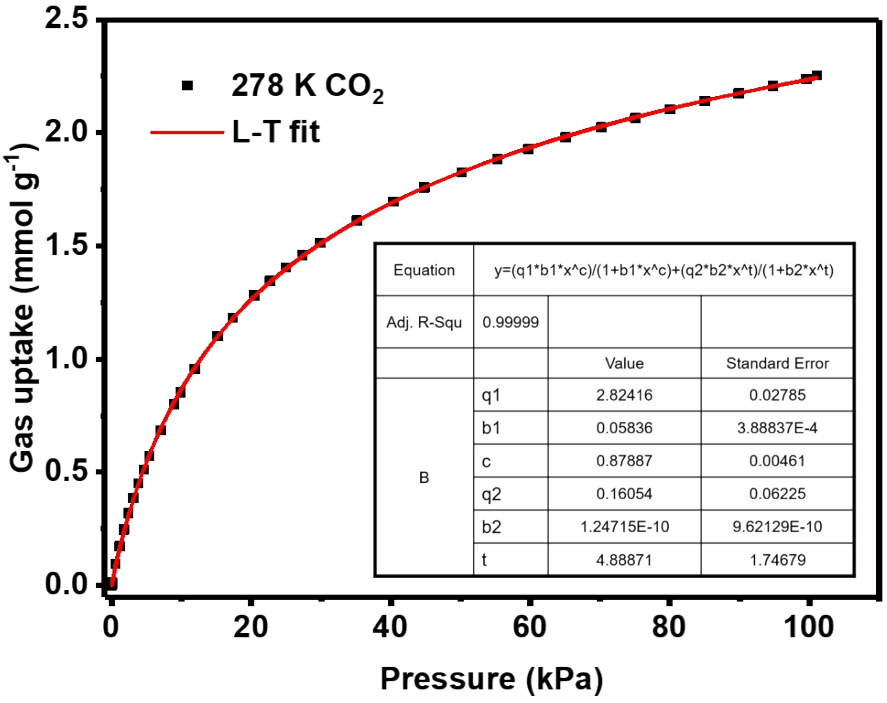
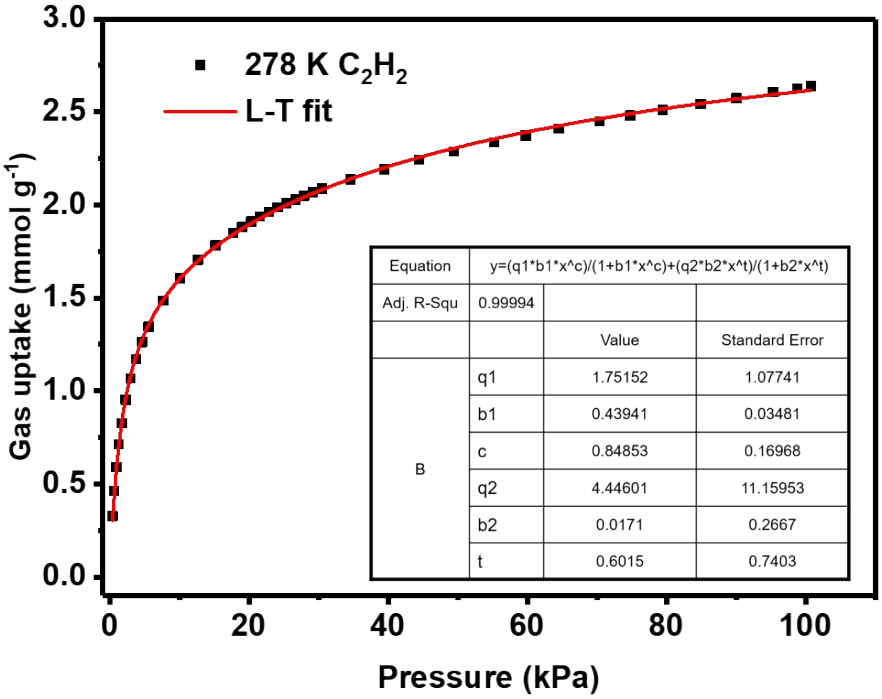


Figure S3. Cycling test of CO_2 adsorption measurements for Bi-BTC at 298 K and 1.0 bar.



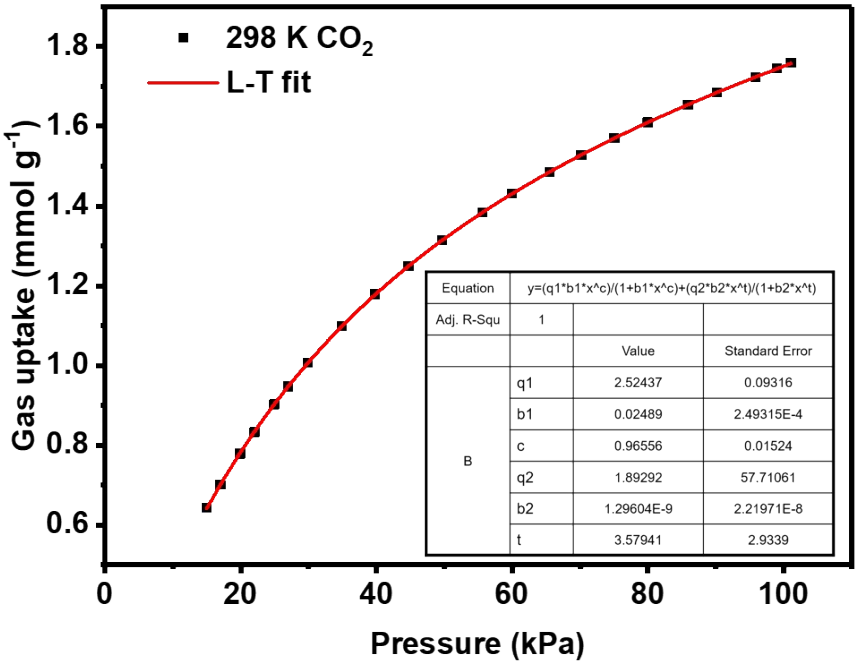
Equation	y=(q1*b1*x^c)/(1+b1*x^c)+(q2*b2*x^t)/(1+b2*x^t)		
Adj. R-Squ	0.99999		
		Value	Standard Error
B	q1	2.82416	0.02785
	b1	0.05836	3.88837E-4
	c	0.87887	0.00461
	q2	0.16054	0.06225
	b2	1.24715E-10	9.62129E-10
	t	4.88871	1.74679

Figure S4. Dual-site Langmuir-Freundlich model for CO_2 adsorption isotherm on Bi-BTC at 278 K.



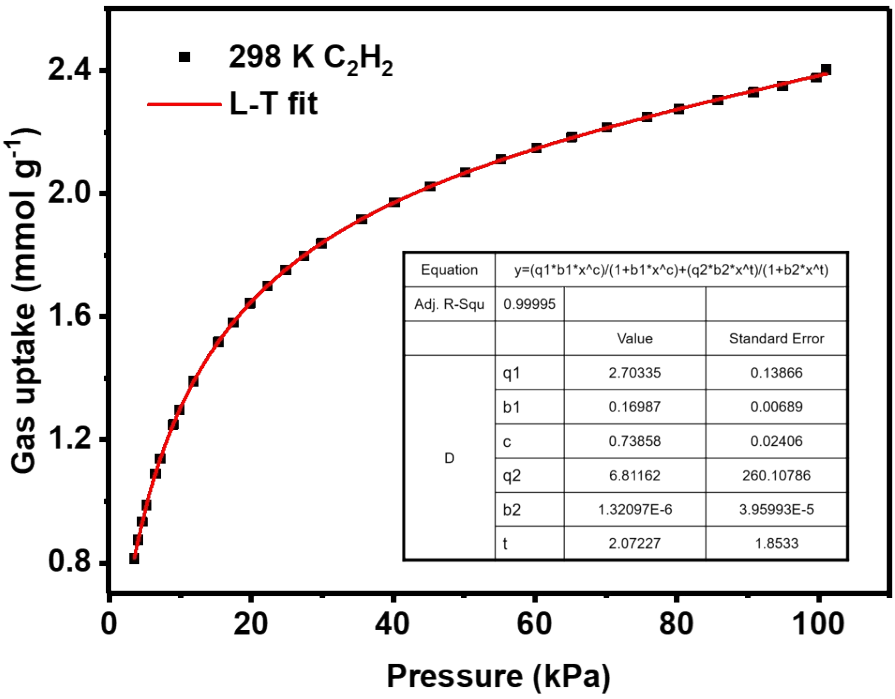
Equation	y=(q1*b1*x^c)/(1+b1*x^c)+(q2*b2*x^t)/(1+b2*x^t)		
Adj. R-Squ	0.99994		
		Value	Standard Error
B	q1	1.75152	1.07741
	b1	0.43941	0.03481
	c	0.84853	0.16968
	q2	4.44601	11.15953
	b2	0.0171	0.2667
	t	0.6015	0.7403

Figure S5. Dual-site Langmuir-Freundlich model for C_2H_2 adsorption isotherm on Bi-BTC at 278 K.



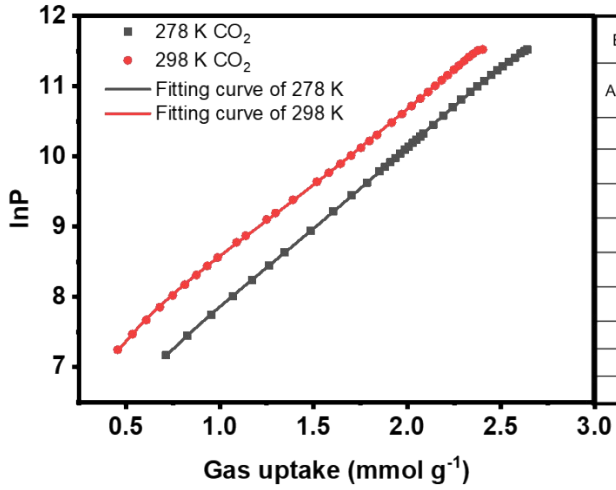
Equation	y=(q1*b1*x^c)/(1+b1*x^c)+(q2*b2*x^t)/(1+b2*x^t)		
Adj. R-Squ	1		
		Value	Standard Error
B	q1	2.52437	0.09316
	b1	0.02489	2.49315E-4
	c	0.96556	0.01524
	q2	1.89292	57.71061
	b2	1.29604E-9	2.21971E-8
	t	3.57941	2.9339

Figure S6. Dual-site Langmuir-Freundlich model for CO_2 adsorption isotherm on Bi-BTC at 298 K.



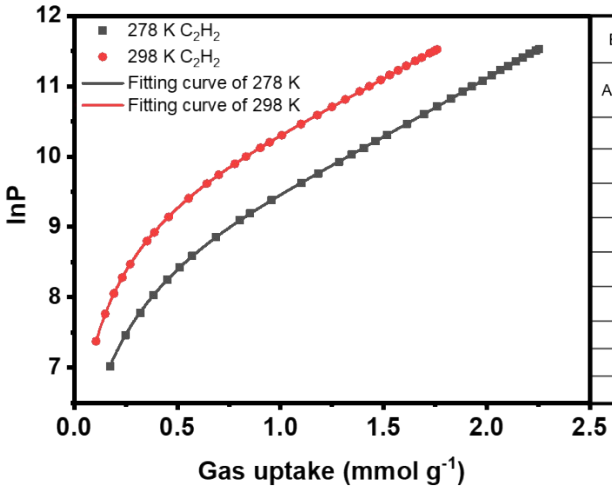
Equation	y=(q1*b1*x^c)/(1+b1*x^c)+(q2*b2*x^t)/(1+b2*x^t)		
Adj. R-Squ	0.99995		
		Value	Standard Error
D	q1	2.70335	0.13866
	b1	0.16987	0.00689
	c	0.73858	0.02406
	q2	6.81162	260.10786
	b2	1.32097E-6	3.95993E-5
	t	2.07227	1.8533

Figure S7. Dual-site Langmuir-Freundlich model for C_2H_2 adsorption isotherm on Bi-BTC at 298 K.



Equation	Y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4)+(b0+b1*x+b2*x^2)	
Adj. R-Squ	0.99994	
	Value	Standard Error
a0	-4253.81677	109.72315
a1	1761.16754	153.07344
a2	-699.65763	64.3579
a3	241.05458	20.1345
a4	-41.05665	3.17943
b0	21.61402	0.35967
b1	-3.96042	0.48029
b2	0.96714	0.14818

Figure S8. The details of virial equation (solid lines) fitting to the experimental CO_2 adsorption data (symbols) for Bi-BTC.



Equation	Y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4)+(b0 +b1*x+b2*x^2)	
Adj. R-Squ	0.99999	
	Value	Standard Error
a0	-3871.3019	16.67702
a1	698.8783	39.99044
a2	-448.93949	22.13862
a3	164.79709	6.18104
a4	-27.93593	1.29369
b0	22.47553	0.05651
b1	-1.05527	0.13297
b2	0.56979	0.06493

Figure S9. The details of virial equation (solid lines) fitting to the experimental C_2H_2 adsorption data (symbols) for Bi-BTC

Table S1. Summary and cooperation of C_2H_2 and CO_2 adsorption capacities at 298 K and isosteric heat of adsorption.

Adsorbent	S_{BET} ($m^2\ g^{-1}$)	C_2H_2 uptake ($cm^3\ g^{-1}$)	CO_2 uptake ($cm^3\ g^{-1}$)	Q_{st} (C_2H_2) (kJ mol^{-1})	IAST Selectivity	Temperature (K)	Ref.
SIFSIX-DPA-Cu-i	898.74	75.59	50.17	46.53	9.3	298	1
Zn-MUC-TRZ	696.3	46.4	42.2	33.06	1.47	298	2
Zn(adenine)(TCPE)	180.1	48.1	33.8	35.1	4.1	298	3
$[Co_2(F\text{-}PyIP)_2DMF]$	509.1	61.7	34.3	34	6.3	298	4
JXNU-18	622	55.2	31.5	37.4	2.81	298	5
ZNU-11	148.8	45.5	22.5	36.1	8.2	298	6
Bi-BTC	91.35	53.8	39.4	35.37	5.14	298	This work
ZNU-9	1623	177.9	100.8	33.1	10.3	298	7
ZNU-8	1402	113.1	58.2	27.2	3.7	298	7
$Cu_3(fbptc)_2$	432.1	119.3	56.5	27.2	3.6	298	8
NBU-7-Cl	123.7	34.3	25.0	33	3.3	298	9
FJU-83	872	123	106	26.9	2.93	298	10
SNNU-29-Mn	1077	115	50		2.9	298	11
CoV-bdc-tppy		164	87.2		2.8	298	12
Cu-AD-GA	517	74	58		2.2	298	13

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