Supporting Information

Solvent-Induced Framework-Interpenetration isomer in Cu MOFs for Efficient Light Hydrocarbon Separation

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Calculation of isosteric heat of adsorption (Q_{st})

The CH_4 adsorption isotherms measured at 273 K and 298 K were first fitted to a virial equation (eqn (1)). The fitting parameters were then used to calculate the isosteric heat of adsorption (Q_{st}) using eqn (2),

$$\ln P = \ln N + \frac{1}{T}\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \quad (1)$$

$$Q_{st} = -R\sum_{i=0}^{m} a_i N^i \quad (2)$$

where P is the pressure (mmHg), N is the adsorbed quantity (mmol g^{-1}), T is the temperature (K), R is the gas constant (8.314 J K^{-1} mol^{-1}), a_i and b_i are virial coefficients, and *m* and *n* represent the number of coefficients required to adequately describe the isotherms (herein, *m*=5, and *n*=2).

Calculation of selectivity via ideal adsorption solution theory (IAST)

The C_2H_2 and CH_4 adsorption isotherms were first fitted to a dual-site Langmuir–Freundlich (DSLF) model (eqn (3)),

$$q = \frac{q_{sat,A} b_A p^{a_A}}{1 + b_A p^{a_A}} + \frac{q_{sat,B} b_B p^{a_B}}{1 + b_B p^{a_B}} \quad (3)$$

where q is the amount of adsorbed gas (mmol g^{-1}), P is the bulk gas phase pressure (atm), q_{sat} is the saturation amount (mmol g^{-1}), *b* is the Langmuir–Freundlich parameter (atm$^{-\alpha}$), and α is the Langmuir–Freundlich exponent (dimensionless) for two adsorption sites A and B indicating the presence of weak and strong adsorption sites.

IAST starts from the Raoult's Law type of relationship between the fluid and adsorbed phase,

$$P_i = Py_i = P_i^0 x_i \quad (4)$$

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \frac{P_i}{P_i^0} = 1 \quad (5)$$

where P_i is the partial pressure of component i (atm), P is the total pressure (atm), and y_i and x_i represent mole fractions of component i in gas and the adsorbed phase (dimensionless). P_i^0 is the equilibrium vapour pressure (atm).

In IAST, P_i^0 is defined by relating to spreading pressure π,

$$\frac{\pi S}{RT} = \int_0^{P_i^0} \frac{q_i(P_i)}{P_i} dP_i = \Pi(constant) \quad (6)$$

where π is the spreading pressure, S is the specific surface area of the adsorbent ($m^2\ g^{-1}$), R is the gas constant (8.314 $J\ K^{-1}\ mol^{-1}$), T is the temperature (K), and $q_i(P_i)$ is the single component equilibrium obtained from isotherms ($mmol\ g^{-1}$).

For a DSLF model, we have an analytical expression for the integral,

$$\int_0^{P_i^0} \frac{q_i(P_i)}{P_i} dP_i = \Pi(constant) = \frac{q_{sat,A}}{\alpha_A} \ln\left[1 + b_A (P_i^0)^{\alpha_A}\right] + \frac{q_{sat,B}}{\alpha_B} \ln\left[1 + b_B (P_i^0)^{\alpha_B}\right] \quad (7)$$

The isotherm parameters are derived from the previous fitting. For a binary component system the unknowns will be Π, P_1^0, and P_2^0 which can be obtained by simultaneously solving eqn (5) and (7).

The adsorbed amount of each compound in a mixture is

$$q_i^{mix} = x_i q_t \quad (8)$$

$$\frac{1}{q_T} = \sum_{i=1}^{n} \frac{x_i}{q_i(P_i^0)} \quad (9)$$

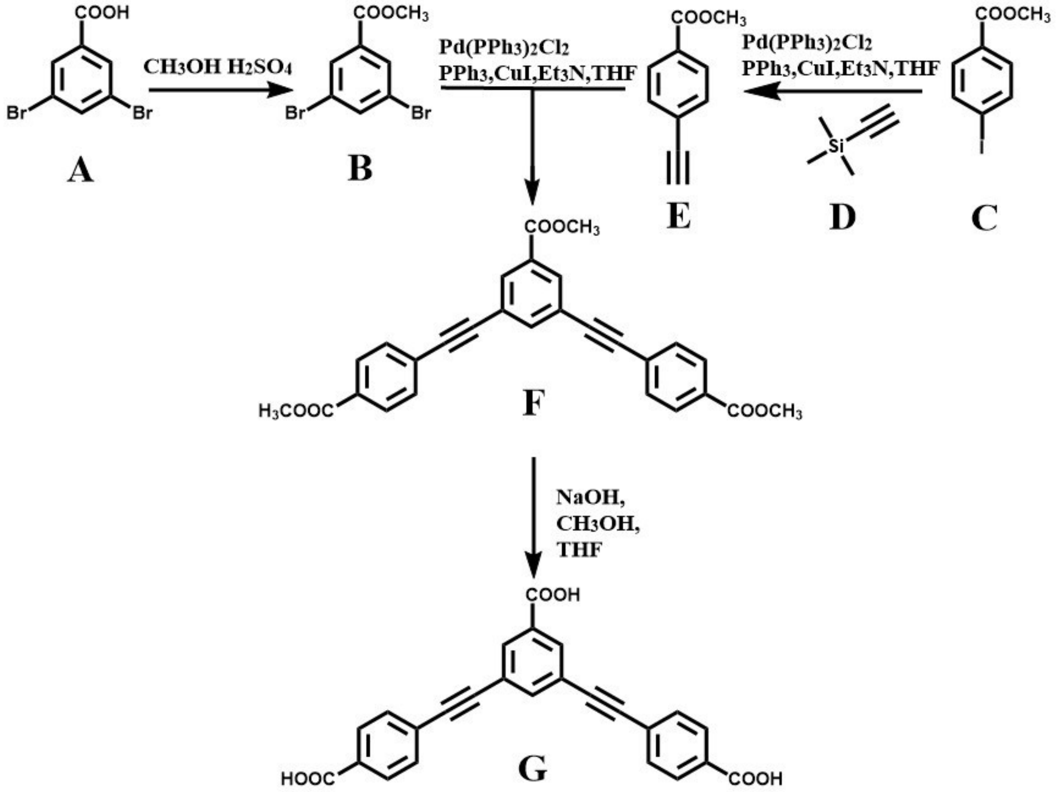
where q_i^{mix} is the adsorbed amount of component i (mmol g^{-1}), and q_T is the total adsorbed amount (mmol g^{-1}).

The adsorption selectivities S_{ads} were calculated using eqn (10).

$$S_{ads} = \frac{q_1/q_2}{p_1/p_2} \quad (10)$$

In this study, IAST calculations were carried out assuming a C_2H_2/CH_4 binary mixed gas with a molar ratio of 50:50 at 273 K and 298 K and pressures up to 1 atm.

Synthesis of H_3L



Scheme. S1 Synthetic procedures of H_3**L** ligand.

(1) Methyl 3,5-dibromobenzoate (B)

3,5-dibromobenzoic acid (20.0 g, 0.072 mol), anhydrous methanol (250 ml), and concentrated sulfuric acid (10 ml) were added into a three-neck round-bottom flask. After the mixture was refluxed for 5 h by stirring, the excessive methanol was removed by air distillation. Then, the mixture was precipitated into a large amount of water and some saturated sodium carbonate solution was added. Then, the mixture was filtered and the resulting solid was collected and dried at 40 ℃ under vacuum for 48 h to constant weight. White sheet-shape crystal was obtained.

(2) Methyl 4-ethynylbenzoate (E)

The mixture of 4-iodobenzaldehyde (3.93 g, 15 mmol), $Pd(PPh_3)_2Cl_2$ (0.75 mmol, 572 mg), PPh_3 (1.5 mmol, 393 mg) and CuI (0.9 mmol, 173 mg) in freshly distilled Et_3N (30 mL) was added dropwise a solution of (trimethylsilyl)acetylene (30mmol, 4.2ml) in Et_3N (5 mL) at 90 ℃ under nitrogen atmosphere for 24 h. After the mixture was cooled to room temperature, the mixture was filtered and the solvent was removed under reduced pressure. Then methanol (30ml) and K_2CO_3 (3.0 g) were added at RT for 3h. Upon completion, methanol was removed under reduced pressure, and water was added to the residue, which was extracted with CH_2Cl_2. The organic phase was washed with saturated salt water and finally dried over $MgSO_4$. The CH_2Cl_2 was removed under reduced pressure and a purification by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate=10/1). 4-ethynylbenzoate (1.68 g, 70%). ^{1}H NMR (CDCl3): δ = 7.54 (d, 2H), 7.98 (d, 2H), 3.92 (s, 3H), 3.22 (s, 1H).

(3) Dimethyl 4,4'-((5-(methoxycarbonyl)-1,3-phenylene) bis (ethyne-2,1diyl)) dibenzoate (F)

B (1.17 g, 4.0 mmol), $Pd(PPh_3)_2Cl_2$ (0.38 g, 0.54 mmol), CuI (0.20 g, 1.12 mmol) and PPh_3 (0.29 g, 1.12 mmol) were placed in a 250 mL two-necked round bottom flask. The flask was degassed and refilled with nitrogen, which was repeated for three times, and degassed Et_3N (100 ml) was added. Then 30 ml THF containing E (1.54 g, 9.60 mmol) was added. The mixture was stirred under reflux for 48 h. After the mixture was cooled to room temperature, the solvent was removed and the residual powder was suspended in CH_2Cl_2/H_2O. The water phase was washed with CH_2Cl_2 three times. The mixed organic phases were dried with $MgSO_4$. After the solvent was removed, the crude product was purified by column chromatography with CH_2Cl_2 as the eluent (yield: 79%).^{1}H NMR (400 MHz, $CDCl_3$) 3.94(s, 6H), 3.96(d, 3H), 7.59(d, 4H), 7.88(s, 1H), 8.05(d, 4H), 8.15(s, 2H). Anal. Calcd. For $C_{28}H_{20}O_6$ (MW 452): C, 74.34; H, 4.42. Found: C, 74.52; H, 4.26.

(4) 4,4'-((5-carboxy-1,3-phenylene)bis(ethyne-2,1-diyl))dibenzoic acid (G)

F (0.75 g, 1.67 mmol) was dissolved in 30 ml MeOH, 30 ml 2 mol L^{-1} NaOH aqueous solution was added. The mixture was stirred at toom temperature overnight. The organic phase was removed, the aqueous phase was acidified with diluted hydrochloric acid (2 mol L^{-1}, 20ml) to give white precipitate, which was filtered and wased with water several times (yield: 95%). ^{1}H NMR (400 MHz, DMSO-d6) 7.75(d, 4H), 8.01(d, 4H), 8.05(s, 1H),8.12(s, 2H), 13.27(s, 3H). Anal. Calcd. For $C_{25}H_{14}O_6$ (MW 410): C, 73.17; H, 3.41. Found: C, 73.38; H, 3.35.

Synthesis of UPC-34 and UPC-35

$[Cu_3(L)_2(H_2O)_3]_2(DMF)_3(EtOH)_3(H_2O)$ (**UPC-34**)

UPC-34 was prepared by the solvothermal reaction. A mixture of H_3L (0.015 mmol, 6.0 mg) and $Cu(NO_3)_2 \cdot 2.5H_2O$ (0.15 mmol, 35.0 mg) was ultrasonically dissolved in a solution of DMF/EtOH/H_2O (3.0 mL, V:V:V=5:2:1) in 10 mL vial. The mixture was heated to 75 °C within 100 min and kept at 75 °C for 1440 min followed by cooled to 30℃ within 200 min. The blue crystals were acquired and washed with DMF and then dried in the air with a yield of 47% based on Cu. FT-IR (cm^{-1}): 3416m, 3071w, 2935w, 1606s, 1402s, 1261w, 1171m, 1012m, 862w, 776m, 740m, 699w, 590w, 482m. Anal. Calcd for $C_{62}H_{64}Cu_3O_{23}N_2$: C, 53.34; H, 4.62; N, 2.01. Found: C, 52.56; H, 4.54; N, 1.85.

$[Cu_3(L)_2(H_2O)_3]_2(DMF)_2(Diox)_3(H_2O)$ (**UPC-35**)

UPC-35 was prepared by the solvothermal reaction. A mixture of H_3L (0.015 mmol, 6.0 mg) and $Cu(NO_3)_2 \cdot 2.5H_2O$ (0.15 mmol, 35.0 mg) was ultrasonically dissolved in a solution of DMF/ Diox /H_2O (3.0 mL, V:V:V=5:2:1) in 10 mL vial. The mixture was heated to 75 °C within 100 min and kept at 75 °C for 1440 min followed by cooled to 30℃ within 200 min. The blue crystals were acquired and washed with DMF and then dried in the air with a yield of 58% based on Cu. FT-IR (cm^{-1}): 3416m, 3071w, 2935w, 1606s, 1402s, 1261w, 1171m, 1012m, 862w, 776m, 740m, 699w, 590w, 482m. Anal. Calcd for $C_{64}H_{60}Cu_3O_{25}N_2$: C, 53.09; H, 4.17; N, 1.93. Found: C, 52.78; H, 4.24; N, 1.13.

Activation of **UPC-34** and **UPC-35**

The as-synthesized crystals of **UPC-34** and **UPC-35** were solvent exchanged three times with dry acetone, then the samples were degassed at 298 K for one night and at 353 K for 12 hours with the outgas rate of 5 mm $Hg \cdot min^{-1}$ to produce the activated samples for the gas adsorption measurements.

Table S1 Crystal data and structure refinement for **UPC-34** and **UPC-35**

Compound	UPC-34	UPC-35
CCDC	1835837	1835836
Formula	$C_{50}H_{26}Cu_3O_{15}$	$C_{50}H_{22}Cu_3O_{15}$
Formula weight	1057.33	1053.29
Temperature/K	150	150
Crystal system	tetragonal	tetragonal
Space group	I4/mcm	I4/m
a/Å	31.3382(11)	31.038(2)
b/Å	31.3382(11)	31.038(2)
c/Å	31.3382(11)	20.6449(18)
α/°	90	90
β/°	90	90
γ/°	90	90
Volume/$Å^3$	38378(3)	19888(3)
Z	8	8
ρ g/cm^3	0.366	0.704
μ/mm^{-1}	0.531	1.025
F(000)	4264.0	4232.0
2Θ range for data collection	7.232 to 134.118	7.674 to 134.152
Index ranges	$-28 \leq h \leq 37$, $-33 \leq k \leq 21$, $-46 \leq l \leq 18$	$-37 \leq h \leq 13$, $-27 \leq k \leq 31$, $-24 \leq l \leq 20$
Reflections collected	34407	18347
Independent reflections	8965 [Rint = 0.0848, Rsigma = 0.1119]	9114 [R_{int}= 0.0863, R_{sigma}= 0.2720]
Data/restraints/parameters	8965/0/166	9114/0/314
Goodness-of-fit on F^2	0.731	0.865
Final R indexes [I>=2σ (I)]	$R_1 = 0.0640$, $wR_2 = 0.1436$	R_1= 0.1103, wR_2= 0.3025
Final R indexes [all data]	$R_1 = 0.1478$, $wR_2 = 0.1698$	R_1= 0.2211, wR_2= 0.3261
Largest diff. peak/hole / e $Å^{-3}$	0.37/-0.32	1.84/-0.32

Table S2. Selected bond lengths (Å) for **UPC-34.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	$O3^1$	1.975(7)	Cu2	$O2^6$	1.967(7)
Cu1	$O3^2$	1.975(7)	Cu2	$O2^7$	1.967(7)
Cu1	O3	1.975(7)	Cu3	O4	1.946(7)
Cu1	$O3^3$	1.975(7)	Cu3	$O4^1$	1.946(7)
Cu1	O5	2.174(17)	Cu3	$O4^2$	1.946(7)
Cu2	O1	2.137(13)	Cu3	$O4^3$	1.946(7)
Cu2	$O2^5$	1.967(7)	Cu3	O6	2.132(19)
Cu2	O2	1.966(7)			

Table S3. Selected bond angles (°) for **UPC-34.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O3^3$	Cu1	O3	90.3(4)	O2	Cu2	O1	96.8(2)
$O3^2$	Cu1	O3	169.1(6)	O2	Cu2	$O2^5$	89.19(5)
$O3^1$	Cu1	O3	88.7(4)	O2	Cu2	$O2^6$	166.3(4)
$O3^1$	Cu1	$O3^2$	90.3(4)	O4	Cu3	$O4^1$	88.1(5)
$O3^1$	Cu1	$O3^3$	169.1(6)	$O4^1$	Cu3	$O4^3$	169.2(6)
$O3^3$	Cu1	$O3^2$	88.7(4)	$O4^1$	Cu3	$O4^2$	90.9(5)
O3	Cu1	O5	95.5(3)	O4	Cu3	O6	95.4(3)

Table S4. Selected bond lengths (Å) for **UPC-35.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	2.115(10)	Cu2	O5^{4}	2.037(9)
Cu1	O2^{1}	1.988(8)	Cu2	O8	2.116(14)
Cu1	O2	1.988(8)	Cu3	O6	1.912(9)
Cu1	O4	1.970(9)	Cu3	O6^{1}	1.912(9)
Cu1	O4^{1}	1.970(9)	Cu3	O7^{1}	2.027(11)
Cu2	O3^{3}	1.919(8)	Cu3	O7	2.027(11)
Cu2	O3	1.919(8)	Cu3	O12^{1}	2.117(15)
Cu2	O5^{2}	2.037(9)	Cu3	O12	2.117(15)

Table S5. Selected bond angles (º) for **UPC-35.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2^{1}	Cu1	O1	97.2(3)	O5^{4}	Cu2	O5^{3}	160.9(6)
O2^{1}	Cu1	O2	87.2(4)	O5^{4}	Cu2	O8	99.5(3)
O4^{1}	Cu1	O1	97.5(4)	O6^{1}	Cu3	O6	90.0(5)
O4^{1}	Cu1	O2	165.3(4)	O6^{1}	Cu3	O7	168.1(5)
O4^{1}	Cu1	O2^{1}	91.2(3)	O6^{1}	Cu3	O7^{1}	89.1(4)
O4^{1}	Cu1	O4	86.6(5)	O6	Cu3	O7^{1}	168.1(5)
O3	Cu2	O3^{2}	174.2(6)	O6	Cu3	O12	84.6(9)
O3	Cu2	O5^{3}	88.9(4)	O6^{1}	Cu3	O12	100.5(10)
O3	Cu2	O5^{4}	90.2(4)	O7^{1}	Cu3	O7	89.3(6)
O3	Cu2	O8	92.9(3)	O7	Cu3	O12	91.2(10)
O3^{2}	Cu2	O8	92.9(3)	O7^{1}	Cu3	O12	107.2(9)

Table S6. Single component gas adsorption Data for **UPC-35.**

Gas	T [K]	Vads [$cm^3 \cdot g^{-1}$]	Amount [$mmol \cdot g^{-1}$]	[wt%]	Qst [$KJ \cdot mol^{-1}$]
CH_4	273	11.0	0.49	0.79	18.5
	298	4.8	0.21	0.34	
C_2H_2	273	72.5	3.24	8.42	22.7
	298	44.4	1.98	5.15	
C_2H_4	273	56.4	2.52	7.05	18.4
	298	35.9	1.60	4.49	
C_2H_6	273	70.1	3.13	9.39	22.7
	298	40.9	1.83	5.48	
C_3H_6	273	138.1	6.17	25.89	24.5
	298	118.3	5.28	22.18	
C_3H_8	273	128.6	5.74	25.26	29.9
	298	111.3	4.97	21.86	

Table S7. Adsorption selectivity of hydrocarbon at 1 bar for different molar fraction of binary mixtures.

Binary gas mixtures	Molar fraction	Selectivity(273K)	Selectivity(298K)
C_2H_2/CH_4	50:50	12.12	13.16
	10:90	12.33	12.99
C_2H_4/CH_4	50:50	8.56	10.39
	10:90	8.68	10.07
C_2H_6/CH_4	50:50	11.22	11.56
	10:90	10.98	11.18
C_3H_6/CH_4	50:50	121.61	86.96
	10:90	56.68	61.76
C_3H_8/CH_4	50:50	159.51	87.67
	10:90	74.04	53.79
C_3H_6/C_2H_2	50:50	4.79	4.93
	10:90	5.23	5.13
C_3H_6/C_2H_4	50:50	7.53	6.95
	10:90	7.29	6.44
C_3H_6/C_2H_6	50:50	5.29	5.56
	10:90	5.56	5.71
C_3H_8/C_2H_2	50:50	5.40	4.96
	10:90	6.36	5.04
C_3H_8/C_2H_4	50:50	8.72	6.99
	10:90	9.01	6.25
C_3H_8/C_2H_6	50:50	6.03	5.59
	10:90	6.78	5.59

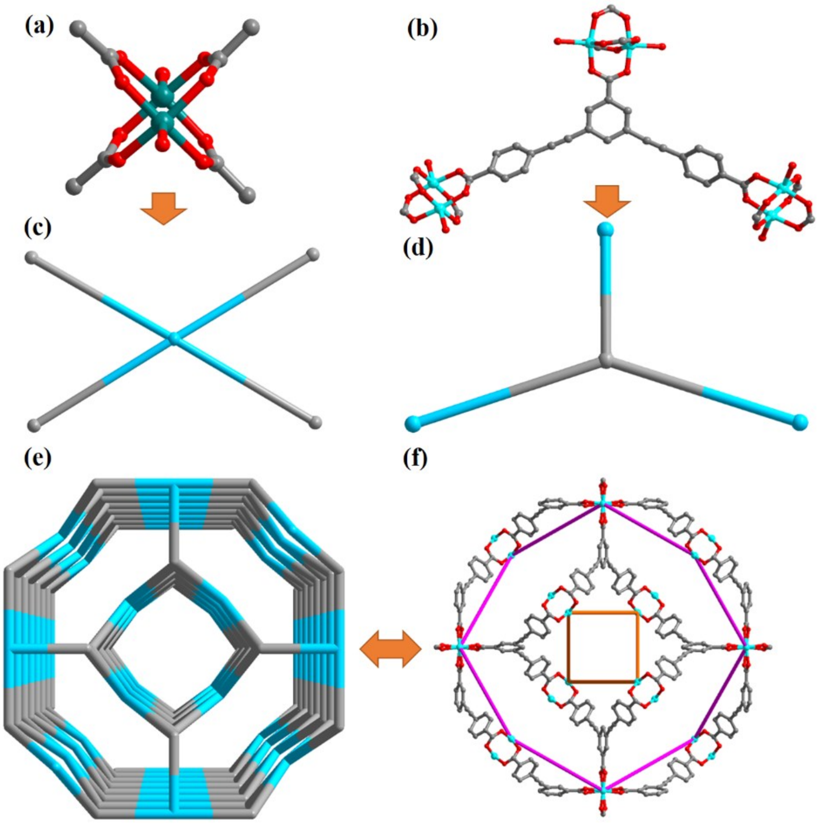


Fig. S1 (a) The Secondary Building Unit ($Cu_2(COO)_4$ SBU) of **UPC-34**; (b) The coordination modes of **L**$^{3-}$; (c) and (c) Simplified $Cu_2(COO)_4$ SBU and **L**$^{3-}$; (e) Topological structures of **UPC-34**; (f) Schematic representation of a simplified 3D network of **UPC-34.**

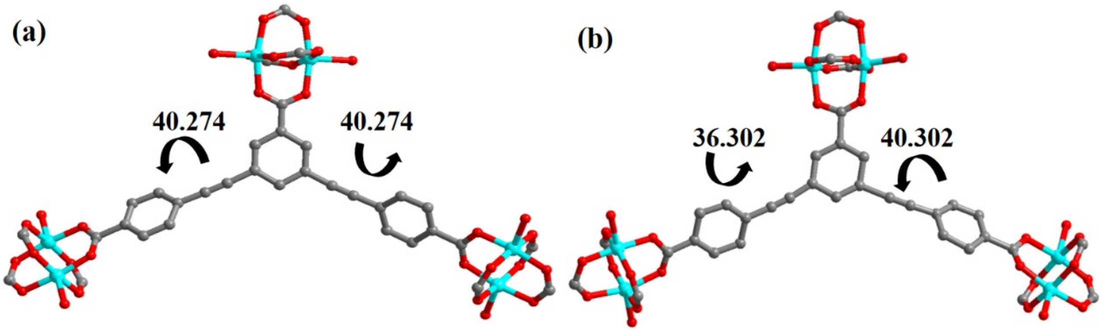


Fig. S2 (a) The dihedral angles of H_3L in **UPC-34**; (b) The dihedral angles of H_3L in **UPC-35.**

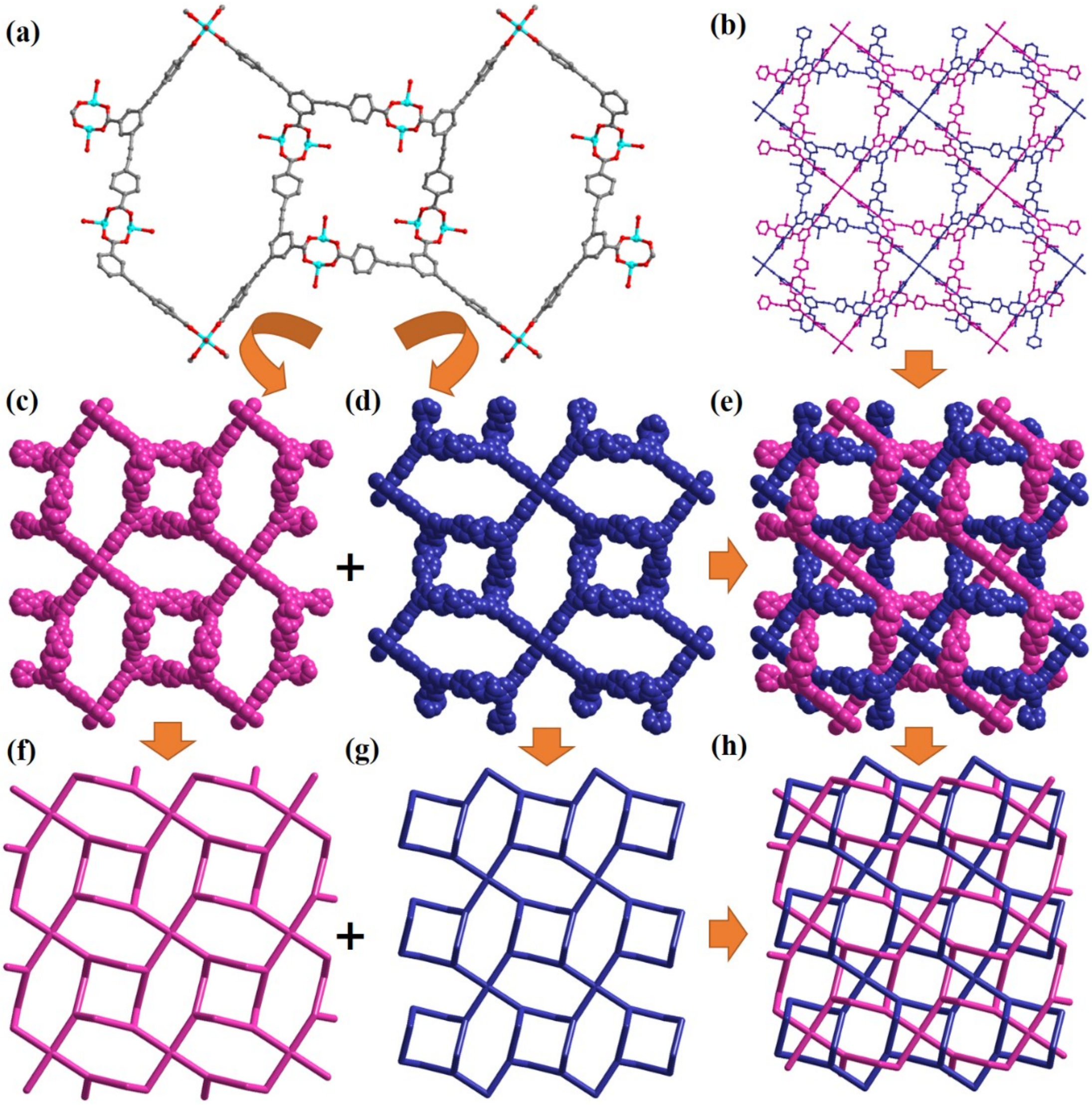


Fig. S3 Schematic representation of a simplified 3D network of **UPC-35**; (a), (c) and (d) Single interpenetrated network; (b) and (e) 2-fold interpenetrating framework of **UPC-35;** (f) and (g) Simplified single interpenetrated network; (h) Topological structures of **UPC-35**.

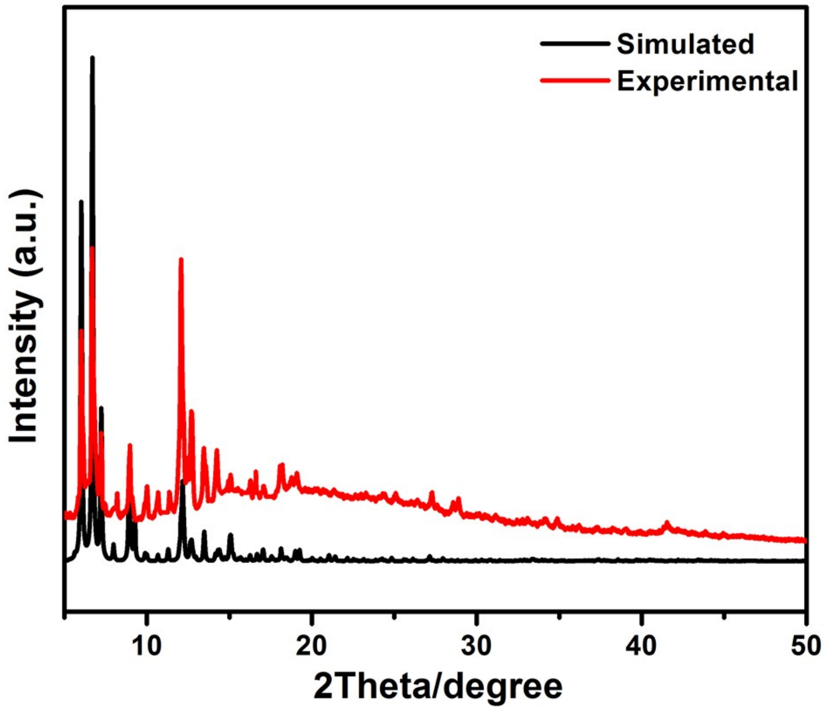


Fig. S4 The XRD pattern of complex **UPC-34.**

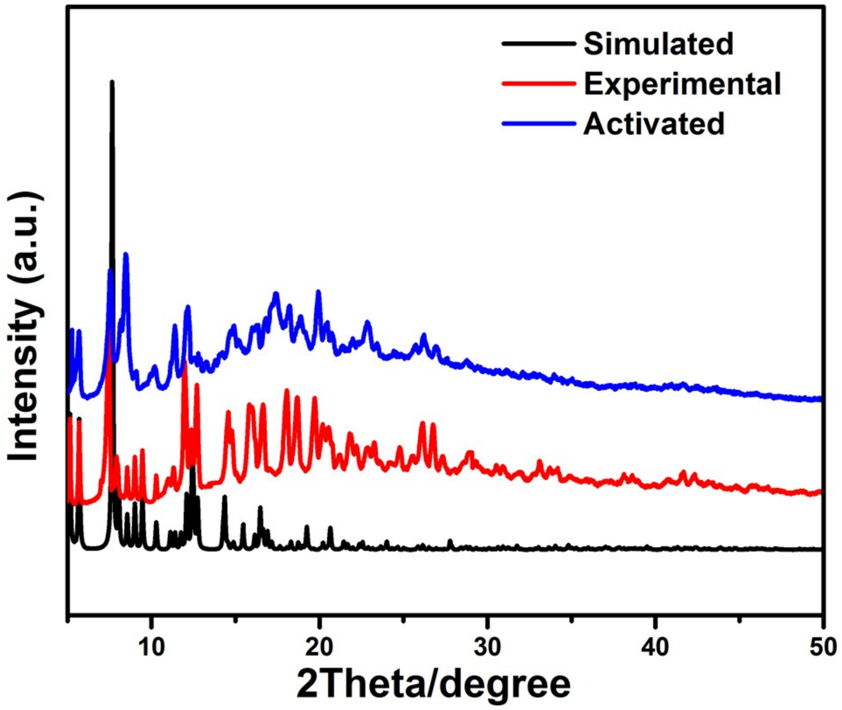


Fig. S5 The XRD pattern of complex **UPC-35.**

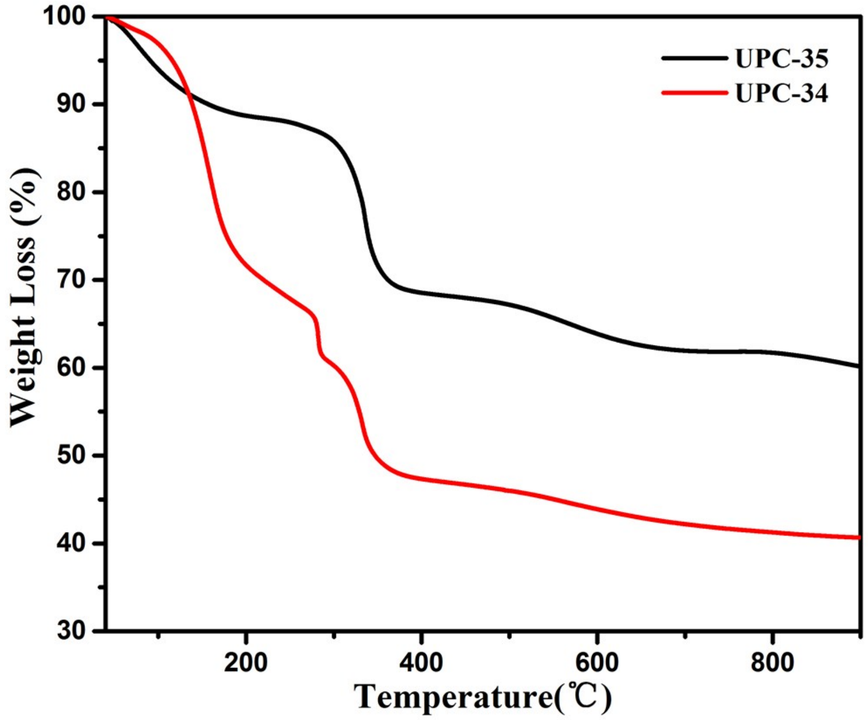


Fig. S6 The TGA curves of **UPC-34** and **UPC-35.**

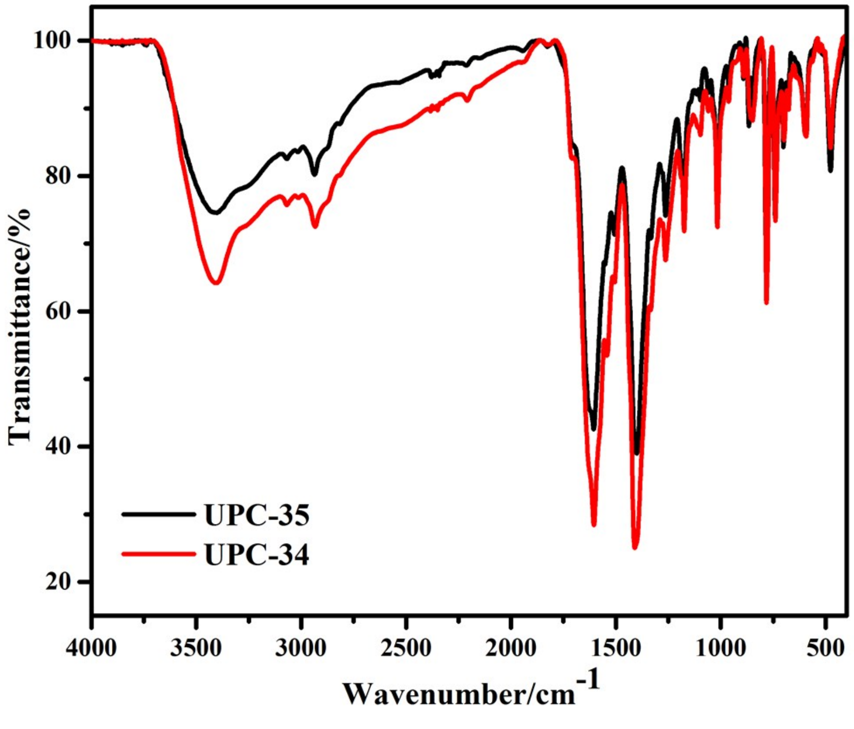
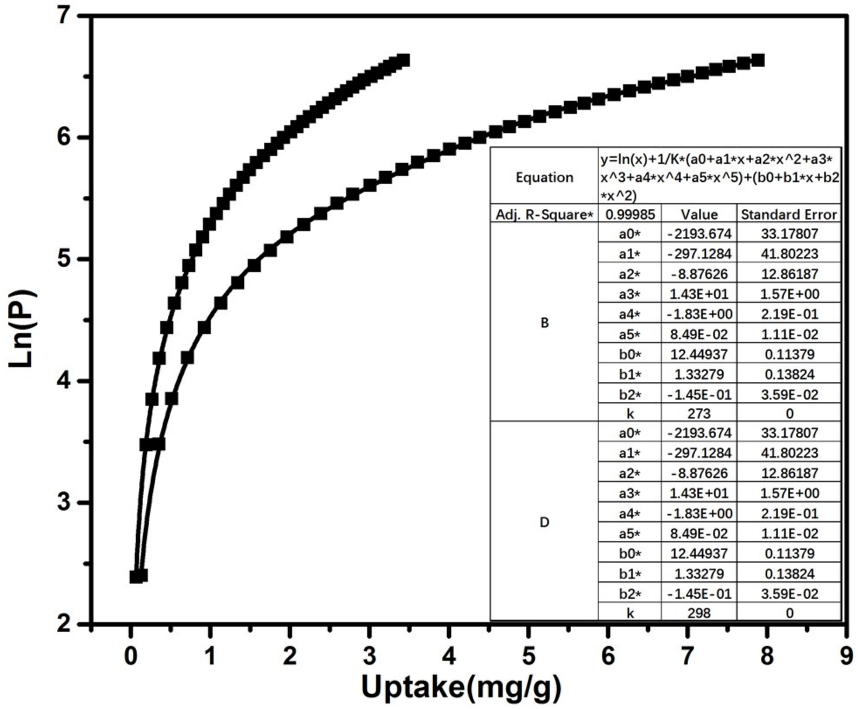
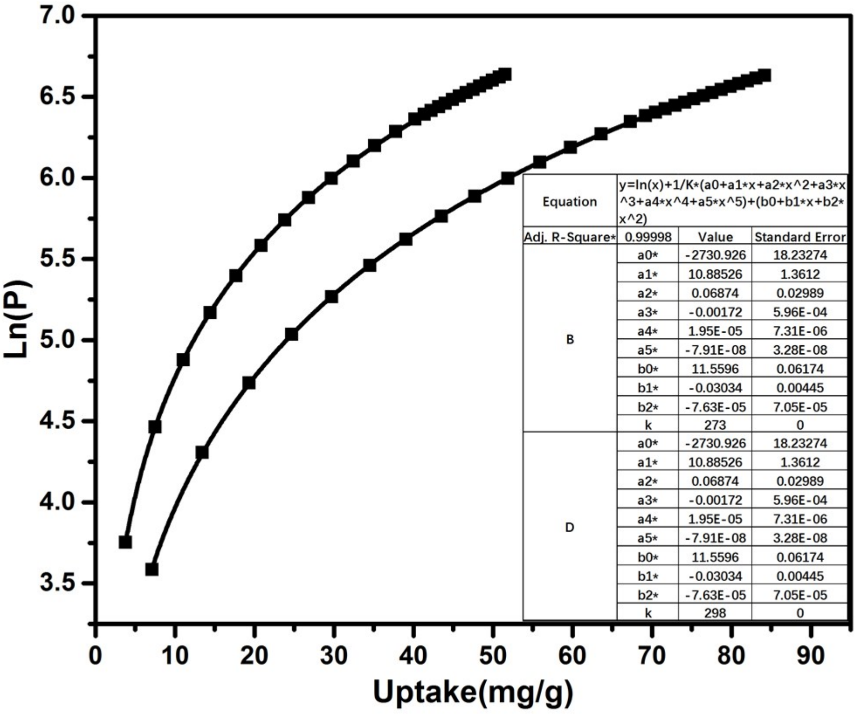


Fig. S7 The IR of **UPC-34** and **UPC-35.**



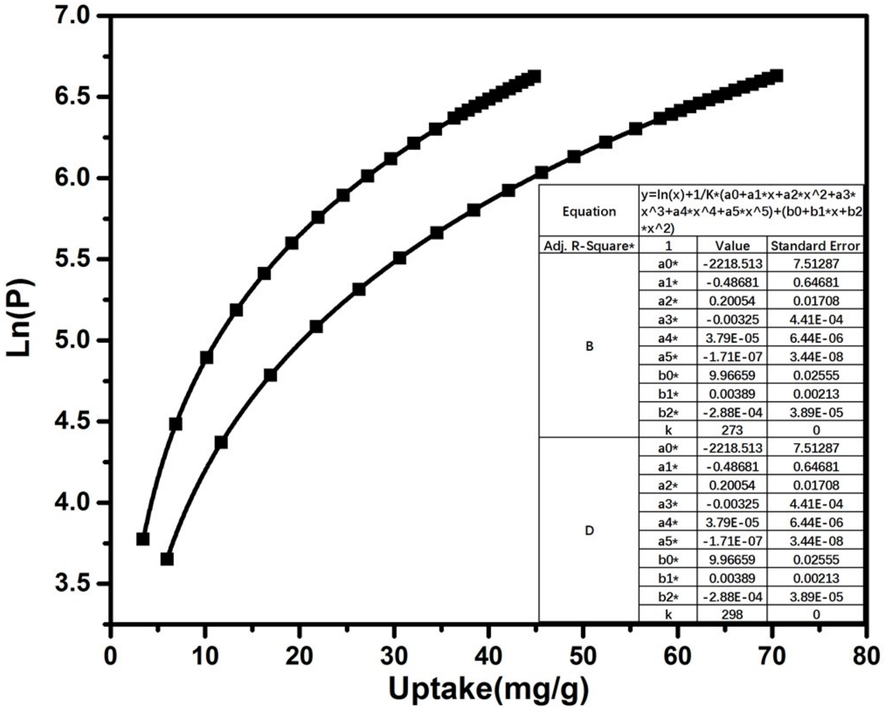
Equation	y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4+a5*x^5)+(b0+b1*x+b2*x^2)		
Adj. R-Square*	0.99985	Value	Standard Error
B	a0*	-2193.674	33.17807
	a1*	-297.1284	41.80223
	a2*	-8.87626	12.86187
	a3*	1.43E+01	1.57E+00
	a4*	-1.83E+00	2.19E-01
	a5*	8.49E-02	1.11E-02
	b0*	12.44937	0.11379
	b1*	1.33279	0.13824
	b2*	-1.45E-01	3.59E-02
	k	273	0
D	a0*	-2193.674	33.17807
	a1*	-297.1284	41.80223
	a2*	-8.87626	12.86187
	a3*	1.43E+01	1.57E+00
	a4*	-1.83E+00	2.19E-01
	a5*	8.49E-02	1.11E-02
	b0*	12.44937	0.11379
	b1*	1.33279	0.13824
	b2*	-1.45E-01	3.59E-02
	k	298	0

Figure S14. The parameters and optimized adsorption isotherms for calculated Q_{st} of CH_4 using a variant of the Clausius-Clapeyron equation.



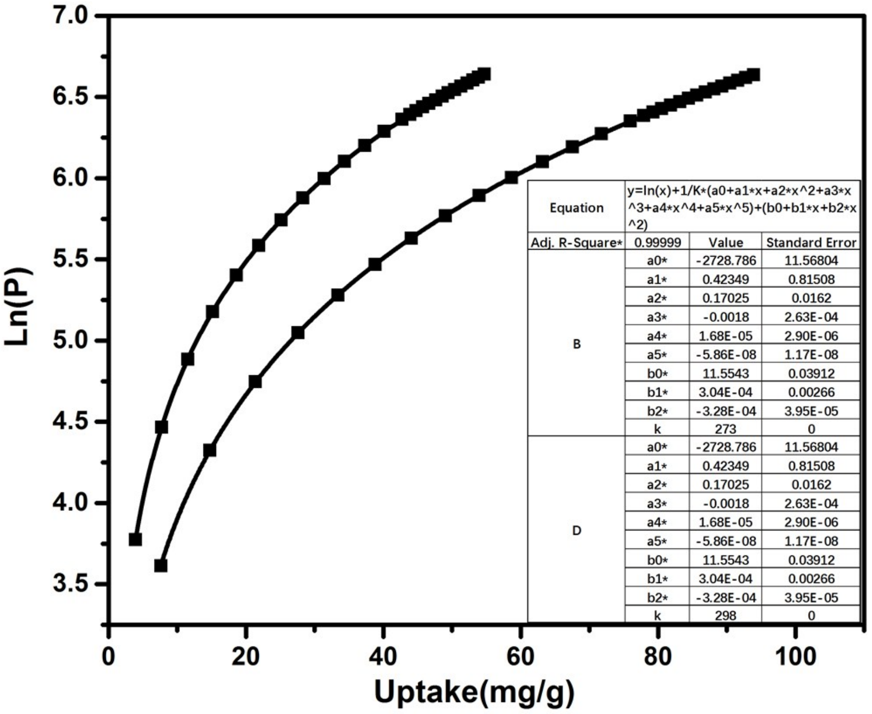
Equation	y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4+a5*x^5)+(b0+b1*x+b2*x^2)		
Adj. R-Square*	0.99998	Value	Standard Error
B	a0*	-2730.926	18.23274
	a1*	10.88526	1.3612
	a2*	0.06874	0.02989
	a3*	-0.00172	5.96E-04
	a4*	1.95E-05	7.31E-06
	a5*	-7.91E-08	3.28E-08
	b0*	11.5596	0.06174
	b1*	-0.03034	0.00445
	b2*	-7.63E-05	7.05E-05
	k	273	0
D	a0*	-2730.926	18.23274
	a1*	10.88526	1.3612
	a2*	0.06874	0.02989
	a3*	-0.00172	5.96E-04
	a4*	1.95E-05	7.31E-06
	a5*	-7.91E-08	3.28E-08
	b0*	11.5596	0.06174
	b1*	-0.03034	0.00445
	b2*	-7.63E-05	7.05E-05
	k	298	0

Figure S15. The parameters and optimized adsorption isotherms for calculated Q_{st} of C_2H_2 using a variant of the Clausius-Clapeyron equation.



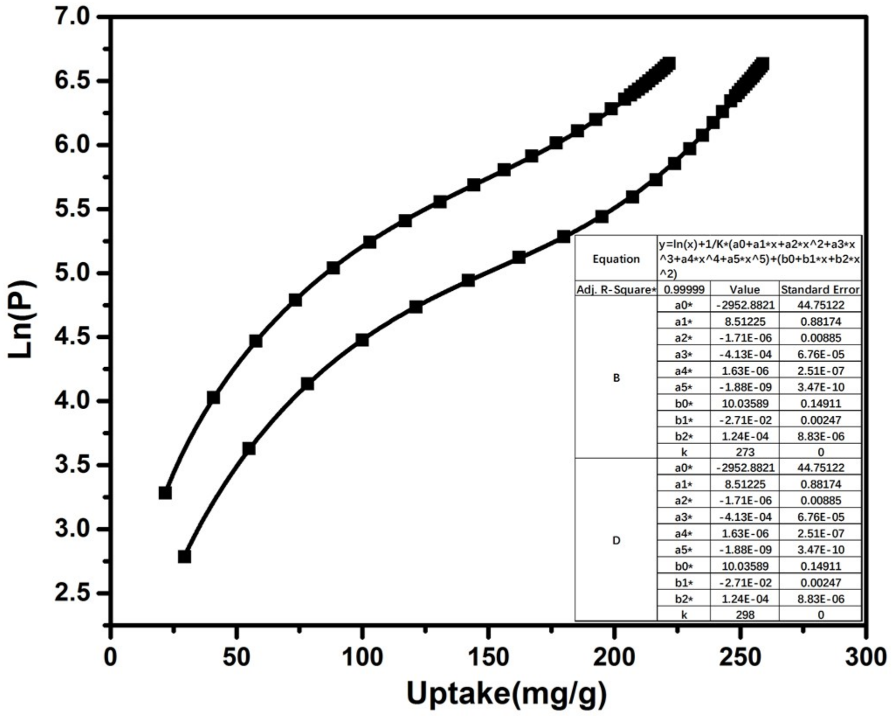
Equation	y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4+a5*x^5)+(b0+b1*x+b2*x^2)		
Adj. R-Square*	1	Value	Standard Error
B	a0*	-2218.513	7.51287
	a1*	-0.48681	0.64681
	a2*	0.20054	0.01708
	a3*	-0.00325	4.41E-04
	a4*	3.79E-05	6.44E-06
	a5*	-1.71E-07	3.44E-08
	b0*	9.96659	0.02555
	b1*	0.00389	0.00213
	b2*	-2.88E-04	3.89E-05
	k	273	0
D	a0*	-2218.513	7.51287
	a1*	-0.48681	0.64681
	a2*	0.20054	0.01708
	a3*	-0.00325	4.41E-04
	a4*	3.79E-05	6.44E-06
	a5*	-1.71E-07	3.44E-08
	b0*	9.96659	0.02555
	b1*	0.00389	0.00213
	b2*	-2.88E-04	3.89E-05
	k	298	0

Figure S16. The parameters and optimized adsorption isotherms for calculated Q_{st} of C_2H_4 using a variant of the Clausius-Clapeyron equation.



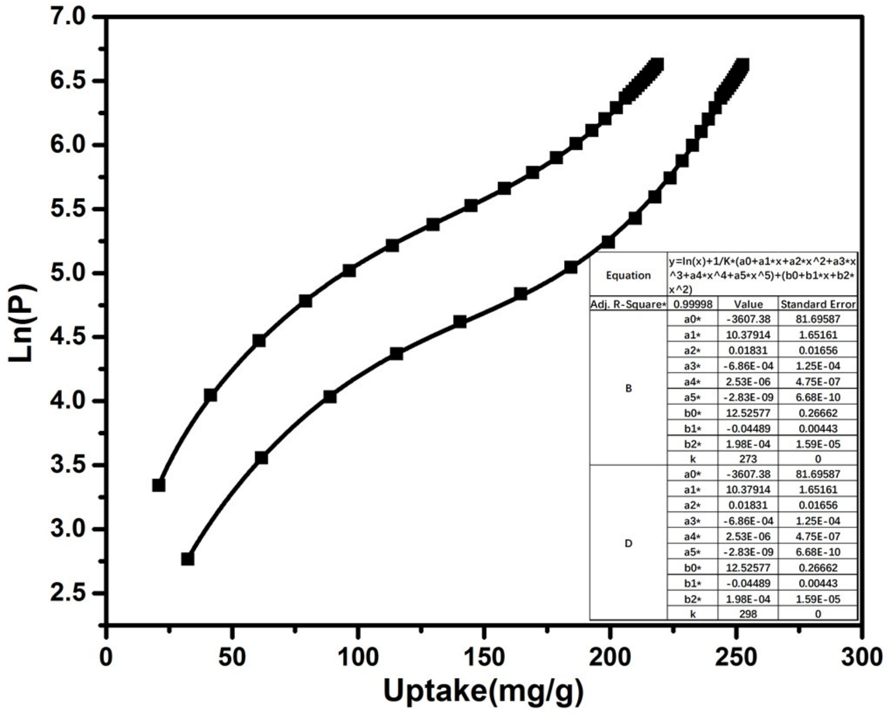
Equation	y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4+a5*x^5)+(b0+b1*x+b2*x^2)		
Adj. R-Square*	0.99999	Value	Standard Error
B	a0*	-2728.786	11.56804
	a1*	0.42349	0.81508
	a2*	0.17025	0.0162
	a3*	-0.0018	2.63E-04
	a4*	1.68E-05	2.90E-06
	a5*	-5.86E-08	1.17E-08
	b0*	11.5543	0.03912
	b1*	3.04E-04	0.00266
	b2*	-3.28E-04	3.95E-05
	k	273	0
D	a0*	-2728.786	11.56804
	a1*	0.42349	0.81508
	a2*	0.17025	0.0162
	a3*	-0.0018	2.63E-04
	a4*	1.68E-05	2.90E-06
	a5*	-5.86E-08	1.17E-08
	b0*	11.5543	0.03912
	b1*	3.04E-04	0.00266
	b2*	-3.28E-04	3.95E-05
	k	298	0

Figure S17. The parameters and optimized adsorption isotherms for calculated Q_{st} of C_2H_6 using a variant of the Clausius-Clapeyron equation.



Equation	y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4+a5*x^5)+(b0+b1*x+b2*x^2)		
Adj. R-Square*	0.99999	Value	Standard Error
B	a0*	-2952.8821	44.75122
	a1*	8.51225	0.88174
	a2*	-1.71E-06	0.00885
	a3*	-4.13E-04	6.76E-05
	a4*	1.63E-06	2.51E-07
	a5*	-1.88E-09	3.47E-10
	b0*	10.03589	0.14911
	b1*	-2.71E-02	0.00247
	b2*	1.24E-04	8.83E-06
	k	273	0
D	a0*	-2952.8821	44.75122
	a1*	8.51225	0.88174
	a2*	-1.71E-06	0.00885
	a3*	-4.13E-04	6.76E-05
	a4*	1.63E-06	2.51E-07
	a5*	-1.88E-09	3.47E-10
	b0*	10.03589	0.14911
	b1*	-2.71E-02	0.00247
	b2*	1.24E-04	8.83E-06
	k	298	0

Figure S18. The parameters and optimized adsorption isotherms for calculated Q_{st} of C_3H_6 using a variant of the Clausius-Clapeyron equation.



Equation	y=ln(x)+1/K*(a0+a1*x+a2*x^2+a3*x^3+a4*x^4+a5*x^5)+(b0+b1*x+b2*x^2)		
Adj. R-Square*	0.99998	Value	Standard Error
B	a0*	-3607.38	81.69587
	a1*	10.37914	1.65161
	a2*	0.01831	0.01656
	a3*	-6.86E-04	1.25E-04
	a4*	2.53E-06	4.75E-07
	a5*	-2.83E-09	6.68E-10
	b0*	12.52577	0.26662
	b1*	-0.04489	0.00443
	b2*	1.98E-04	1.59E-05
	k	273	0
D	a0*	-3607.38	81.69587
	a1*	10.37914	1.65161
	a2*	0.01831	0.01656
	a3*	-6.86E-04	1.25E-04
	a4*	2.53E-06	4.75E-07
	a5*	-2.83E-09	6.68E-10
	b0*	12.52577	0.26662
	b1*	-0.04489	0.00443
	b2*	1.98E-04	1.59E-05
	k	298	0

Figure S19. The parameters and optimized adsorption isotherms for calculated Q_{st} of C_3H_8 using a variant of the Clausius-Clapeyron equation.