Electronic Supplementary Information (ESI)

Construction of Indium-Organic Frameworks with *flu*-Topology for Efficient Acetylene Separation

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Table S1. The crystal data and structure refinements for compound SNNU-400.

Compound	SNNU-400
CCDC number	2445424
Empirical formula	$C_{42}H_{30}In_3O_{18}P_2$
Formula weight	1229.06
Temperature/K	153(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.407(2)
b/Å	13.1276(18)
c/Å	20.156(3)
α/°	90
β/°	109.181(4)
γ/°	90
Volume/Å^3	3850.5(9)
Z	2
ρ_{calc}g/cm^3	1.060
μ/mm^{-1}	7.896
F(000)	1206.0
Crystal size/mm^3	0.270 × 0.250 × 0.230
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.074 to 137.148
Index ranges	-18 ≤ h ≤ 18, -15 ≤ k ≤ 15, -24 ≤ l ≤ 24
Reflections collected	21092
Independent reflections	6764 [R_{int} = 0.0623, R_{sigma} = 0.0558]
Data/restraints/parameters	6764/72/313
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0627, wR_2 = 0.1689
Final R indexes [all data]	R_1 = 0.0689, wR_2 = 0.1789

Table S2. The selected bond length (Å) for SNNU-400.

Atom-Atom	Length/Å	Atom-Atom	Length/Å
In1-O9	2.079(4)	In2-O1^3	2.155(4)
In1- O2	2.186(4)	In2-O5^4	2.178(4)
In1- O4	2.184(4)	In2-O7	2.110(5)
In2-O9	2.094(4)	In2-O3^6	2.122(4)
In2-O8	2.157(5)		

^{1}-X,1-Y,1-Z; ^{2}1-X,-1/2+Y,3/2-Z; ^{3}-1+X,3/2-Y,-1/2+Z; ^{4}1-X,1/2+Y,3/2-Z; ^{5}-1+X,1/2-Y,-1/2+Z; ^{6}1-X,1-Y,1-Z

Table S3. The selected bond angles (°) for SNNU-400.

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O9[1]- In1-O9	180.0	O1[3]-In2-O3[6]	85.24(16)
O2[2]- In1-O9	89.95(15)	O5[5]-In2-O9	91.65(16)
O2[3]- In1-O9	94.05(15)	O5[5]-In2-O3[6]	171.93(17)
O6[1]- In1-C8[2]	86.66(8)	O5[5]-In2-O1[3]	88.18(18)
O9[1]-In1-O9	180.0	O7-In2-O9	96.72(18)
O2[2]-In1-O2[3]	180.0	O7-In2-O3[6]	93.39(18)
O4[4]-In1-O9[1]	91.10(16)	O7-In2-O13	175.37(18)
O4[5]-In1-O9[1]	88.90(16)	O7-In2-O5[5]	92.82(19)
O4[4]-In1-O2[2]	91.64(17)	O8-In2-O9	174.0(2
O4[4]-In1-O2[3]	88.36(17)	O8-In2-O3[6]	90.04(18)
O4[4]-In1-O4[5]	180.0	O8-In2-O1[3]	87.2(2)
O3[6]-In2-O9	92.74(16)	O8-In2-O5[5]	84.98(18)
O1[3]-In2-O9	87.76(18)	O8-In2-O7	88.4(2)

[1]-X,1-Y,1-Z; [2]1-X,-1/2+Y,3/2-Z; [3]-1+X,3/2-Y,-1/2+Z; [4]-1+X,1/2-Y,-1/2+Z; [5]1-X,1/2+Y,3/2-Z; [6]1-X,1-Y,1-Z; [7]1+X,3/2-Y,1/2+Z

Calculation of ideal adsorption solution theory (IAST)

Langmuir–Freundlich (LF)：

$$q = q_m * \frac{b * p^{1/n}}{1 + b * p^{1/n}} \quad \text{.....Eq1}$$

Where p is the pressure when the volume gas is in equilibrium with the adsorption phase (kPa), q is the adsorption capacity per unit mass of the adsorbent (mmol g^{-1}), q_m is the saturation capacity of the site (mmol g^{-1}), b is the affinity coefficient of the site (1/kPa), and n represents the deviation from the ideal homogeneous surface.

Separation ratio calculation：

$$S_{A/B} = \frac{x_A / y_A}{x_B / y_B} \quad \text{.....Eq2}$$

Where *x*i and *y*i are the molar fractions of components i (i = A and B) in the adsorption phase and bulk phase, respectively. Note that in the Henry system, $S_{A/B}$ is the same ratio as the Henry constant for both species.

Isosteric heat of adsorption calculations

To calculate heats of adsorptions, the corresponding adsorption isotherms at different temperatures were simultaneously fitted using the virial type:

$$ln\, P = ln\, N + \frac{1}{T}\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \quad \text{.....Eq3}$$

$$Q_{st} = -R\sum_{i=0}^{m} a_i N^i \quad \text{.....Eq4}$$

In this equation, P represents pressure, N denotes the adsorption amount, T signifies temperature, and m together with N establishes the number of terms required to sufficiently characterize the isotherm.

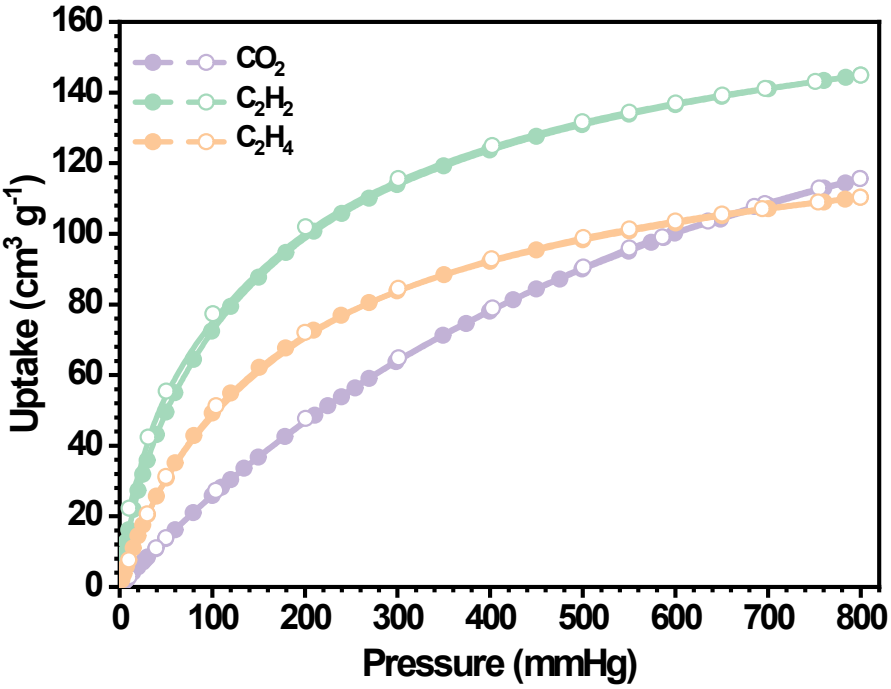

Fig. S1 The gas adsorption curves at 273 K

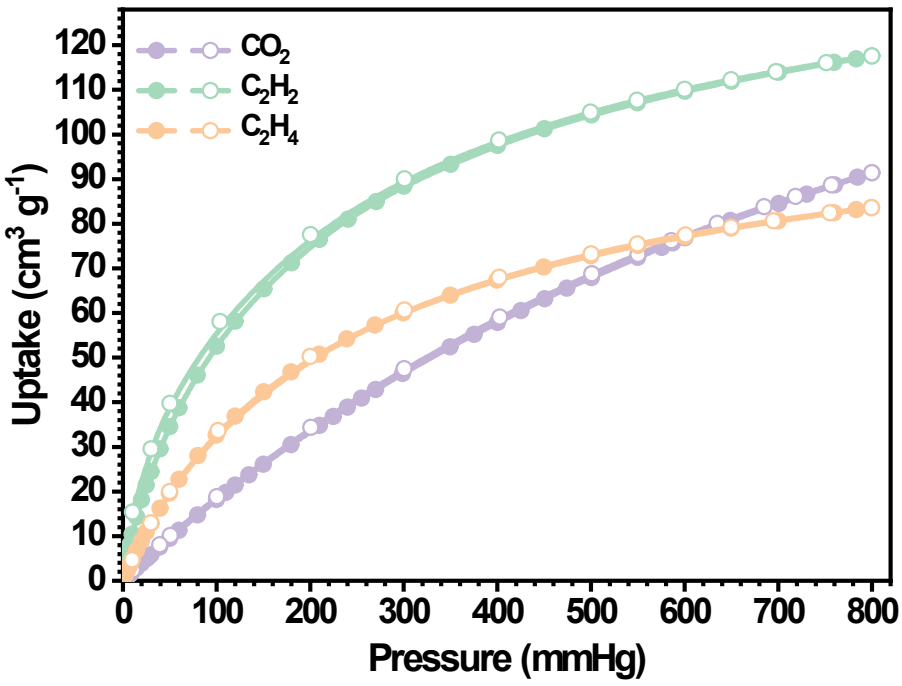

Fig. S2 The gas adsorption curves at 283 K

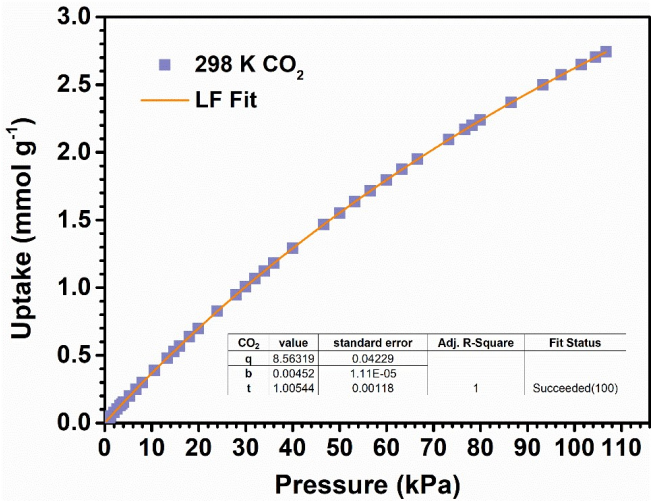

Fig. S3 LF fitting parameters for CO_2 adsorption by SNNU-400 at 298 K.

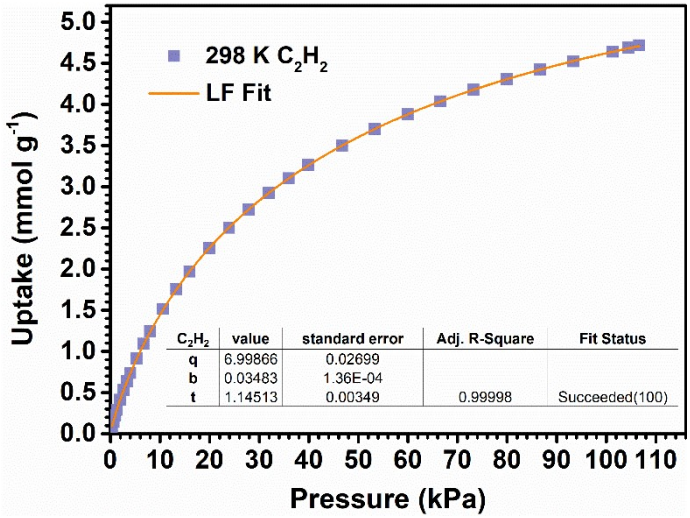

Fig. S4 LF fitting parameters for C_2H_2 adsorption by SNNU-400 at 298 K.

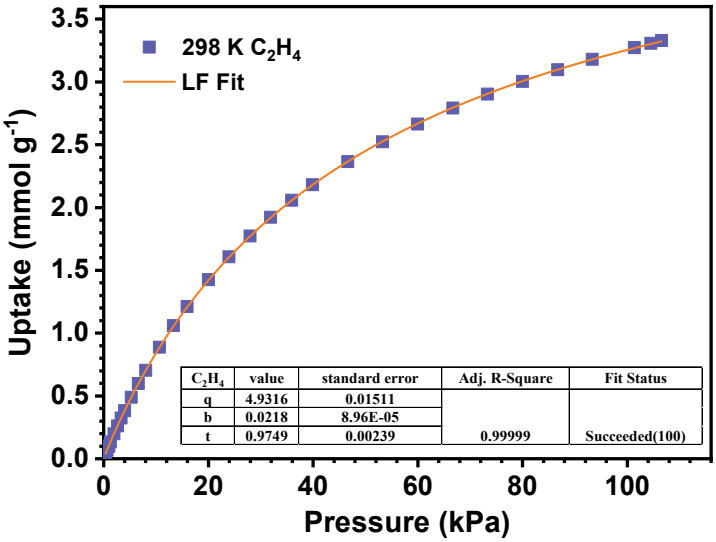

Fig. S5 LF fitting parameters for C_2H_4 adsorption by SNNU-400 at 298 K.

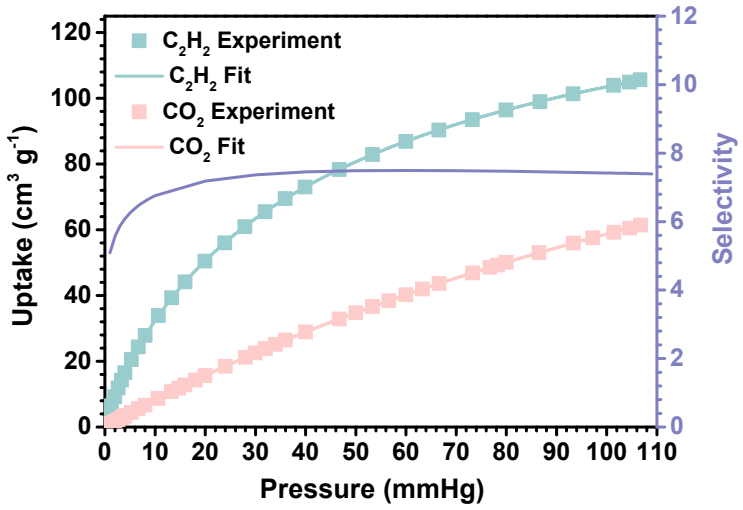

Fig. S6 The gas uptakes-selectivity for C_2H_2 and CO_2 at 298 K.

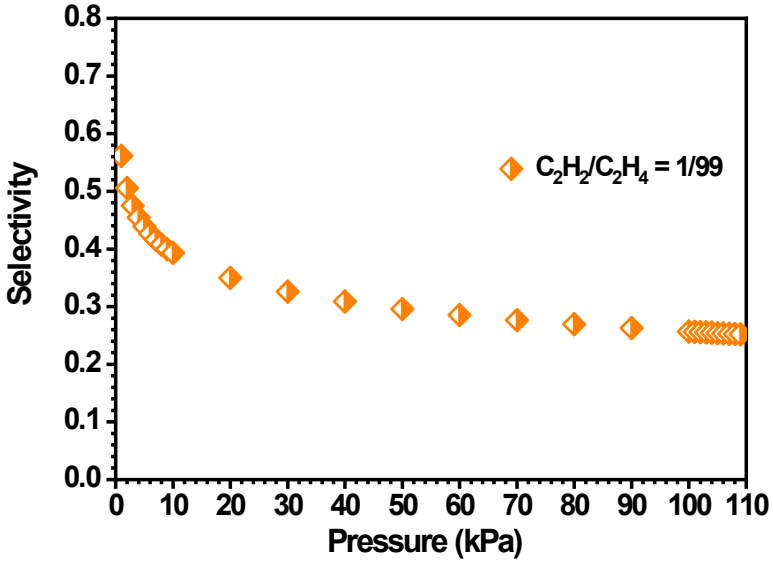

Fig. S7 The selectivity ratio of SNNU-400 for C_2H_2/C_2H_4 (1/99, v/v).

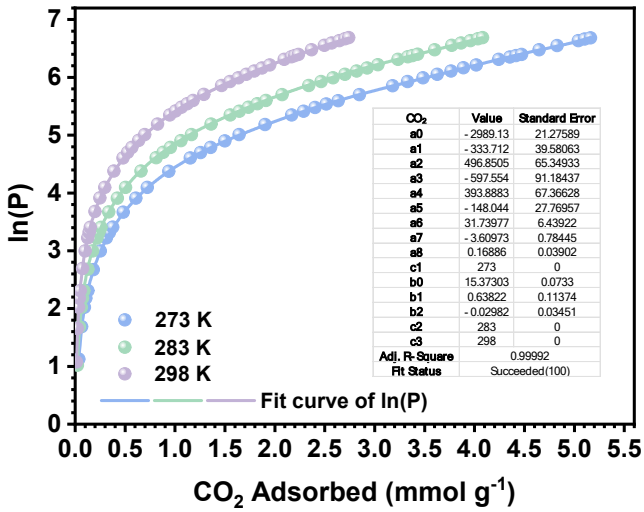

Fig. S8 The fitting parameters of CO_2 by the virial equation in SNNU-400.

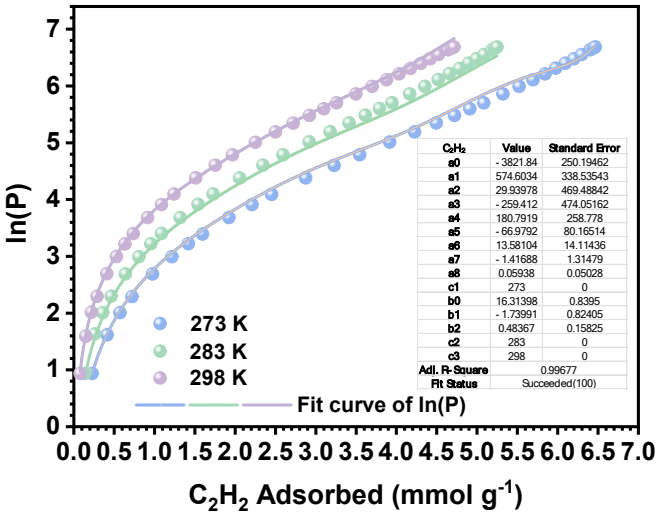

Fig. S9 The fitting parameters of C_2H_2 by the virial equation in SNNU-400.

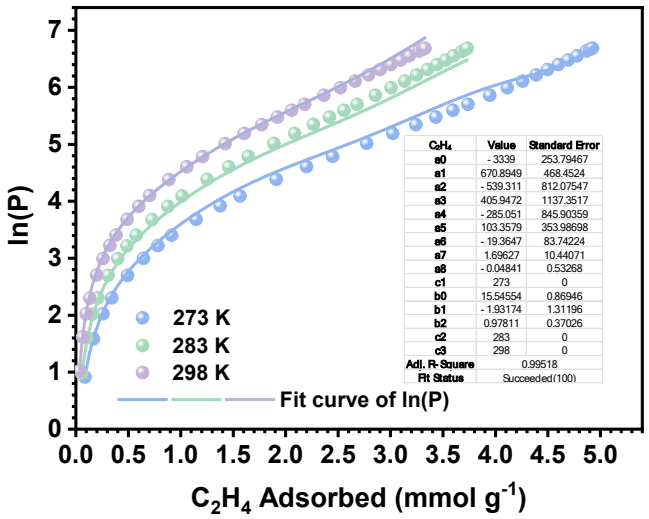

Fig. S10 The fitting parameters of C_2H_4 by the virial equation in SNNU-400.