Electronic Supplementary Information (ESI)

Assembly of indium-porphyrin framework JLU-Liu7: a mesoporous metal-organic framework with high gas adsorption and separation of light hydrocarbons

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Calculation procedures of the Gas Adsorption Selectivity by IAST

The measured experimental data is excess loadings (q^{ex}) of the pure components CO_2, CH_4, C_2H_6 and C_3H_8 for **JLU-Liu7**, which should be converted to absolute loadings (q) firstly.

$$q = q^{ex} + \frac{pV_{pore}}{ZRT}$$

Here Z is the compressibility factor. The Peng-Robinson equation was used toestimate the value of compressibility factor to obtain the absolute loading, while the measure pore volume 0.56 cm^3g^{-1} is also necessary.

The dual-site Langmuir-Freundlich equation is used for fitting the isotherm data at 298K.

$$q = q_{m_1} \times \frac{b_1 \times p^{1/n_1}}{1 + b_1 \times p^{1/n_1}} + q_{m_2} \times \frac{b_2 \times p^{1/n_2}}{1 + b_2 \times p^{1/n_2}}$$

Here p is the pressure of the bulk gas at equilibrium with the adsorbed phase (kPa), q is the adsorbed amount per mass of adsorbent (mol kg^{-1}), q_{m1} and q_{m2} are the saturation capacities of sites 1 and 2 (mol kg^{-1}), b_1 and b_2 are the affinity coefficients

of sites 1 and 2 (1/kPa), n_1 and n_2 are the deviations from an ideal homogeneous surface.

The selectivity of preferential adsorption of component 1 over component 2 in amixture containing 1 and 2, perhaps in the presence of other components too, can beformally defined as

$$S = \frac{q_1/q_2}{p_1/p_2}$$

q_1 and q_2 are the absolute component loadings of the adsorbedphase in the mixture. These component loadings are also termed the uptake capacities.We calculate the values of q_1 and q_2 using the Ideal Adsorbed Solution Theory (IAST) of Myers and Prausnitz.[1]

Calculations of the Isosteric Heats of Gas Adsorption (Q_{st}):

A virial-type[2] expression comprising the temperature-independent parameters a_i and b_j was employed to calculate the enthalpies of adsorption for CO_2, CH_4, C_2H_4, C_2H_6 and C_3H_8 (at 273 and 298 K) on compounds. In each case, the data were fitted using the equation:

$$ln^P = ln^N + {}^1/_T \sum_{i-0}^{m} a_i N^i + \sum_{j-0}^{n} b_j N^j$$

Here, P is the pressure expressed in Torr, N is the amount adsorbed in mmol g^{-1}, T is the temperature in K, a_i and b_j are virial coefficients, m, n represent the number of coefficients required to adequately describe the isotherms (m and n were gradually increased until the contribution of extra added a and b coefficients was deemed to be statistically insignificant towards the overall fit, and the average value of the squared deviations from the experimental values was minimized). The values of the virial coefficients a_0 through a_m were then used to calculate the isosteric heat of adsorption using the following expression.

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

Q_{st} is the coverage-dependent isosteric heat of adsorption and R is the universal gas constant. The heats of gas sorption for **JLU-Liu7** in this manuscript are determined by using the sorption data measured in the pressure range from 0-1 atm (273 and 298 K for gases), which is fitted by the virial-equation very well.

Table S1 Crystal data and structure refinement for compound **JLU-Liu7**.

Name	**JLU-Liu7**
Empirical formula	$In_2C_{66}H_{78}N_{10}O_{20}$
Formula weight	1561.02
Temperature (K)	100(2)
Wave length (Å)	1.54178
Crystal system	Orthorhombic
Space group	*Cmmm*
a (Å)	7.1665(6)
b (Å)	32.669(2)
c (Å)	17.0604(14)
Volume ($Å^3$)	3994.2(5)
Z, D_{calc}(Mg/m^3)	16, 1.219
Absorption coefficient (mm^{-1})	5.095
F (000)	1604
θ range (deg)	1.73 to 24.68
Limiting indices	-8<=h<=4 -37<=k<=35 -12<=l<=19
reflections collected/ unique (Rint)	5265/1819 [R(int) = 0.0319]
Crystal size (mm^3)	0.04×0.08×0.1
Data/restraints/parameters	1819/ 12 / 92
Completeness to theta = 24.68	92.8 %
Goodness-of-fit on F^2	1.135
R_1, wR_2 ($I>2\sigma(I)$)	0.0489, 0.1412
R_1, wR_2 (all data))	0.0632, 0.1507
largest difference in peak and hole (e $Å^{-3}$)	1.512, -0.911

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[\ w\ (F_o^2-F_c^2)^2]\ /\ \sum[\ w\ (F_o^2)^2]]^{1/2}$

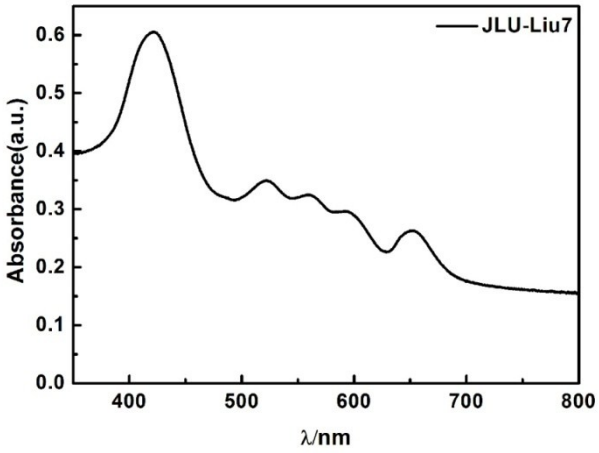

Figure S1UV/Vis solid-state absorption spectra of **JLU-Liu7**.

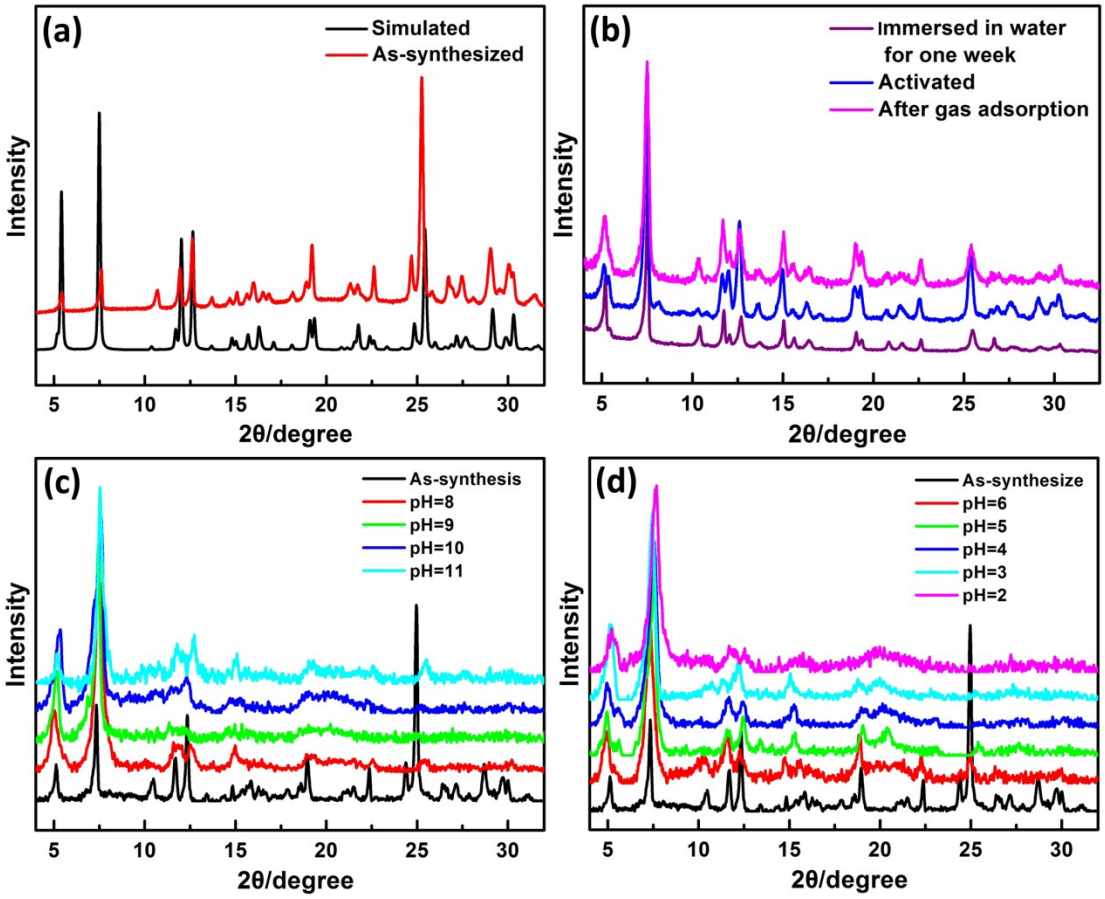

Figure S2 The powder X-ray diffraction (PXRD) patterns of**JLU-Liu7**:(a) as-synthesized (red) and simulated (black); (b) activated by continuously extracted with acetone(blue), immersed in water for one week (purple) and after gas adsorption (pink); (c) soaked in base aqueous solutions of varying pH from 8 to 11; (d) soaked in acid aqueous solutions of varying pH from 2 to 6.

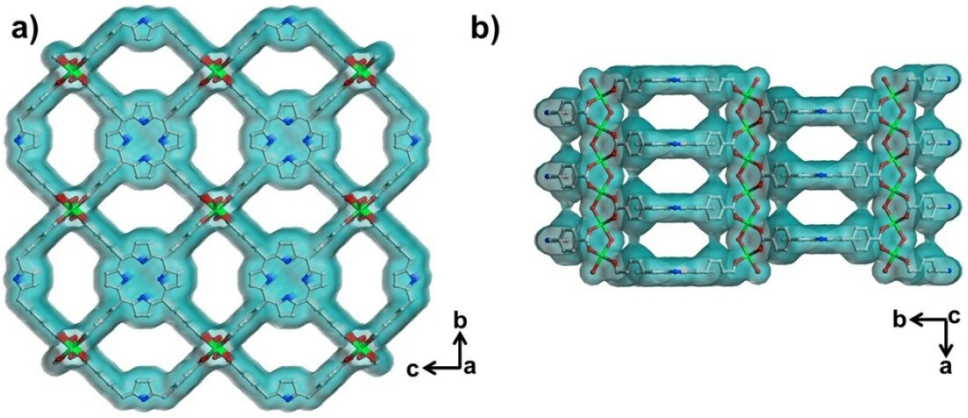

Figure S3 Thevan der Waals surfacesview of the framework through [100] and [001] directions.

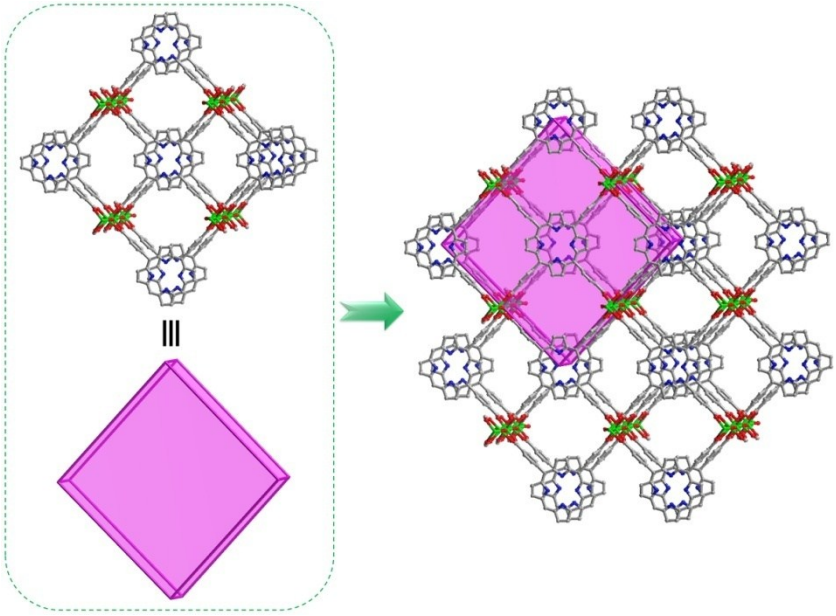

Figure S4 The mesoporous pore of the framework.

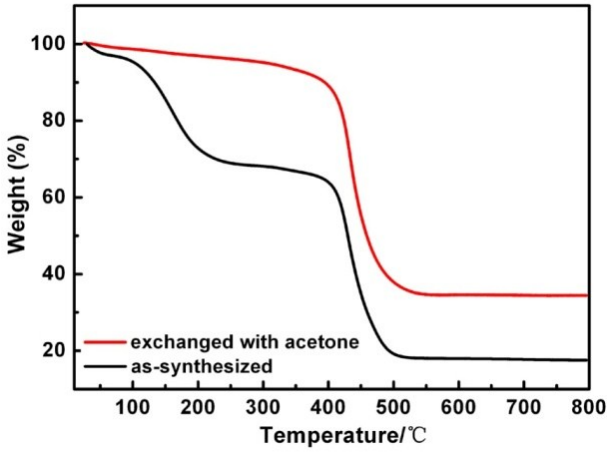

Figure S5 TGA curves of **JLU-Liu7** for the as-synthesized (black) and extracted by Soxhlet extraction with acetone (red)**.**

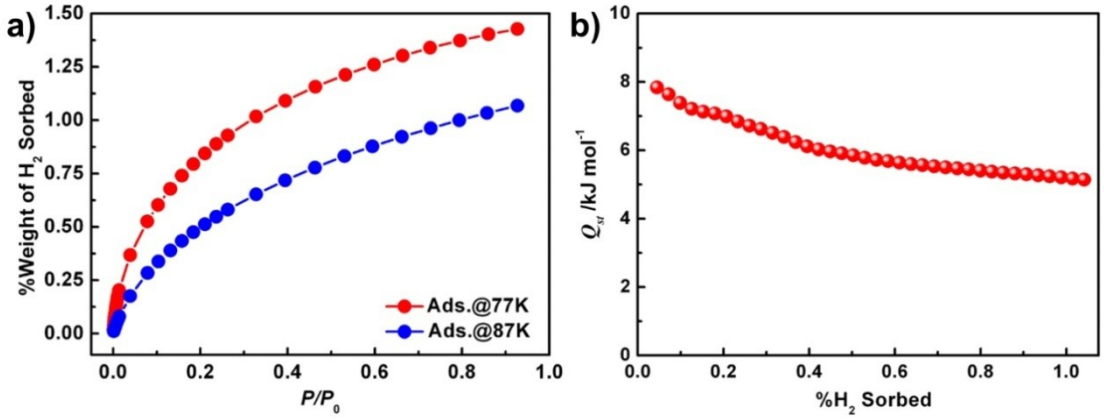

Figure S6 The hydrogen isotherms of activated **JLU-Liu7** at 77and 87 K (a) are used to calculate theheat of adsorption (b).

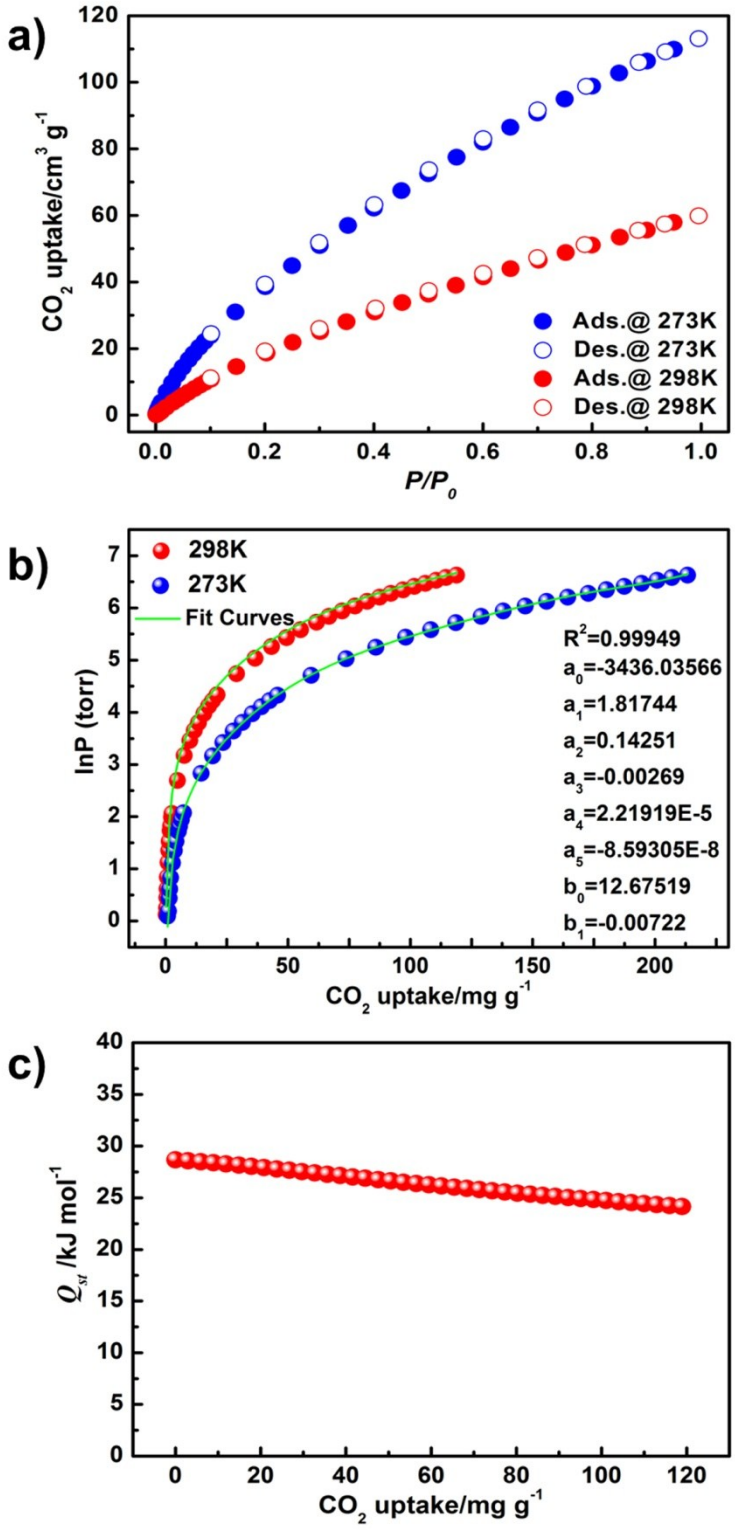

Figure S7 Adsorption isotherms (a), nonlinear curves fitting data (b) and the Q_{st} of CO_2 for **JLU-Liu7** at 273 and 298 K under 1 atm (c).

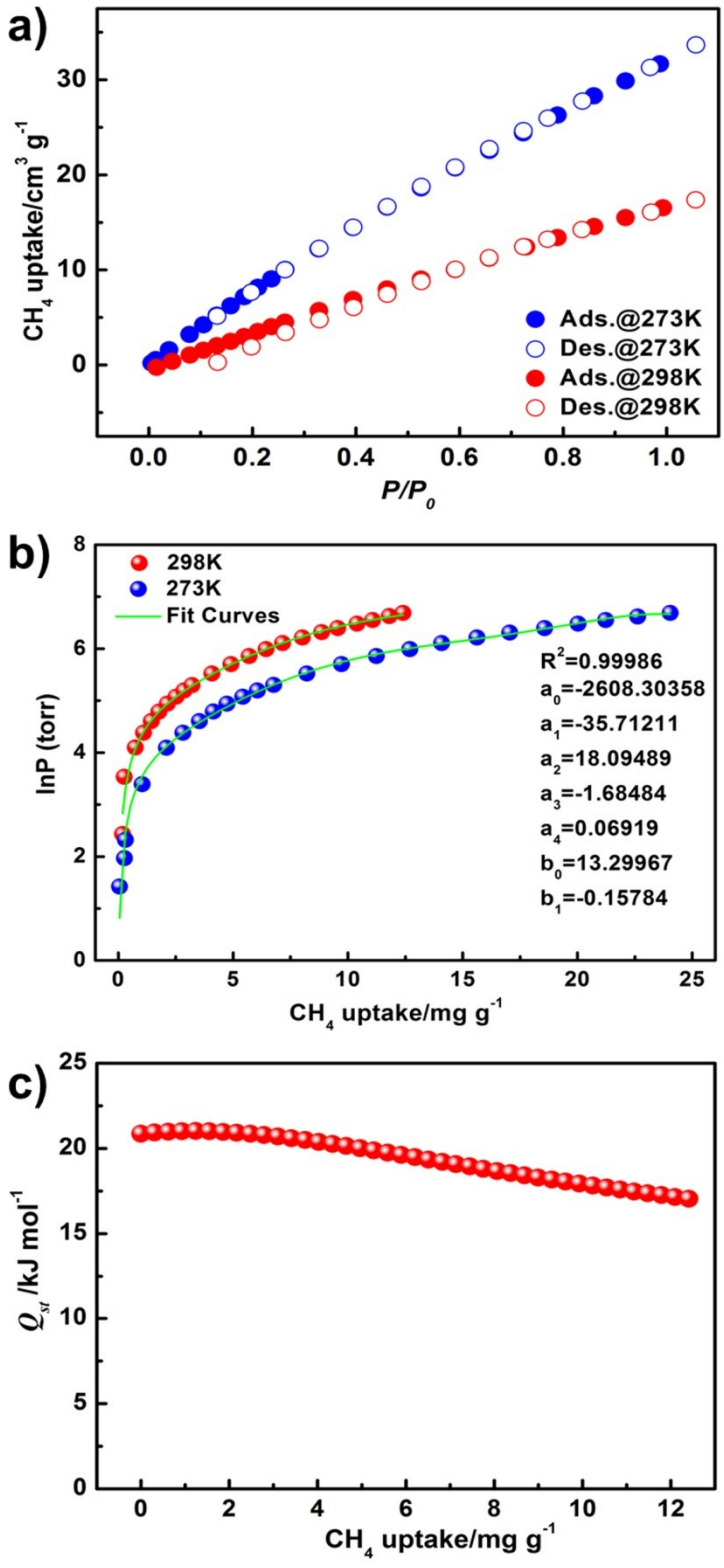

Figure S8 Adsorption isotherms (a), nonlinear curves fitting data (b) and the Q_{st}(c) of CH_4 for **JLU-Liu7** at 273 and 298 K under 1 atm.

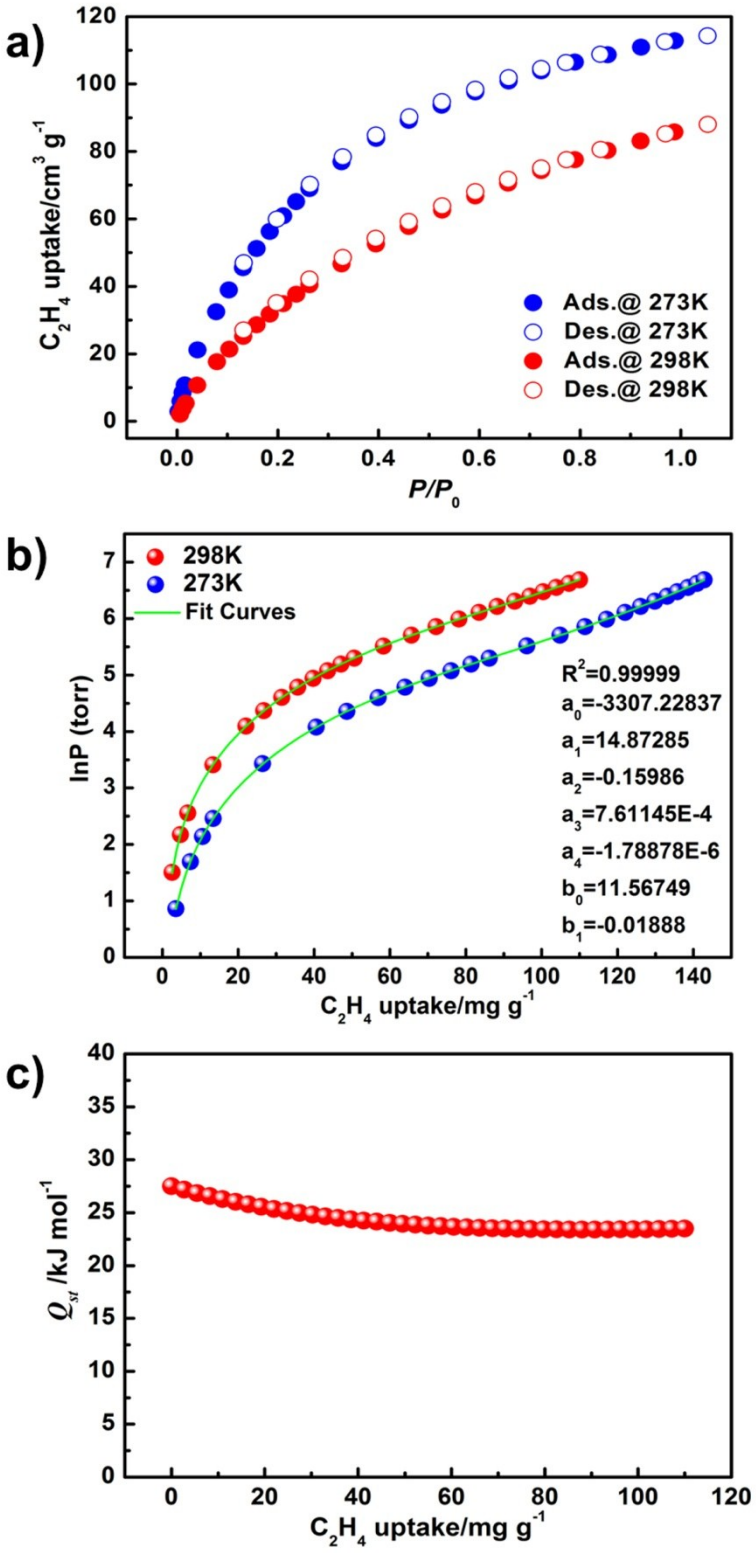

Figure S9 Adsorption isotherms (a), nonlinear curves fitting data (b) and the Q_{st} (c) of C_2H_4 for **JLU-Liu7** at 273 and 298 K under 1 atm.

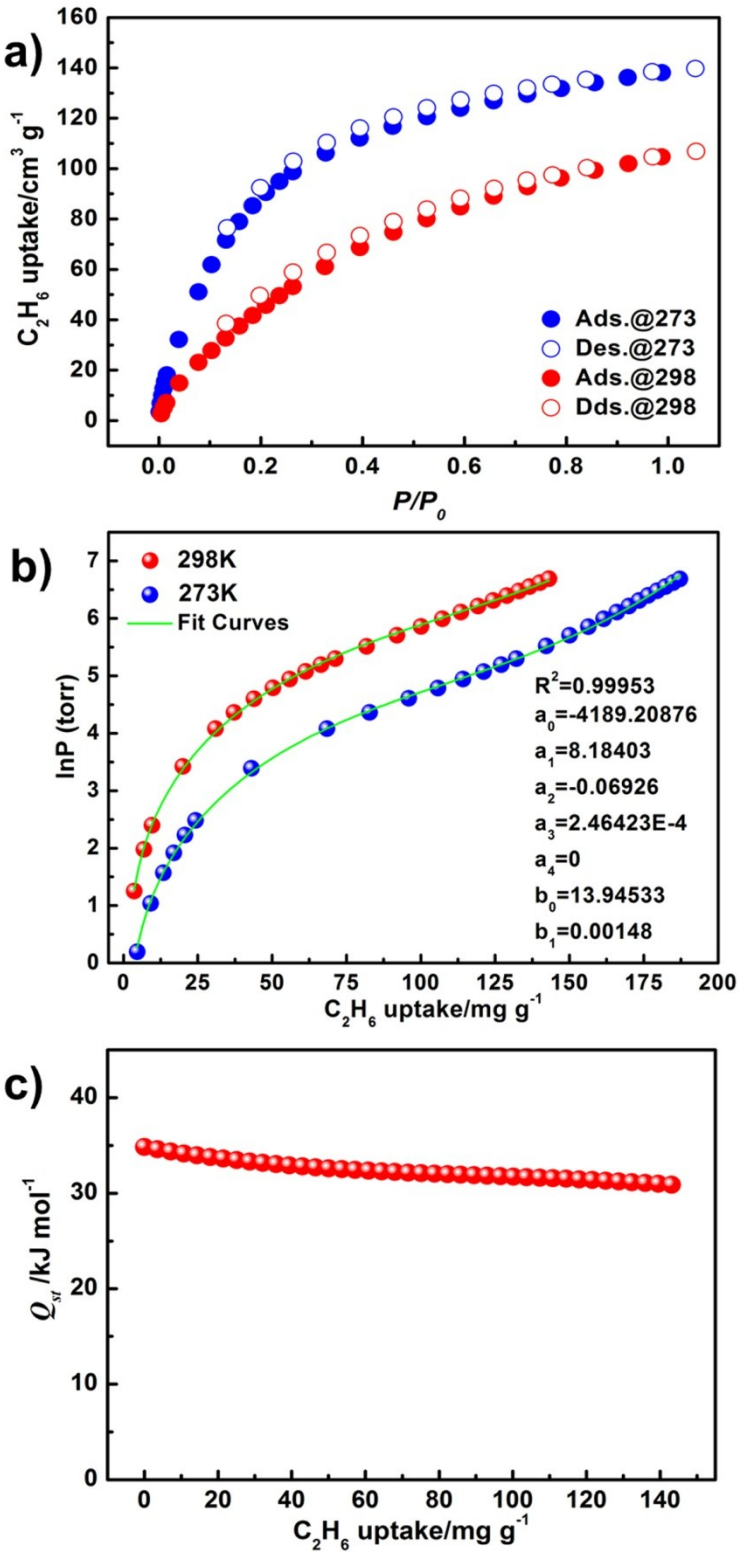

Figure S10 Adsorption isotherms (a), nonlinear curves fitting data (b) and the Q_{st}(c) of C_2H_6 for **JLU-Liu7** at 273 and 298 K under 1 atm.

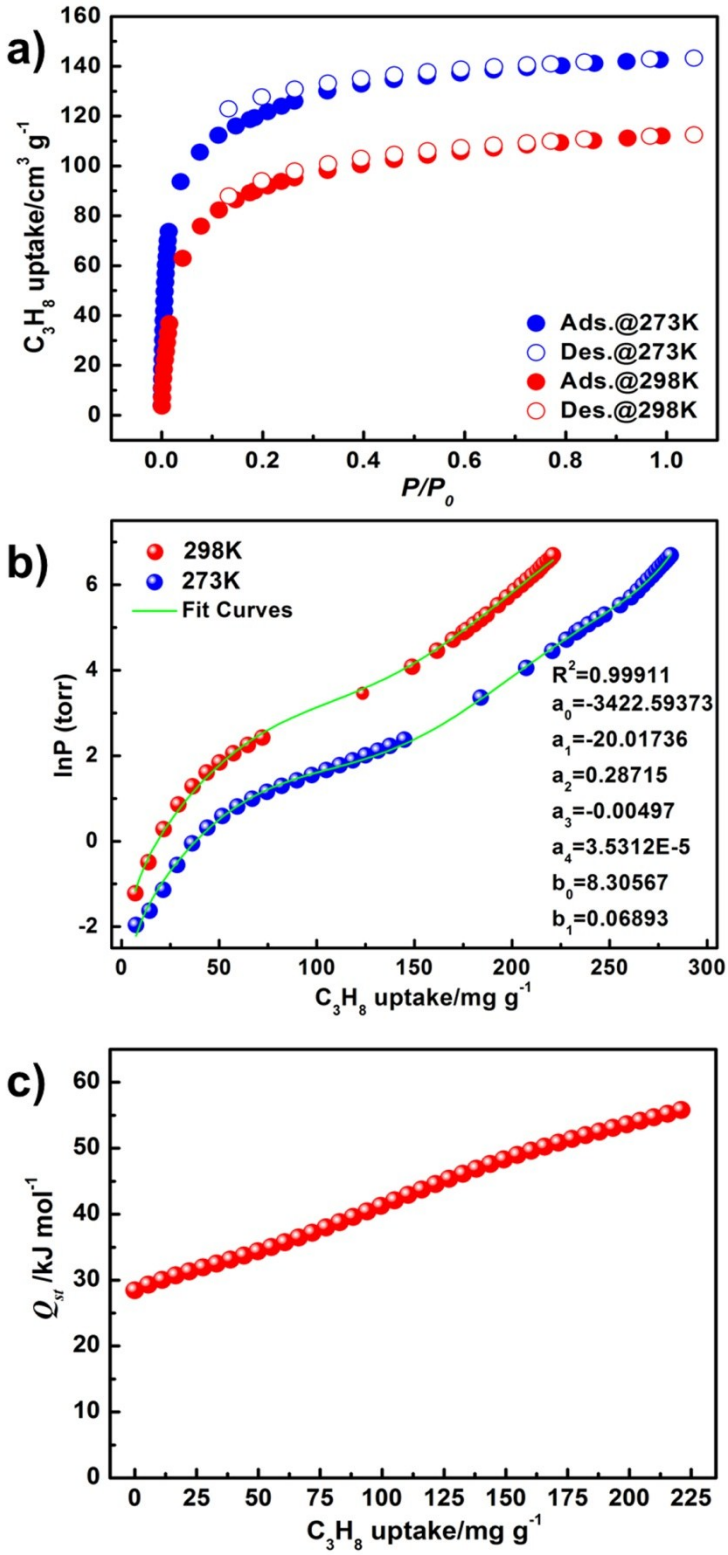

Figure S11 Adsorption isotherms (a), nonlinear curves fitting data (b) and the Q_{st}(c) of C_3H_8 for **JLU-Liu7** at 273 and 298 K under 1 atm.

Table S2 Summary of MOFs materials with high light hydrocarbons uptakes.

MOF compound	C_2H_4 uptake (mmol g^{-1})	C_2H_6 uptake (mmol g^{-1})	C_3H_8 uptake (mmol g^{-1})	Condition	Reference
FIR-7a	2.64	4.06	7.24	298K, 100 kPa	3
ZnP-CTF-500	N. A.	4.02	7.19	298K, 100kPa	4
MOF-74-Fe	6.02	6.89	5.87	318K, 1atm	5
UTSA-35	2.71	3.26	5.84	296K, 100kPa	6
JLU-Liu18	N. A.	4.11	5.18	298K, 100kPa	7
JLU-Liu7	3.93	4.77	5.02	298K, 100kPa	This work
ZnP-CTF-400	N. A.	3.13	5.00	298K, 100kPa	4
ZnP-CTF-600	N. A.	2.41	4.60	298K, 100kPa	4
JLU-Liu22	N. A.	3.30	4.15	298K, 100kPa	8
JLU-Liu15	N. A.	3.47	3.88	298K, 100kPa	9
JLU-Liu5	N. A.	3.17	3.12	298K, 100kPa	10
JLU-Liu6	N. A.	2.19	2.54	298K, 100kPa	10
MCOF-1	1.61	1.96	2.46	298K, 100kPa	11
UTSA-33	3.40	3.71	N. A.	296K, 100kPa	12
UTSA-34	3.75	3.76	N. A.	296K, 100kPa	13
$[Cu_3(TDPAH)(H_2O)_3]13H_2O8DMA$	5.21	4.79	N. A.	298K, 100kPa	14
La(BTB)	7.9	7.0	N. A.	195K, 100kPa	15
	7.0	6.4	N. A.	273K, 900kPa	15

N. A.: Not Available. The articles do not list the data.

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Table S3 The refined parameters for the Dual-site Langmuir-Freundlich equations fit for the pure isotherms of CH_4, C_2H_4, C_2H_6, C_3H_8 and CO_2 for **JLU-Liu7** at 298 K.

	q_{m1}	b_1	n_1	q_{m2}	b_2	n_2	R^2
CH_4	0.0435	8.73566E-29	0.06859	1.7842	0.00222	0.81382	0.99995
C_2H_4	6.27965	0.0255	1.21604	0.67502	6.77304E-5	0.432645	0.99998
C_2H_6	7.85102	0.03141	1.34050	0.87621	2.84603E-4	0.44327	0.99995
C_3H_8	0.28669	8.74328E-8	0.26073	5.07392	0.35325	1.22312	0.99996
CO_2	0.63368	0.05483	0.9041	10.97388	0.00163	0.926981	0.99999