# Electronic Supplementary Information (ESI) Significant enhancement of gas uptake capacity and selectivity by judiciously increasing open metal sites and Lewis basic sites within two polyhedron-based metal-organic frameworks

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# **Materials and Methods**

All the reagents were obtained from commercial sources and used without further purification. Powder X-ray diffraction (PXRD) data was collected on a Rigaku D/max-2550 diffractometer with CuK $\alpha$  radiation ( $\lambda = 1.5418$  Å). Elemental analyses (C, H, and N) were performed on a vario MICRO (Elementar, Germany). Infrared (IR) spectra were recorded within the 4000-400 cm<sup>-1</sup> region on a Nicolet Impact 410 FTIR spectrometer with KBr pellets. Thermogravimetric (TG) analyses were performed on TGA Q500 V20.10 Build 36 thermogravimetric analyzer in the temperature range of 35-800 °C under air flow with the heating rate of 10 °C min<sup>-1</sup>.

## Synthesis of Compound JLU-Liu20

A mixture of Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O (3 mg, 0.0125 mmol), 5-5'-(1*H*-1,2,4-triazole-3,5-diyl) diisophthalic acid (H<sub>4</sub>TADIPA) (5 mg, 0.0125 mmol), 1,4-diazabicyclo[2.2.2]-octane (DABCO) (0.05 mL, 2 g in 10 mL DMF), N,N-dimethylformamide (DMF) (1 mL), ethanol (0.25 mL), H<sub>2</sub>O (0.25 mL) and 0.35 mL HNO<sub>3</sub> (2.7M in DMF) were added to a 20 mL vial, then the solution was heated at 85 °C for 12h. Blue crystals were collected and air-dried (58% yield based on Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O). Elemental analysis (%) Calcd for **JLU-Liu20**  $C_{87}H_{126}Cu_6N_{20}O_{48}$ : C, 40.17; H, 4.88; N, 10.77. Found: C, 41.39; H, 5.026; N, 11.23. The agreement between the experimental and simulated PXRD patterns indicated the phase purity of the as-synthesized product.

## Synthesis of Compound JLU-Liu21

A mixture of Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O (5 mg, 0.021 mmol), H<sub>4</sub>TADIPA (3 mg, 0.0075 mmol), DMF (2 mL), ethanol (0.25 mL), H<sub>2</sub>O (0.25 mL) and 0.45 mL HNO<sub>3</sub> (2.7 M in DMF) were added to a 20 mL vial, then the solution was heated at 85 °C for 12h. Blue crystals were collected and air-dried (54% yield based on Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O). Elemental analysis (%) Calcd for **JLU-Liu21** C<sub>87</sub>H<sub>121</sub>Cu<sub>6</sub>N<sub>17</sub>O<sub>54</sub>: C, 39.43; H, 4.60; N, 8.99. Found: C, 38.94; H, 4.61; N, 9.78. The agreement between the experimental and simulated PXRD patterns indicated the phase-purity of the as-synthesized product.

## Single Crystal X-ray Structure Determination

Data were collected on a BRUKER SMART APEX II CCD diffractometer for JLU-Liu20

and **JLU-Liu21**, with graphite-monochromated Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å). The structure was solved by direct methods and refined by full-matrix least-squares methods with SHELXTL.<sup>1</sup> All non-hydrogen atoms were easily found from the difference Fourier map. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms of the ligands were generated theoretically onto the specific atoms and refined isotropically with fixed thermal factors. The guest molecules were highly disordered and could not be modeled properly, the diffused electron densities resulting from them were removed by the SQUEEZE routine in PLATONS3 and the results were appended in the CIF file. The reported refinements are of the guest-free structures using the \*.hkp files produced using the SQUEEZE routine. The final formula of **JLU-Liu20** and **JLU-Liu21** were derived from crystallographic data combined with elemental and thermogravimetric analysis data. Crystallographic data for **JLU-Liu20** and **JLU-Liu21** (1436216 and 1435683) have been deposited with Cambridge Crystallographic Data Centre. Data can be obtained free of charge upon request at www.ccdc.cam.ac.uk/data\_request/cif. Crystal data and structure refinement is summarized in Table S1. Topology information for the two compounds were calculated by TOPOS 4.0.<sup>2</sup>

Name	JLU-Liu20	JLU-Liu21
Empirical formula	$C_{87}H_{126}Cu_6N_{20}O_{48}$	$C_{87}H_{121}Cu_6N_{17}O_{54}$
Formula weight	2601.32	2542.16
Temperature (K)	100(2)	253(2)
Wave length (Å)	0.71073	0.71073
Crystal system	Tetragonal	Tetragonal
Space group	P4/mnc	P4/mnc
a (Å)	27.405(4)	26.956(4)
b (Å)	27.405(4)	26.956(4)
c (Å)	39.362(8)	39.145(8)
a (deg)	90	90
β (deg)	90	90
γ (deg)	90	90
Volume (Å <sup>3</sup> )	29562(8)	28443(8)
Z, $D_{calc}$ (Mg/m <sup>3</sup> )	8, 1.169	8, 1.187
Absorption coefficient (mm <sup>-1</sup> )	0.923	0.960
F (000)	10768	10512
Crystal size (mm <sup>3</sup> )	$0.28\times0.26\times0.24$	$0.24 \times 0.22 \times 0.21$
$\theta$ range (deg)	0.91 to 24.82	0.92 to 20.81
index range (deg)	-29≤h≤18, -31≤k≤31, -45≤l≤37	-26≤h≤25,-16≤k≤22, -38≤l≤19
Reflections collected / unique	86393/12745 [R(int) = 0.0862]	26837/7460 [R(int) = 0.0971]
Data / restraints / parameters	12745 / 2 / 506	7460 / 18 / 453
Goodness-of-fit on $F^2$	0.982	0.934
$\mathbf{R}_1, \mathbf{w}\mathbf{R}_2 \left( I \ge 2\sigma(I) \right)$	0.0720, 0.1896	0.0856, 0.2344
$R_1$ , w $R_2$ (all data)	0.0866, 0.2002	0.1246, 0.2587
Largest diff. peak and hole (e Å-3)	0.625, -3.183	0.807, -1.005

Table S1. Crystal data and structure refinement for the JLU-Liu20 and LU-Liu21.

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



**Figure S1.** 5-5'-(1*H*-1,2,4-triazole-3,5-diyl) diisophthalic acid ligands with different dihedral angles in **JLU-Liu20** (a, b) and **JLU-Liu21** (c, d).



**Figure S2.**View of three different cages in **JLU-Liu20** (cuboctahedron = cuo-*Oh* (green), truncated tetrahedron = T-Td (blue) and truncated octahedron = T-Oh (yellow)).



**Figure S3.**View of three different cages in **JLU-Liu21** (cuboctahedron = cuo-*Oh* (blue), truncated tetrahedron = T-Td (green) and truncated octahedron = T-Oh (purple)).



**Figure S4.** The 3D framework of **JLU-Liu20** with DABCO ligand located between two paddlewheels (a) and **JLU-Liu21** without DABCO ligand (b), exhibiting more OMSs.



**Figure S5.** Space-filling view of the structure of **JLU-Liu20** showing multiple pores in different directions (regardless of van der Waals radii).



**Figure S6.** Space-filling view of the structure of **JLU-Liu21** showing multiple pores in different directions (regardless of van der Waals radii).

#### **Topology Analysis**

The two compounds are assembled by one kind of inorganic SBU and two kinds of organic SBUs. The Cu(II) paddlewheel MBBs can be regarded as 4-c nodes, while the H<sub>4</sub>TADIPA ligands considered as two 3-c nodes, **JLU-Liu20** and **JLU-Liu21** can be regarded as novel (3,4)-c net, respectively (Fig. S7, Table S2). Alternatively, the H<sub>4</sub>TADIPA ligand is regarded as linear rods and the MOP-1 can be viewed as a **cuo** (12 paddlewheels as vertices) SBB, which gives rise to 12-c **fcu** topology with a Schläfli symbol of  $\{3^{24}, 4^{36}, 5^6\}$ .



**Figure S7.** Illustration of topology of **JLU-Liu20** and **JLU-Liu21**: simplification of the inorganic  $Cu_2(CO_2)_4$  (4-connected node, green) and the organic  $H_4TADIPA$  linker (two 3-connected nodes, red), leading to the new (3,4)-c net.

	Coordin	Coordination Sequnce									
Vertex	CS1	CS2	CS3	CS4	CS5	CS6	CS7	CS8	CS9	CS10	Cum10
V <sub>1</sub> (4-c)	5	13	30	63	116	198	299	442	624	843	2633
V <sub>2</sub> (4-c)	5	13	30	64	112	187	290	437	625	824	2587
V <sub>3</sub> (3-c)	4	12	28	57	106	176	285	425	600	826	2519
V <sub>4</sub> (3-c)	4	12	28	58	110	176	282	421	594	820	2505
V <sub>5</sub> (3-c)	4	12	28	58	110	180	289	420	595	827	2523
Vertex	Extend	led point s	ymbols								
V <sub>1</sub> (4-c)	[6.6(2).	[6.6(2).8.8.9.9]									
V <sub>2</sub> (4-c)	[6.6.6.8	[6.6.6.8.10(3).10(3)]									
V <sub>3</sub> (3-c)	[6.6.9(2)]										
V <sub>4</sub> (3-c)	[6.6.8]	[6.6.8]									
V <sub>5</sub> (3-c)	[6.6.8]										

 Table S2 Topological information for JLU-Liu20 and JLU-Liu21.

Compounds	Topology	Point symbol	Vertex	Transitivity	reference
	type		number		
PCN-12 <sup>a</sup>	sty	$\{6^2.8\}_4\{6^3.8.10^2\}_2\{6^3\}_8$	V <sub>(3-c)</sub> : 4	[89(11)7]	3
		$\{6^4.10^2\}_3\{6^4.8^2\}$	V <sub>(4-c)</sub> : 4		
Cu(bcpm) <sub>3</sub> (DMF)(H <sub>2</sub> O) <sub>5</sub> <sup>b</sup>	ucp	${6^3}_2{6^4.10^2}$	V <sub>(3-c)</sub> : 3	[5886]	4
			$V_{(4-c)}$ : 4		
JLU-Liu20&21°	new	$\{6^2.8^2.9^2\}_2\{6^2.8\}_4\{6^2.9\}_2$	V <sub>(3-c)</sub> : 3	[5863]	This work
		$\{6^3.8.10^2\}$	V <sub>(4-c)</sub> : 2		
$Cu_{24}(bdpb)_{12}(DMF)_8(H_2O)_{16}^{d}$	zmj	$\{6^2.8\}_4\{6^3.8.10^2\}_2\{6^3\}_2\{6^6\}$	V <sub>(3-c)</sub> : 2	N.A.	5
			V <sub>(4-c)</sub> : 2		
PCN-21 <sup>e</sup>	new	$\{5.8^2\}_2\{5^2.6.8.9^2\}\{5^2.6\}$	V <sub>(3-c)</sub> : 3	[5674]	6
		$\{5^2.8^2.9^2\}\{5^2.8\}$	V <sub>(4-c)</sub> : 4		
$Cu_{24}(bmbdb)_{12}(H_2O)_{16}(DMSO)_8^{f}$	zmj	$\{6^2.8\}_4\{6^3.8.10^2\}_2\{6^3\}_2\{6^6\}$	V <sub>(3-c)</sub> : 4	N.A.	7
			V <sub>(4-c)</sub> : 4		
$Zn_5L_3(H_2O)_5^g$	zjz	$\{6.8.10\}_{12}\{6^6\}_3\{8^3\}_4$	V <sub>(3-c)</sub> : 1	[3334]	8
			V <sub>(4-c)</sub> : 2		

 Table S3. Topology information of some related MOFs base on MOP-1 SBBs and tetracarboxylate ligands.

a)-g) Ligands are corresponding with the above compounds. N.A.: Not Available. The article do not list the data.





**Figure S8.** (a) Three types of tiles with face symbol; (b) Natural tiling of **JLU-Liu20** and **JLU-Liu21**.



**Figure S9.** (a) Simulated, as-synthesized and activated PXRD patterns for **JLU-Liu20** samples; (b) The variable-temperature PXRD patterns for **JLU-Liu20**.



**Figure S10.** (a) Simulated, as-synthesized and activated PXRD patterns for **JLU-Liu21** samples; (b) The variable-temperature PXRD patterns for **JLU-Liu21**.

# Thermogravimetric Analysis (TGA)

Thermogravimetric analysis (TGA) for compound **JLU-Liu20** shows a weight loss of 50.65 % between 35 and 280 °C, which corresponding to the loss of coordinated  $H_2O$  molecules, guest DMF molecules and DABCO ligand. The further weight loss of 33.23% occurs between 280 and 380°C should be attributed to the release of organic  $H_4TADIPA$  ligands (calcd 34.3%).

Thermogravimetric analysis (TGA) for compound **JLU-Liu21** shows a weight loss of 43.9 % between 35 and 280 °C, which corresponding to the loss of coordinated  $H_2O$  molecule and guest DMF molecules. The further weight loss of 37.2% between 280 and 400°C, should be attributed to the release of organic  $H_4$ TADIPA ligands (calcd 36.8%).



Figure S11. TGAs curves for the as-synthesized and activated samples of JLU-Liu20.



Figure S12. TGAs curves for the as-synthesized and activated samples of JLU-Liu21.



Figure S13. The infrared spectra for JLU-Liu20 (red) and JLU-Liu21 (blue).

### Gas adsorption measurements

The N<sub>2</sub>, H<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> and C<sub>3</sub>H<sub>8</sub> gas adsorption measurements were performed on a Micromeritics ASAP 2420, Micromeritics ASAP 2020 and Micromeritics 3-Flex instruments. Before gas adsorption measurements, the samples were degassed under a dynamic vacuum at 100 °C for 10 hours after solvent exchange with ethanol for 7 days to completely remove the non-volatile solvent molecules. A colour changed from bright-blue to deep purple-blue is a typical feature for Cu paddlewheel to generate open Cu sites.

Compounds	<b>SA</b> <sub>BET</sub> (m <sup>2</sup> g <sup>-1</sup> )	SA <sub>Langmuir</sub> (m <sup>2</sup> g <sup>-1</sup> )	<b>Pore volume</b> (cm <sup>3</sup> g <sup>-1</sup> ) (Experimental/Theoretical)	OMSs (nm <sup>-3</sup> )	LBSs (nm <sup>-3</sup> )
JLU-Liu20	1807	2434	0.87/0.91	1.08	2.30
JLU-Liu21	2080	2804	1.00/1.06	1.69	2.39

Table S4. N<sub>2</sub> adsorption data and structure information for JLU-Liu20 and JLU-Liu21.

Table S5. Gas adsorpt	tion data f	for JLU-Liu20	and JLU-Liu21.
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Compounds	$H_2^a$		$CO_2^a$		$CH_4{}^a$		C <sub>2</sub> H <sub>6</sub> <sup>a</sup>		$C_3H_8^a$	
	77 K	87 K	273 K	298 K	273 K	298 K	273 K	298 K	273 K	298 K
JLU-Liu20	256	166	162	88	31	18	113	130	202	117
JLU-Liu21	280	187	210	118	37	22	182	195	224	199

<sup>*a*</sup> Gas uptake in cm<sup>3</sup> g<sup>-1</sup>.

Compounds	SA <sub>BET</sub>	$SA_{Langmuir}$	H <sub>2</sub> uptake	Reference
	$(m^2 g^{-1})$	$(m^2 g^{-1})$	(wt%)	
[Cu(Me-4py-trz-ia)]	1473	N.A.	3.07	9
PCN-12	1943	2425	3.05	3
UTSA-20	1156	N.A.	2.92	10
In-soc-MOF	N.A.	1417	2.60	11
PCN-11	1931	2442	2.55	12
$[Cu_{24}L_{12}(H_2O)_{12}]$	1879	2489	2.47	13
Mn-BTT	2100	2800	2.42	14a
PCN-10	1407	1179	2.34	12
$[Cu_{24}L_8(H_2O)_{24}]$	3730	4180	2.29	15
Cu-BTT	1710	1770	2.25	14a, b
PCN-6	N.A.	3800	1.9	16a, b
PCN-6'	N.A.	2700	1.35	16a

**Table S6.** Hydrogen uptake of porous MOFs at 77 K and 1 bar.

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

Compounds	CO <sub>2</sub> uptake	OMS density	LBS density	Reference
	(RT, wt%)	(nm <sup>-3</sup> )	(nm <sup>-3</sup> )	
[Cu(Me-4py-trz-ia)]	26.8	1.4	2.9	9
Cu-TDPAT	25.9	1.76	3.5	17
Cu-TPBTM	23.3	1.3	1.3	18
JLU-Liu-21	23.2	1.69	2.39	This work
Cu-TDPAH	22.8	1.72	5.4	19
NOTT-122	20.4	1.3	3.3	20
JLU-Liu-20	17.3	1.08	2.3	This work
mmen-Mg <sub>2</sub> (dobpdc)	17.0	0.28	1.92	21
CuBTTri	16.4	1.9	3.7	22
SNU-50	15.84	1.2	1.2	23

Table S7. CO<sub>2</sub> adsorption data of selected MOFs with both OMSs and LBSs at 298 K.

MOF compounds	CO <sub>2</sub> uptake	Pressure	Reference
	(wt%)	(bar)	
Cu-TDPAT	44.5	1	17
[Cu <sub>6</sub> (TADIPA) <sub>3</sub> (H <sub>2</sub> O) <sub>6</sub> ]	41.2	1	This work
[Cu(Me-4py-trz-ia)]	40.5	1	9
Cu <sub>2</sub> (abtc) <sub>3</sub>	38.5	1	24
[Cu <sub>6</sub> (TADIPA) <sub>3</sub> (DABCO)(H <sub>2</sub> O) <sub>2</sub> (DMF) <sub>2</sub> ]	31.8	1	This work
Dy(BTC)	27.2	1	25
Cu <sub>2</sub> (EBTC)(H <sub>2</sub> O) <sub>2</sub>	25.9	1	26
Al <sub>4</sub> (OH) <sub>2</sub> (OCH <sub>3</sub> ) <sub>4</sub> (BDC-NH <sub>2</sub> ) <sub>3</sub>	24.1	1	27
$[Zn_2(abtc)(DMF)_2]_3$	20.6	1	24
Zn <sub>2</sub> (BTetB)	19.7	1	28
[Cu <sub>2</sub> (abtc)(DMF) <sub>2</sub> ] <sub>3</sub>	19.2	1	24
Cu <sub>2</sub> (TCM)	18.4	1	29

Table S8. CO<sub>2</sub> adsorption capacities in MOFs at 273 K and 1 bar.



**Figure S14.** (a) Nitrogen sorption isotherms on **JLU-Liu20** (red) and **JLU-Liu21** (blue) at 77 K (Adsorption: closed symbols; desorption: open symbols, respectively); (b)The pore size distribution calculated using the DFT method.



**Figure S15.** (a) The H<sub>2</sub> isotherm for **JLU-Liu20** and **JLU-Liu21** at 77 and 87 K under 1 bar; (b)  $Q_{st}$  of H<sub>2</sub> for **JLU-Liu20** (red) and **JLU-Liu21** (blue).

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

A virial-type<sup>30</sup> expression comprising the temperature-independent parameters  $a_i$  and  $b_j$  was employed to calculate the enthalpies of adsorption for CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> and C<sub>3</sub>H<sub>8</sub> (at 273 and 298 K) on compounds. In each case, the data were fitted using the equation:

$$ln^{P} = ln^{N} + \frac{1}{T} \sum_{i=0}^{m} a_{i}N^{i} + \sum_{j=0}^{n} b_{j}N^{j}$$

Here, *P* is the pressure expressed in Torr, *N* is the amount adsorbed in mmol g<sup>-1</sup>, *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 heat of gas sorption for **JLU-Liu20** and **JLU-Liu21** in this manuscript are determined by using the sorption data measured in the pressure range from 0-1 bar (273 and 298 K for gases), which is fitted by the virial-equation very well.



**Figure S16.** Nonlinear curves fitting of **JLU-Liu20** for CO<sub>2</sub> (a), CH<sub>4</sub> (b), C<sub>2</sub>H<sub>6</sub> (c) and C<sub>3</sub>H<sub>8</sub> (d) at 273 K and 298 K.



**Figure S17.** Nonlinear curves fitting of **JLU-Liu21** for  $CO_2$  (a),  $CH_4$  (b),  $C_2H_6$  (c) and  $C_3H_8$  (d) at 273 K and 298 K.



Figure S18. Isosteric heat of  $CO_2$  (a),  $CH_4$  (b),  $C_2H_6$  (c) and  $C_3H_8$  (d) for JLU-Liu20 (red) and JLU-Liu21 (blue).

# Prediction of adsorption of binary mixture by IAST theory

The excess adsorption data for pure gases measured at 273K and 298 K, were first converted to absolute loadings, along with *Peng-Robinson* equation. In order to perform the IAST calculations, the single-component isotherm was fitted by the dual-site Langmuir-Freundlich (DSLF) adsorption model<sup>31</sup> to correlate the pure-component equilibrium data and further predict the adsorption of mixtures. The DSLF model is described as:

$$N^{0}(f) = \frac{N_{1}k_{1}f}{1+k_{1}f} + \frac{N_{2}k_{2}f}{1+k_{2}f}$$

Where *f* is the fugacity of bulk gs at equilibrium with adsorbed phase,  $N_i$  is the model parameter of the maximum adsorption amount at the site *i* (*i*=1 or 2), and  $k_i$  is the affinity constant.

Based on the above model parameters of pure gas adsorption, we used the IAST model,<sup>32</sup> which was proposed by *Myer* and *Prausnitz* in 1965 to predict the multi-component adsorption. Analogous to *Raoult's* law for vapor-liquid equilibrium, the IAST assumes that the adsorbed solutions are ideal and all activity coefficients in the adsorbed phase are unity. Thus, the adsorption equilibrium between adsorbed and gas phases will lead to the following equation

 $Py_i\varphi_i = x_i f_i^0(\pi)$ 

Where  $f_i^0$  is the fugacity of the equilibrium gas phase corresponding to the spreading pressure  $\pi$  for the adsorption of pure gas *i*,  $\varphi_i$  is the gas fugacity coefficient of component *i* calculated by *PR* equation of state, and  $x_i$  and  $y_i$  are the molar fraction of component *i* at the adsorbed and bulk phases, respectively. The binary gas mixing process is carried out at constant spreading pressure  $\pi$  and indicated by

$$\int_{0}^{f_{1}^{0}} N_{1}^{0}(f_{1}) dlnf_{1} = \int_{0}^{f_{2}^{0}} N_{2}^{0}(f_{2}) dlnf_{2}$$

Where the single-component adsorption amount and selectivity are further obtained from the above equation by numerical integration and root exploration. To investigate the separation of binary mixtures, the adsorption selectivity is defined by

$$S_{ij} = \frac{\frac{x_i}{x_j}}{\frac{y_i}{y_j}}$$

Where the selectivity refers to the first component over the second one, and the  $x_i$ ,  $x_j$  and  $y_i$ ,  $y_j$  denote the molar fractions of species *i*, *j* in the adsorbed and bulk phases, respectively.



**Figure S19.**  $CO_2$ ,  $CH_4$ ,  $C_2H_6$  and  $C_3H_8$  adsorption isotherms at 298 K along with the Dualsite Langmuir Freundich (DSLF) fits (a, c); Gas mixture adsorption selectivity are predicted by IAST at 298K and 100 kPa for **JLU-Liu20** (b, d).

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