

Supporting information

Structural optimization of ZIF-8-derived porous N-doped carbon materials for effective CO₂ capture

Hao Wang, Jiadi Gao, Xianyi Liu, Zhiguo Zhang, Zhigeng Fan, Yange Suo*

School of Mechanical and Energy Engineering, Zhejiang University of Science and
Technology, Liuhe Road 318#, Hangzhou, Zhejiang Province 310023, China
E-mail address: suoyange@zust.edu.cn (Yange Suo);

Standardized formula for multiple linear regression equations:

$$\sigma = \sqrt{\frac{\sum (x_i - \mu)^2}{n}} \quad (S1)$$

$$z_i = \frac{x_i - \mu}{\sigma} \quad (S2)$$

where σ denotes the variance, μ denotes the mean, and z denotes the data after standardization.

Dual-site Langmuir-Freundlich model equation is as follows [1]:

$$q = q_c \frac{K_c p}{1 + K_c p} + q_i \frac{K_i p}{1 + K_i p} \quad (S3)$$

Where, “ q ” denotes the amount adsorbed in unit of mmol g⁻¹, “ q_c ” and “ q_i ” represent saturation capacity of the two adsorption sites in unit of mmol g⁻¹, respectively. “ K_c ” and “ K_i ” is DSLF fitting parameters of the two adsorption sites in unit of bar⁻¹, respectively.

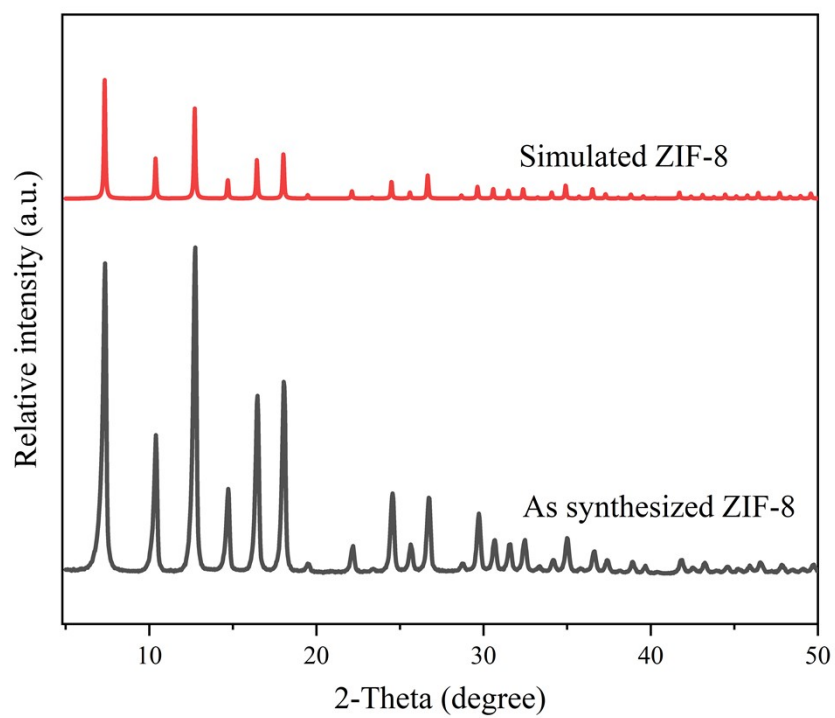


Figure S1. XRD patterns of the simulated ZIF-8 and the as-synthesized ZIF-8.

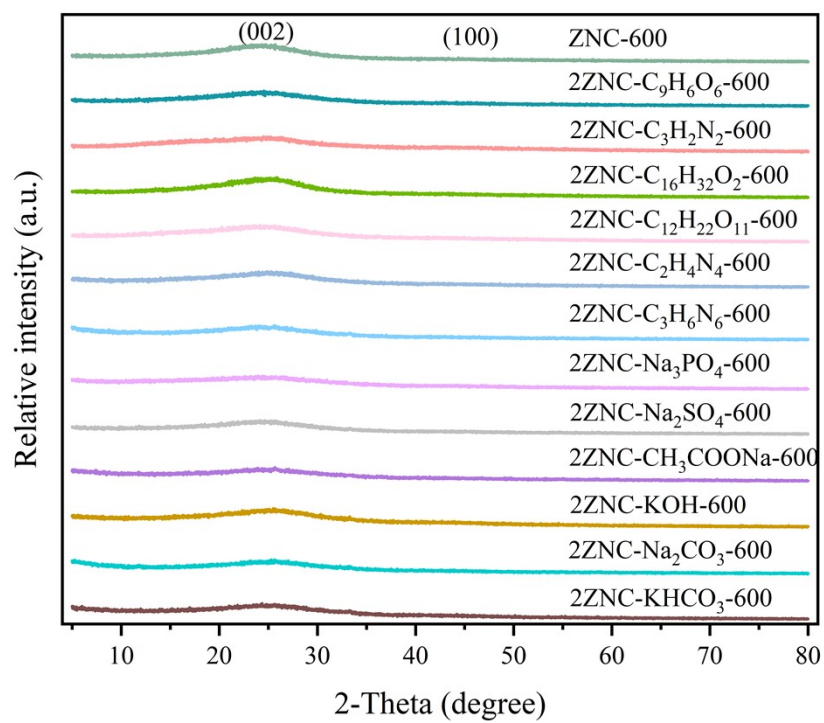


Figure S2. XRD patterns of ZNCs.

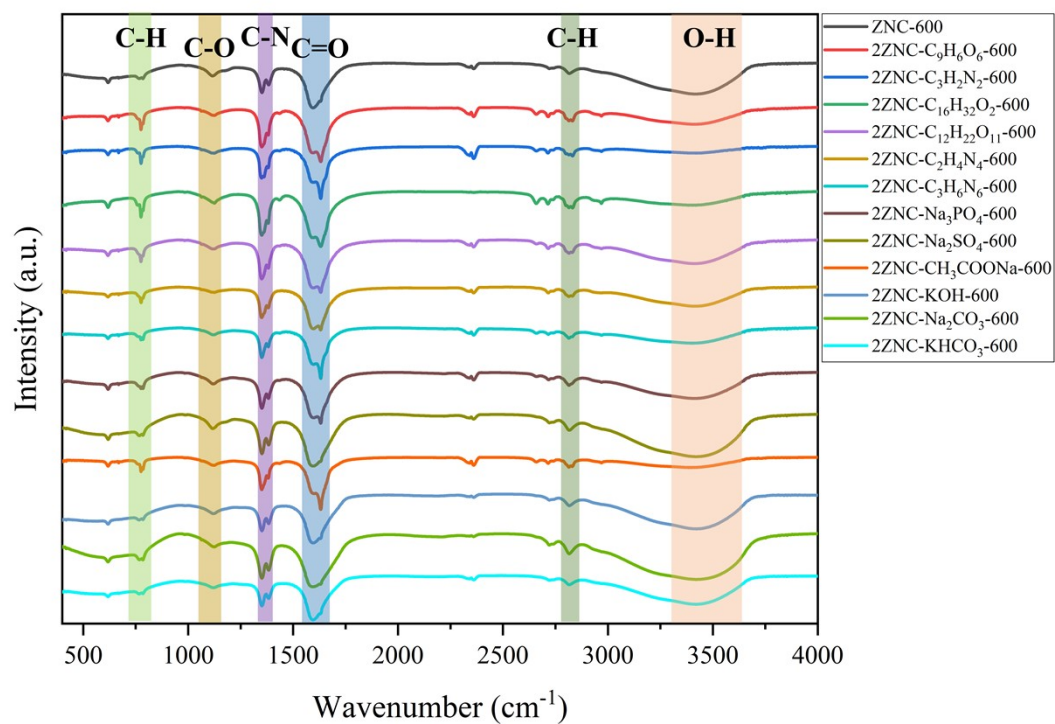


Figure S3. FTIR spectrum of ZNCs.

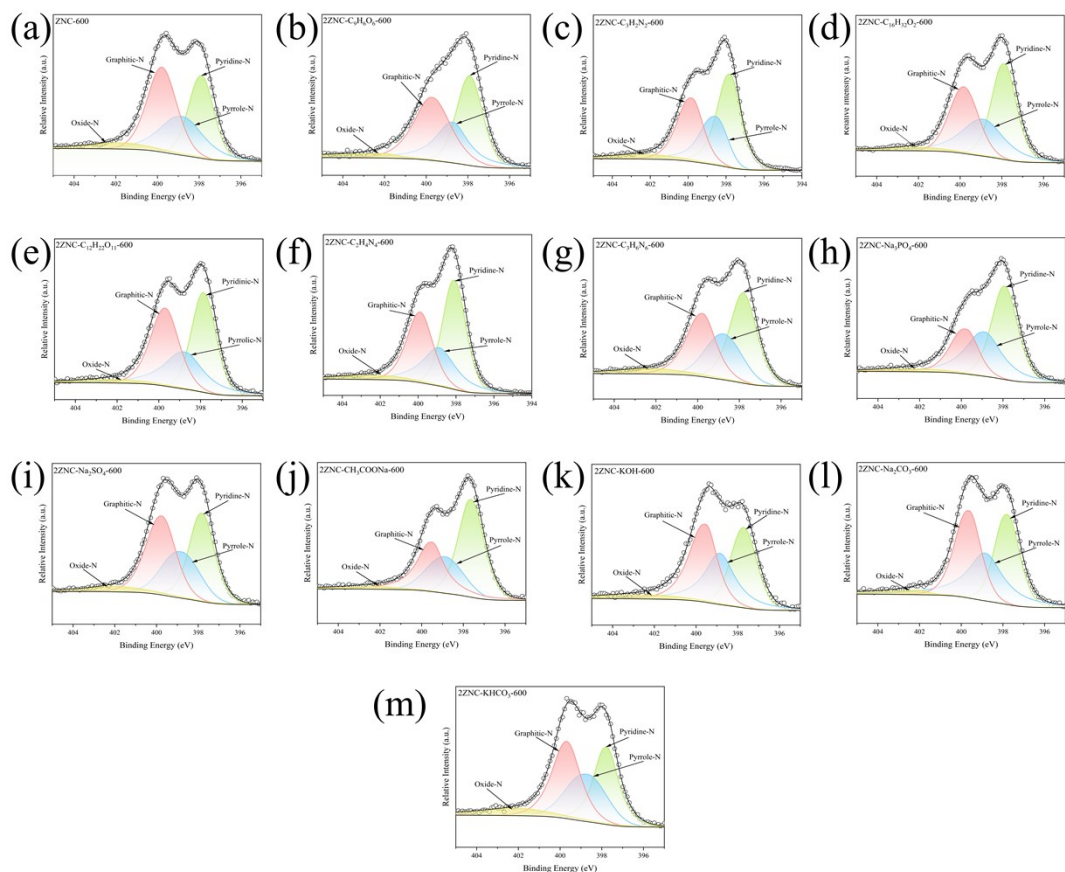


Figure S4. N1s spectrum of (a) ZNC-600, (b) 2ZNC-C₉H₆O₆-600, (c) 2ZNC - C₃H₂N₂-600, (d) 2ZNC-C₁₆H₃₂O₂-600, (e) 2ZNC-C₁₂H₂₂O₁₁-600, (f) 2ZNC-C₂H₄N₄-600, (g) 2ZNC-C₃H₆N₆-600, (h) 2ZNC-Na₃PO₄-600, (i) 2ZNC-Na₂SO₄-600, (j) 2ZNC-CH₃COONa-600, (k) 2ZNC-KOH-600, (l) 2ZNC-Na₂CO₃-600, (m) 2ZNC-KHCO₃-600.

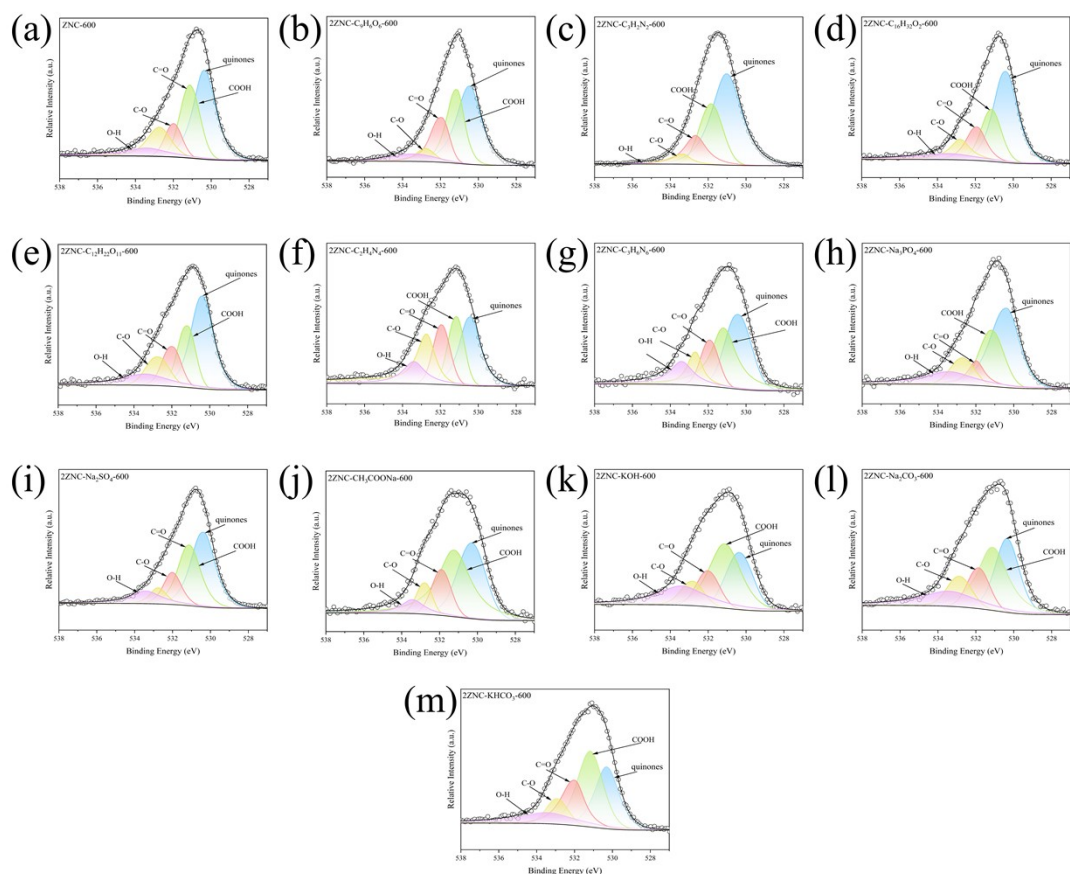


Figure S5. O1s spectrum of (a) ZNC-600, (b) 2ZNC-C₉H₆O₆-600, (c) 2ZNC - C₃H₂N₂-600, (d) 2ZNC-C₁₆H₃₂O₂-600, (e) 2ZNC-C₁₂H₂₂O₁₁-600, (f) 2ZNC-C₂H₄N₄-600, (g) 2ZNC-C₃H₆N₆-600, (h) 2ZNC-Na₃PO₄-600, (i) 2ZNC-Na₂SO₄-600, (j) 2ZNC-CH₃COONa-600, (k) 2ZNC-KOH-600, (l) 2ZNC-Na₂CO₃-600, (m) 2ZNC-KHCO₃-600.

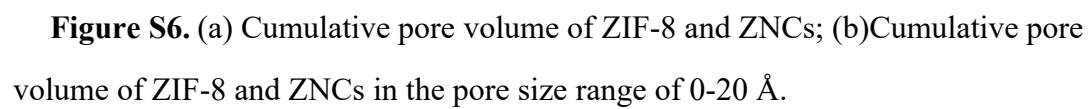


Figure S6. (a) Cumulative pore volume of ZIF-8 and ZNCs; (b) Cumulative pore volume of ZIF-8 and ZNCs in the pore size range of 0-20 Å.

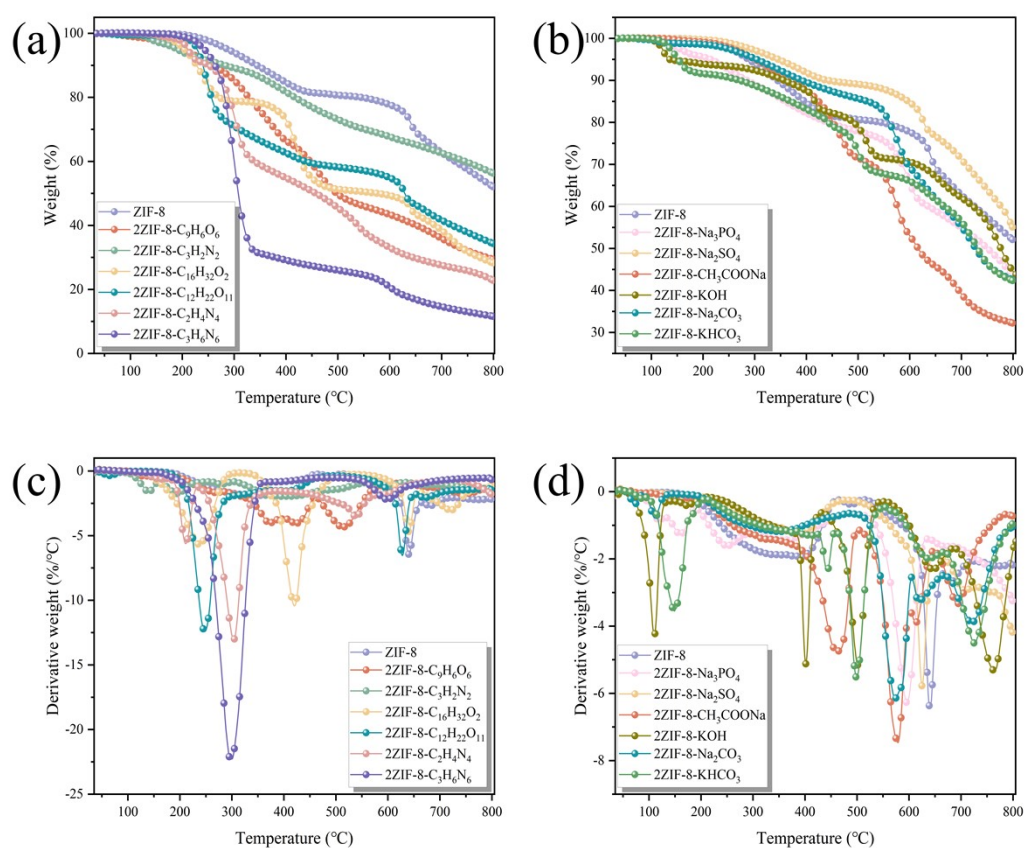


Figure S7. (a) TG curves of ZIF-8 and 2ZNC-organic compounds; (b) TG curves of ZIF-8 and 2ZNC-inorganic compounds; (c) DTG curves of ZIF-8 and 2ZNC-organic compounds; (b) DTG curves of ZIF-8 and 2ZNC-inorganic compounds.

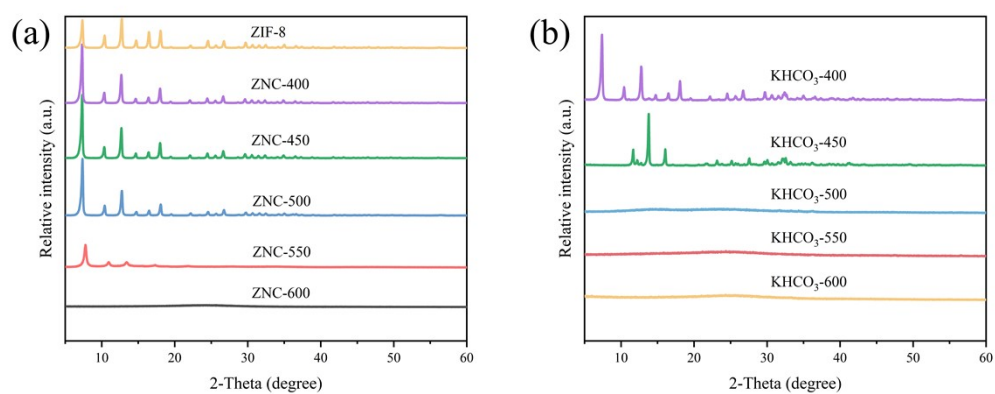


Figure S8. (a) XRD patterns of the ZIF-8 and ZNC-T (400-600°C); (b) XRD patterns of the 2ZNC-KHCO₃-T (400-600°C).

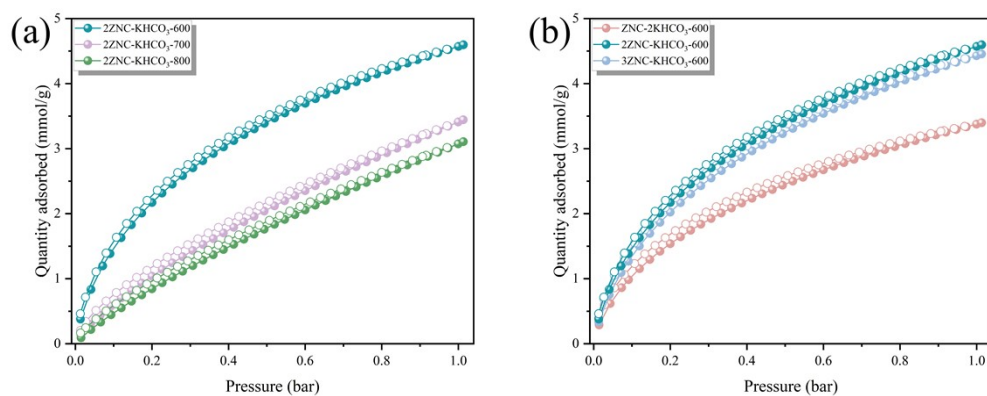


Figure S9. (a) The CO₂ adsorption capacity of 2ZNC-KHCO₃-T at 25 °C and 1 bar;
 (b) The CO₂ adsorption capacity of xZNC-yKHCO₃-600 at 25 °C and 1 bar.

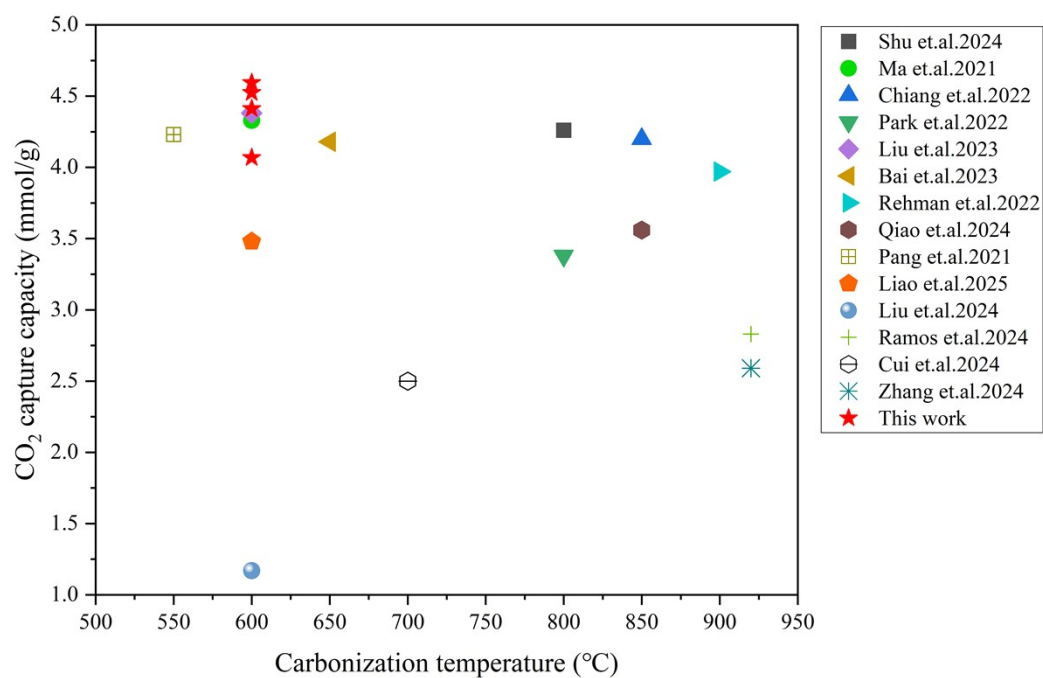


Figure S10. Comparison of CO₂ adsorption capacity of ZNCs from this paper and other carbon materials from existing literature (at 1 bar and 25 °C).

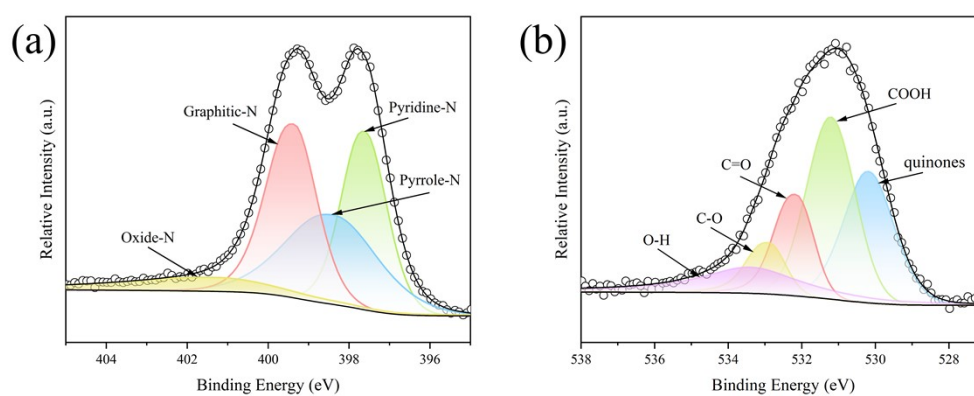


Figure S11. (a) N1s spectra of 2ZNC-KHCO₃-600 after CO₂ adsorption; (b) O1s spectra of 2ZNC-KHCO₃-600 after CO₂ adsorption.

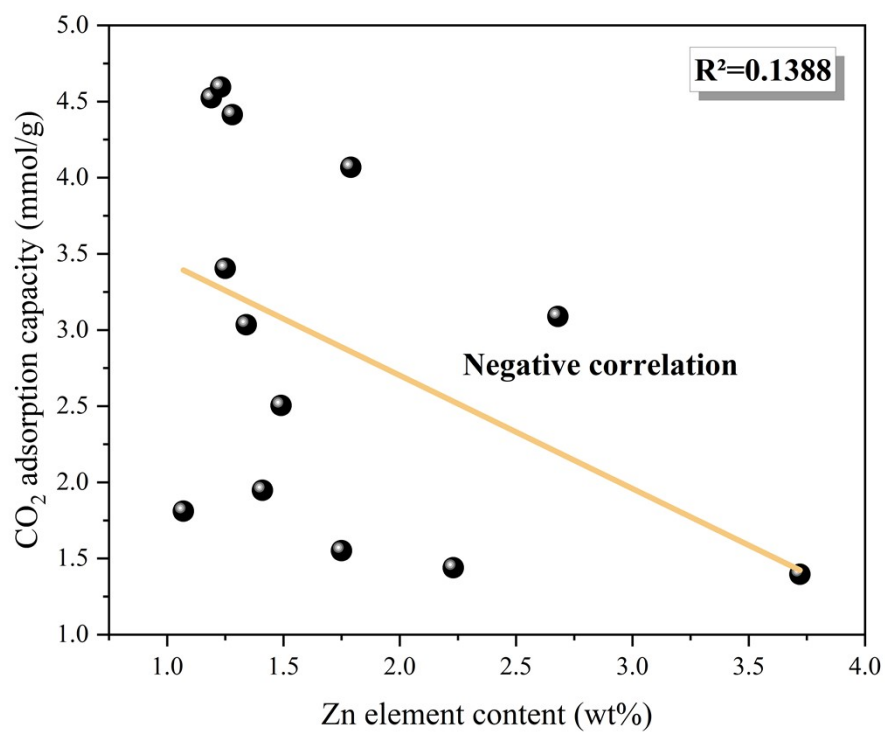


Figure S12. The linear correlation analyses between the CO₂ adsorption capacities (at 25 °C and 1 bar) and contents of Zn element.

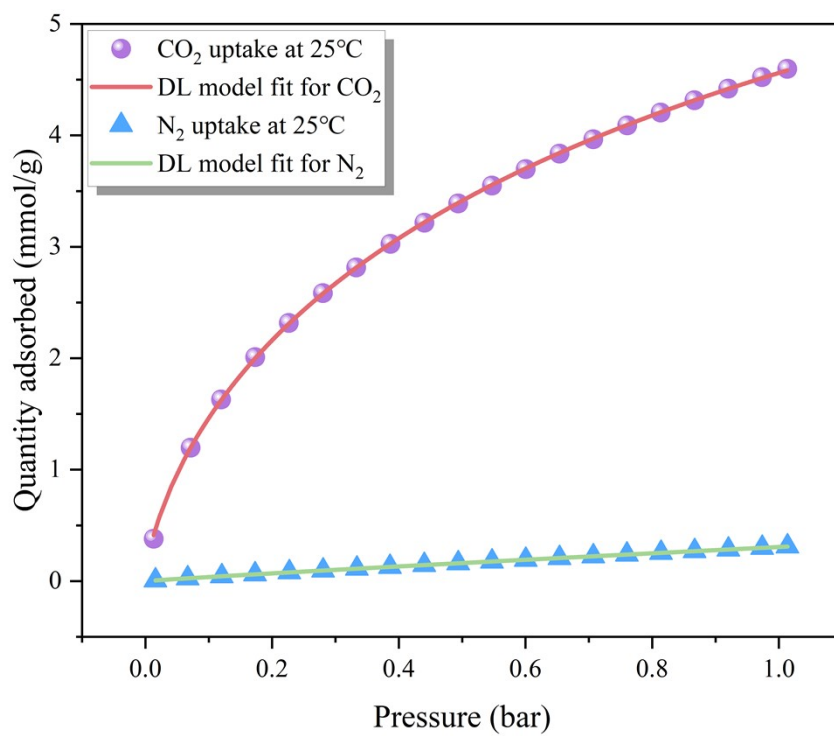


Figure S13. CO₂ and N₂ adsorption for 2ZNC-KHCO₃-600 fitted by Dual-site Langmuir Freundlich model measured at 25°C.

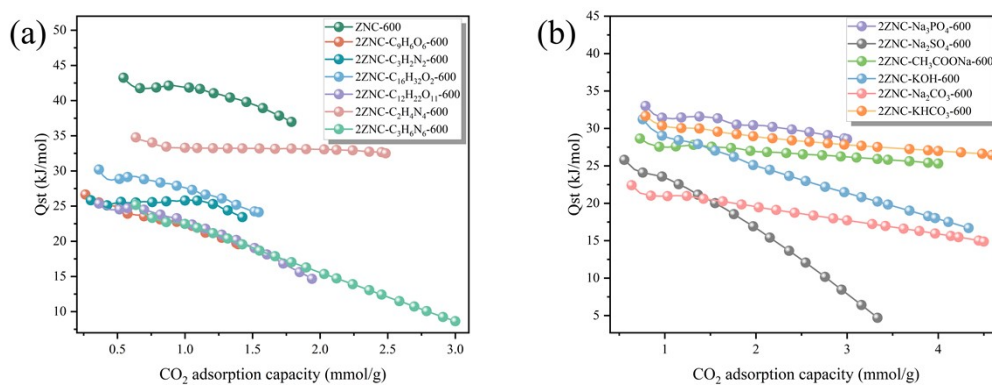


Figure S14. (a) Isosteric heats of CO₂ adsorption on ZIF-8 and 2ZNC-organic compounds; (b) Isosteric heats of CO₂ adsorption on 2ZNC-inorganic compounds.

Table S1. The CO₂ adsorption performance of 2ZNC-KHCO₃-600 and similar materials reported in the literature.

Sample	Original material	CO ₂ adsorption capacity at 1 bar (mmol/g)		Reference
		0 °C	25 °C	
2ZNC-KHCO ₃ -600	ZIF-8	6.55	4.60	This work
ZIF-8/Pan	ZIF-8	/	4.20	[2]
20-ZCMC-800	ZIF-8	7.30	4.26	[3]
HNC-350-850	ZIF-8	6.21	3.56	[4]
2CN61-KCl-700	ZIF-61	6.19	3.91	[5]
mJUC160-900	JUC-160	5.50	3.50	[6]
5C-C ₆ H ₁₄ O ₆ -900	MOF-5	5.18	3.32	[7]
CS3K0U800	Glucose	6.67	4.26	[8]
NSDCS2700	Glucose	5.60	3.40	[9]
MNC-0-800	Magnesium gluconate	6.60	4.22	[10]
CN6-750-KOH	Biomass	5.57	3.91	[11]
OPMK-900	Biomass	6.67	3.97	[12]
LC-C22	Biomass	4.89	4.23	[13]
HSM-550-2	Biomass	6.34	4.23	[14]

Table S2. The contents of C, N, O, Zn in all samples based on XPS characterizations.

Sample	C (wt%)	N (wt%)	O (wt%)	Zn (wt%)
ZIF-8	68.43	18.44	6.25	6.88
ZNC-600	68.82	20.36	9.75	1.07
2ZNC-C ₉ H ₆ O ₆ -600	65.19	20.22	10.87	3.72
2ZNC-C ₃ H ₂ N ₂ -600	67.81	20.46	9.50	2.23
2ZNC-C ₁₆ H ₃₂ O ₂ -600	66.23	21.24	10.78	1.75
2ZNC-C ₁₂ H ₂₂ O ₁₁ -600	71.27	17.33	9.99	1.41
2ZNC-C ₂ H ₄ N ₄ -600	66.87	23.67	7.97	1.49
2ZNC-C ₃ H ₆ N ₆ -600	68.89	23.03	6.74	1.34
2ZNC-Na ₃ PO ₄ -600	65.50	22.83	8.99	2.68
2ZNC-Na ₂ SO ₄ -600	64.76	22.70	11.29	1.25
2ZNC-CH ₃ COONa-600	68.08	22.01	8.12	1.79
2ZNC-KOH-600	63.93	23.54	11.25	1.28
2ZNC-Na ₂ CO ₃ -600	66.71	21.74	10.36	1.19
2ZNC-KHCO ₃ -600	63.27	23.35	12.15	1.23

Table S3. BET specific surface area (S_{BET}), total pore volume (V_{total}), Porosity, and cumulative pore volume in the range of 0–20 Å, 0–10 Å and 5–7 Å of all samples.

Sample	S_{BET} (m^2/g)	V_{total} (cm^3/g)	Porosity (%)	V_{micro} (cm^3/g)	Cumulative pore volume (cm^3/g)		
					5–7(Å)	7–9(Å)	0–10(Å)
ZIF-8	1422.2111	0.582	36.79	0.471	0	0	0.291
ZNC-600	152.0762	0.230	18.70	0.042	0.018	0.011	0.031
2ZNC-C ₉ H ₆ O ₆ -600	14.0545	0.010	0.99	0.004	0	0	0
2ZNC-C ₃ H ₂ N ₂ -600	119.1156	0.121	10.79	0.032	0.013	0.010	0.023
2ZNC-C ₁₆ H ₃₂ O ₂ -600	90.057	0.124	11.03	0.020	0	0.009	0.009
2ZNC-C ₁₂ H ₂₂ O ₁₁ -600	213.34	0.108	9.75	0.060	0	0.048	0.048
2ZNC-C ₂ H ₄ N ₄ -600	522.3894	0.653	39.50	0.135	0.062	0.053	0.116
2ZNC-C ₃ H ₆ N ₆ -600	571.2232	0.476	32.25	0.149	0.078	0.042	0.120
2ZNC-Na ₃ PO ₄ -600	617.3971	0.482	32.52	0.174	0.025	0.137	0.162
2ZNC-Na ₂ SO ₄ -600	808.6519	0.376	27.33	0.257	0.041	0.161	0.202
2ZNC-CH ₃ COONa-600	1052.075	0.393	28.21	0.341	0.045	0.258	0.302
2ZNC-KOH-600	1020.1166	0.367	26.85	0.353	0.177	0.111	0.301
2ZNC-Na ₂ CO ₃ -600	1095.0764	0.497	33.20	0.361	0.187	0.108	0.295
2ZNC-KHCO ₃ -600	1179.73	0.466	31.79	0.388	0.025	0.294	0.320

Table S4. The carbon yields of ZNCs.

Sample	Carbon yield (wt%)
ZNC-600	34
2ZNC-C ₉ H ₆ O ₆ -600	36
2ZNC-C ₃ H ₂ N ₂ -600	50
2ZNC-C ₁₆ H ₃₂ O ₂ -600	38
2ZNC-C ₁₂ H ₂₂ O ₁₁ -600	42
2ZNC-C ₂ H ₄ N ₄ -600	44
2ZNC-C ₃ H ₆ N ₆ -600	45
2ZNC-Na ₃ PO ₄ -600	51
2ZNC-Na ₂ SO ₄ -600	43
2ZNC-CH ₃ COONa-600	48
2ZNC-KOH-600	54
2ZNC-Na ₂ CO ₃ -600	46
2ZNC-KHCO ₃ -600	57

Table S5. CO₂ adsorption capacity of samples at 25 °C and 0 °C (1 bar).

Sample	CO ₂ adsorption capacity at 1 bar (mmol/g)	
	0 °C	25 °C
ZIF-8	1.69	0.43
ZNC-600	2.58	1.81
2ZNC-C ₉ H ₆ O ₆ -600	1.83	1.40
2ZNC-C ₃ H ₂ N ₂ -600	1.86	1.44
2ZNC-C ₁₆ H ₃₂ O ₂ -600	2.05	1.55
2ZNC-C ₁₂ H ₂₂ O ₁₁ -600	2.31	1.95
2ZNC-C ₂ H ₄ N ₄ -600	3.54	2.51
2ZNC-C ₃ H ₆ N ₆ -600	3.31	3.03
2ZNC-Na ₃ PO ₄ -600	4.04	3.09
2ZNC-Na ₂ SO ₄ -600	3.55	3.41
2ZNC-CH ₃ COONa-600	5.51	4.07
2ZNC-KOH-600	5.37	4.41
2ZNC-Na ₂ CO ₃ -600	5.48	4.52
2ZNC-KHCO ₃ -600	6.55	4.60

Table S6. The content of different chemical states of N element before and after CO₂ adsorption on 2ZNC-KHCO₃-600.

2ZNC-KHCO ₃ -600	Pyridine-N (wt%)	Pyrrole-N (wt%)	Graphitic-N (wt%)	Oxide-N (wt%)
after adsorption of CO ₂	6.48	6.66	7.24	2.07
before adsorption of CO ₂	6.95	6.35	7.77	2.28

Table S7. The content of different chemical states of O element before and after CO₂ adsorption on 2ZNC-KHCO₃-600.

2ZNC-KHCO ₃ -600	quinones (wt%)	COOH (wt%)	C=O (wt%)	C-O (wt%)	O-H (wt%)
after adsorption of CO ₂	3.07	4.06	1.87	0.95	1.60
before adsorption of CO ₂	3.06	4.12	2.29	1.06	1.62

Table S8 The contents of N elements of different chemical states in ZNCs.

Sample	Pyridine-N (wt%)	Pyrrole-N (wt%)	Graphitic-N (wt%)	Oxide-N (wt%)
ZNC-600	6.12	5.23	7.48	1.53
2ZNC-C ₉ H ₆ O ₆ -600	6.90	4.99	7.10	1.23
2ZNC-C ₃ H ₂ N ₂ -600	8.22	4.97	5.91	1.36
2ZNC-C ₁₆ H ₃₂ O ₂ -600	8.04	5.71	6.38	1.11
2ZNC-C ₁₂ H ₂₂ O ₁₁ -600	6.18	4.48	5.86	0.81
2ZNC-C ₂ H ₄ N ₄ -600	9.59	5.65	7.11	1.32
2ZNC-C ₃ H ₆ N ₆ -600	8.82	5.76	6.78	1.67
2ZNC-Na ₃ PO ₄ -600	9.53	7.32	5.22	0.76
2ZNC-Na ₂ SO ₄ -600	7.62	5.69	7.95	1.44
2ZNC-CH ₃ COONa-600	8.80	6.07	6.19	0.95
2ZNC-KOH-600	7.20	6.82	8.08	1.44
2ZNC-Na ₂ CO ₃ -600	6.96	6.73	7.21	0.84
2ZNC-KHCO ₃ -600	6.95	6.35	7.77	2.28

Table S9 Contents of O elements of different chemical states in ZNCs.

Sample	quinones (wt%)	COOH (wt%)	C=O (wt%)	C-O (wt%)	O-H (wt%)
ZNC-600	3.85	2.62	1.01	1.44	0.83
2ZNC-C ₉ H ₆ O ₆ -600	4.49	2.97	1.93	0.75	0.73
2ZNC-C ₃ H ₂ N ₂ -600	3.48	3.10	0.98	0.93	1.01
2ZNC-C ₁₆ H ₃₂ O ₂ -600	4.80	2.22	1.49	1.20	1.07
2ZNC-C ₁₂ H ₂₂ O ₁₁ -600	4.03	2.02	1.35	1.21	1.38
2ZNC-C ₂ H ₄ N ₄ -600	2.15	1.51	1.36	2.02	0.93
2ZNC-C ₃ H ₆ N ₆ -600	2.11	2.14	0.89	0.76	0.84
2ZNC-Na ₃ PO ₄ -600	3.71	2.07	0.86	0.96	1.39
2ZNC-Na ₂ SO ₄ -600	4.48	3.39	1.41	0.67	1.34
2ZNC-CH ₃ COONa-600	2.77	3.20	1.07	0.59	0.49
2ZNC-KOH-600	2.70	3.89	1.45	1.00	2.24
2ZNC-Na ₂ CO ₃ -600	2.78	3.39	1.37	1.13	1.69
2ZNC-KHCO ₃ -600	3.06	4.12	2.29	1.06	1.62

Table S10. Results of Lasso regression analysis.

	Non-standardized coefficient	standardized coefficient	P
constant	1.132	-	0.158
V ₀₋₁₀ (Å)	9.034	0.975	0.000
V ₇₋₉ (Å)	0.000	-0.041	1.000
Pyrrolic content	0.059	0.047	0.645
COOH content	0.000	-0.033	1.000
O-H content	0.076	0.050	0.691
R ²		0.980	

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