

Supporting Information

Efficient Selective Capture of Carbon Dioxide from Nitrogen and Methane Using a Metal-Organic Framework-Based Nanotrap

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S1. Fitting parameters of the DSLF model for isotherms of CO₂, N₂, and CH₄ on ZnAtzCO₃

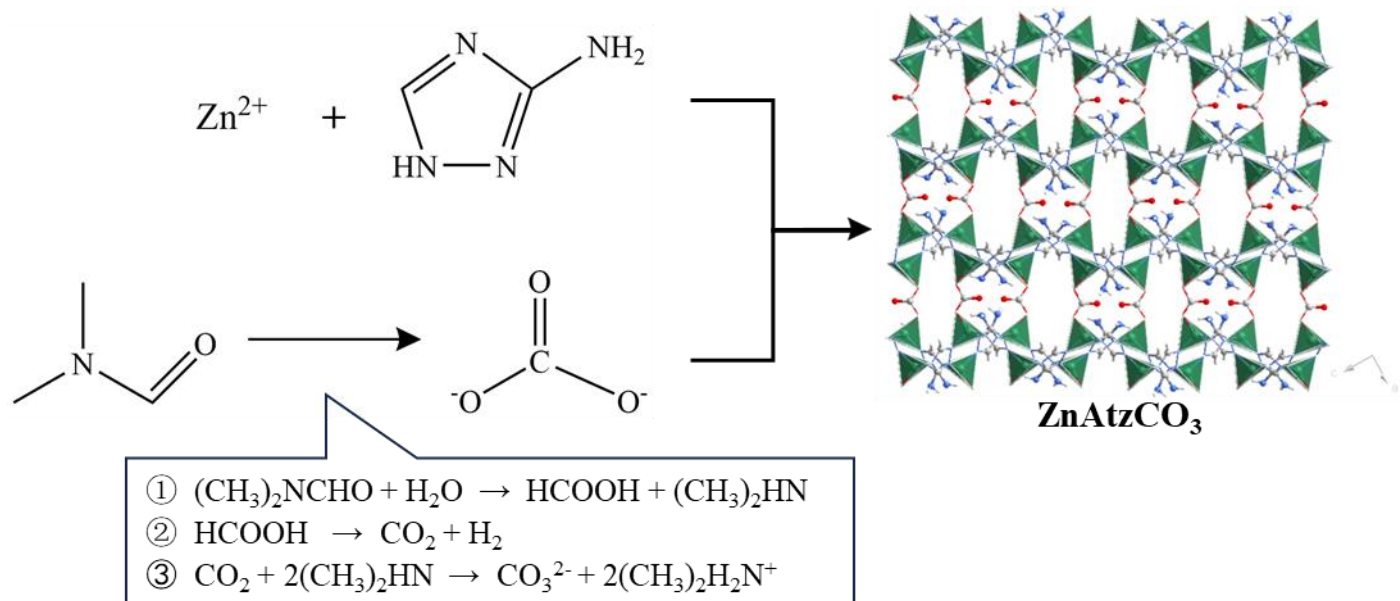
Table S1. Fitting parameters of the DSLF model for isotherms of CO₂, N₂, and CH₄ on ZnAtzCO₃

Parameters	CO ₂	N ₂	CH ₄
q ₁	3.214	0.4353	1.335
b ₁	0.192	0.002757	0.008264
c	0.756	1.063	0.9743
q ₂	1.235	0.2935	0.3774
b ₂	0.00099	0.001972	0.002858
t	0.751	1.122	1.029
R ²	0.9961	0.9993	0.9999

S2. Fitting parameters and correlation coefficients of the Virial equation for all gases on ZnAtzCO₃**Table S2.** Fitting parameters and correlation coefficients of the Virial equation for all gases on ZnAtzCO₃

Gas	a ₀	a ₁	a ₂	a ₃	a ₄	b ₀	b ₁	R ²
CO ₂	-5811.5	3.283	-0.0027	3.37E-6	-1.147E-9	15.72	-0.0074	0.9980
N ₂	-2174.2	-21.24	0.263	-0.00299	1.174E-5	10.03	0.045	0.9958
CH ₄	-2690.9	1.643	0.0145	-8.75E-5	1.52E-7	10.52	-0.0030	0.9976

S3. Synthetic pathways for ZnAtzCO₃



Scheme S1. Synthetic pathways for ZnAtzCO₃ with starting reactants of ZnSO₄/HAtz/DMF/H₂O at 523 K

S4. Asymmetric unit of ZnAtzCO_3

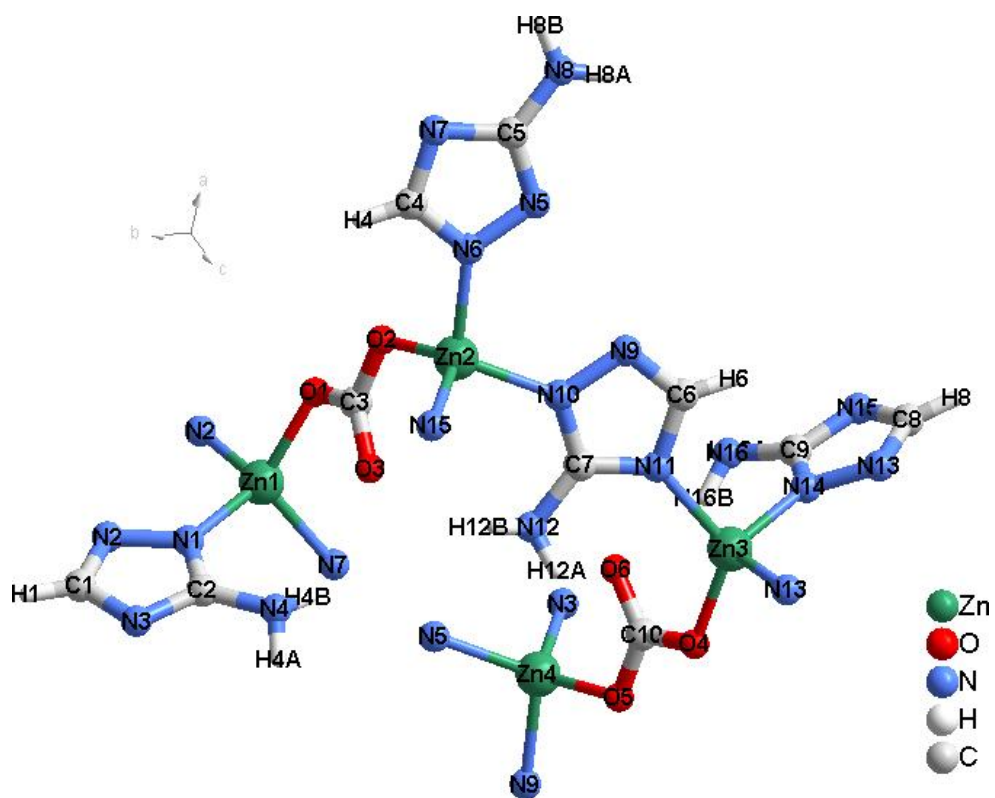


Figure S1. Asymmetric unit of ZnAtzCO_3

S5. Pore size distribution of ZnAtzCO₃ based on the HK model using CO₂ as the probe molecule

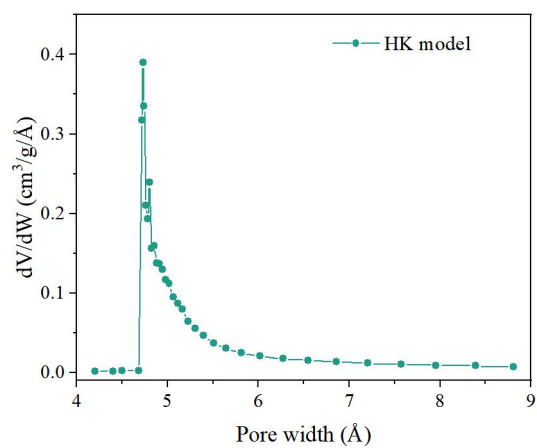


Figure S2. Pore size distribution of ZnAtzCO₃ based on the HK model using CO₂ as the probe molecule

S6. CO₂ breakthrough time for CO₂/N₂ and CO₂/CH₄ mixtures in five cycles of breakthrough experiments on ZnAtzCO₃

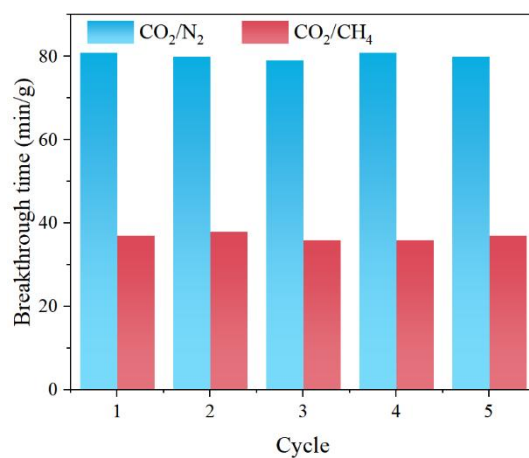


Figure S3. CO₂ breakthrough times of CO₂/N₂ (v:v, 15:85) and CO₂/CH₄ (v:v, 50:50) mixtures in five cycles of breakthrough experiments on ZnAtzCO₃