

Article

# Modulating and Orienting an Anisotropic Zn-Based Metal Organic Framework for Selective CH<sub>4</sub>/CO<sub>2</sub> Gas Separation

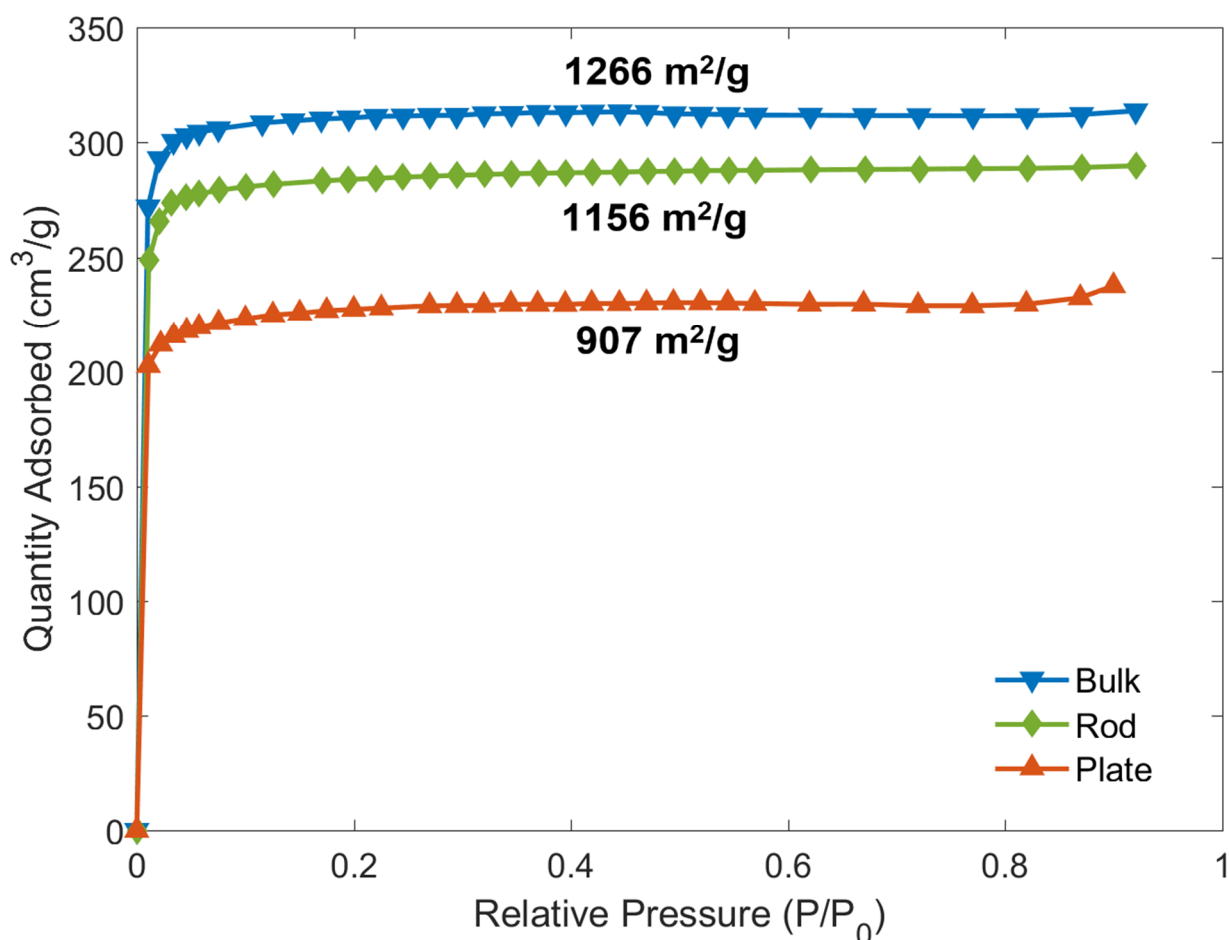
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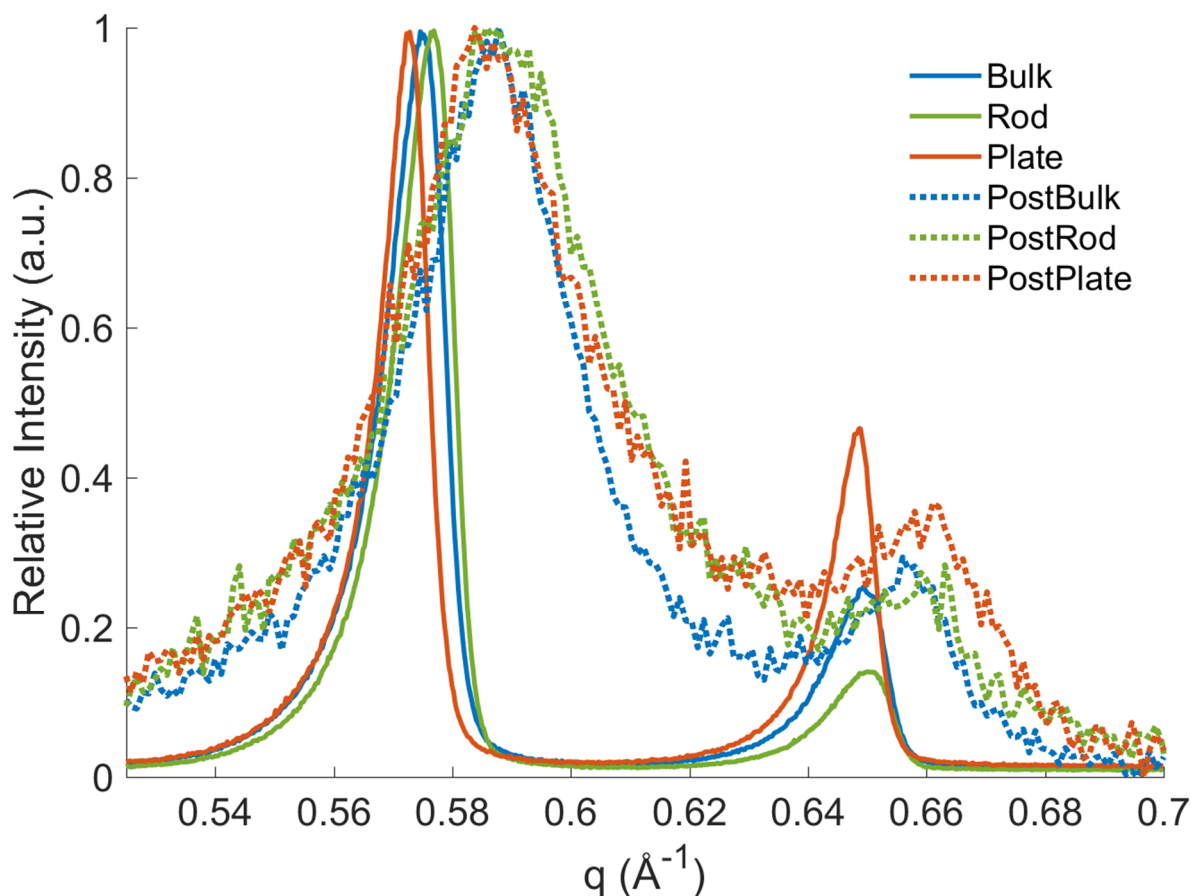
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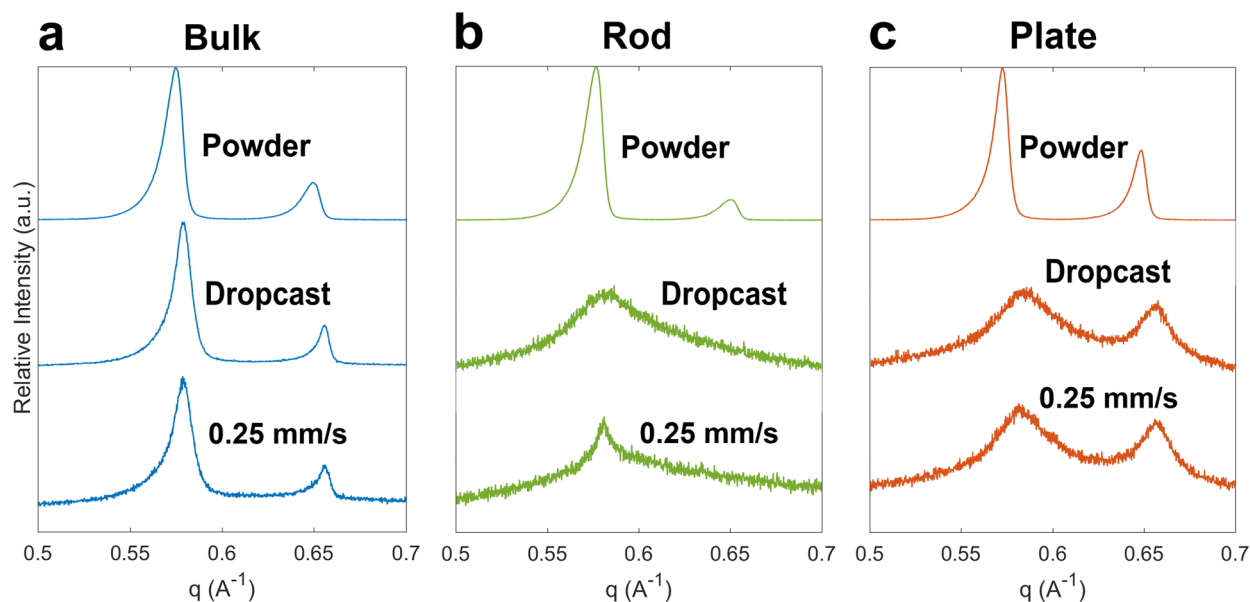
## Supplementary Information



**Figure S1.** Representative nitrogen isotherms for varied morphologies of [Zn<sub>2</sub>(NDC)<sub>2</sub>(DABCO)]<sub>n</sub>.



**Figure S2.** PXRD patterns for MOF material pre and post-competitive gas adsorption procedure showing peak broadening for all samples, indicating sample degradation.



**Figure S3.** PXRD patterns for powder, drop cast and solution sheared MOFs. XRDs were taken with the same XRD geometry reported in the main text, with no revolution during the scans. Additionally, these XRDs were taken parallel to the shearing direction of the material. (a) are the bulk material XRDs, while (b) and (c) are the rod and plate morphologies' XRDs, respectively.

**Table S1.** BET Surface Areas and standard error of  $[\text{Zn}_2(\text{NDC})_2(\text{DABCO})]_n$  with differing drying procedures.

Drying Procedure	BET Surface Area ( $\text{m}^2/\text{g}$ )
Degassed at 90°C, heated at 100°C for 12 h	451 ± 122
Degassed at 80°C, heated at 85°C for 8 h	780
Degassed at 70°C, heated at 80°C for 8 h	1100 ± 68

**Table S2.** Equilibrium adsorption quantities in competitive adsorption environment.

Morphology	CO <sub>2</sub> Uptake (mmol/g)	CH <sub>4</sub> Uptake (mmol/g)	CO <sub>2</sub> /CH <sub>4</sub> Selectivity
<i>Bulk</i>	0.184 ± 0.022	0.042 ± 0.006	4.38 ± 1.16
<i>Rod</i>	0.650 ± 0.300	0.152 ± 0.008	4.27 ± 0.42
<i>Plate</i>	0.232 ± 0.021	0.056 ± 0.006	4.15 ± 0.85

**Table S3.** Diffusion time constant data for CO<sub>2</sub> and CH<sub>4</sub> at 700 mmHg and 273 K for multiple trials.

Rod	D/r <sup>2</sup> CO <sub>2</sub> (1/s)	D/r <sup>2</sup> CH <sub>4</sub> (1/s)	CO <sub>2</sub> /CH <sub>4</sub> Selectivity
<b>700mmHg</b>			
Trial 1	2.11E-03	6.31E-03	
Trial 2		1.22E-02	
Trial 3		1.09E-02	
Trial 4		9.01E-03	
Trial 5	1.80E-03	7.30E-03	
Trial 6	1.50E-03	7.56E-03	
Trial 7	1.50E-03	7.93E-03	
AVG	1.73E-03	8.75E-03	1.97E-01
STDERR	1.26E-04	7.43E-04	2.21E-02
Bulk	D/r <sup>2</sup> CO <sub>2</sub> (1/s)	D/r <sup>2</sup> CH <sub>4</sub> (1/s)	CO <sub>2</sub> /CH <sub>4</sub> Selectivity
<b>700mmHg</b>			
Trial 1	1.46E-03	6.40E-03	
Trial 2	1.53E-03	4.84E-03	
Trial 3	1.73E-03	4.06E-03	
Trial 4		5.65E-03	
AVG	1.57E-03	5.24E-03	3.00E-01
STDERR	6.74E-05	4.38E-04	2.82E-02
Plate	D/r <sup>2</sup> CO <sub>2</sub> (1/s)	D/r <sup>2</sup> CH <sub>4</sub> (1/s)	CO <sub>2</sub> /CH <sub>4</sub> Selectivity
<b>700mmHg</b>			
Trial 1	2.21E-03	6.25E-03	
Trial 2	2.50E-03	4.03E-03	
Trial 3	2.03E-03	4.21E-03	
Trial 4	1.53E-03	4.61E-03	
Trial 5	1.55E-03	4.61E-03	
Trial 6	1.47E-03	4.61E-03	
AVG	1.88E-03	4.72E-03	3.99E-01
STDERR	1.48E-04	2.73E-04	3.90E-02