Electronic Supplementary Information

First-Order and Gradual Phase Transitions of Ethane confined in MCM-41

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Experimental data of capillary condensation

Table S1. Experimental data of capillary condensation of ethane in MCM-41.

92 mg MCM-41			150 mg MCM-41			210 mg MCM-41		
T, K	*P*, bar	*h*, J	*T*, K	*P*, bar	*h*, J	*T*, K	*P*, bar	*h*, J
249.1	6.58	0.262	266.8	11.24	0.133	258.6	8.94	0.354
234.4	3.85	0.483	256.2	8.15	0.320	251.0	6.95	0.676
206.3	1.14	0.909	249.8	6.65	0.443	239.1	4.62	1.014
			240.5	4.85	0.597	224.4	2.62	1.531
			227.3	2.94	0.902	208.3	1.28	2.052
			212.2	1.52	1.265			

The uncertainties of capillary-condensation data

With the same procedure as that used in our previous work[1] for determining the uncertainties of capillary-condensation of methane in MCM-41 and SBA-15, we use the bulk condensation of ethane along with the melting points of standard substances from literature to derive the uncertainties of measurements in this work. More details can be referred to the Supporting Information in our previous work. We define the temperature correction as

$$\Delta T_{corr} = T - T_{\exp} \tag{S1}$$

where T is the temperature obtained from literature ('true' temperature) and $T_{\exp}$ is the measured temperature. The temperature correction data obtained are statistically averaged to obtain the mean temperature correction ($\Delta T_{\text{corr, mean}} = -0.320$ K) and standard deviation ($\sigma = 0.237$ K ≈ 0.2 K), as shown in Figure S2. The mean temperature correction is then applied to all temperature measurements in this work, and the standard deviation is the uncertainty of the measurements. The corrected temperature is then given by

$$T_{corr} = T_{\exp} + \Delta T_{\text{corr,mean}} \tag{S2}$$

with an uncertainty of ± 0.2 K.

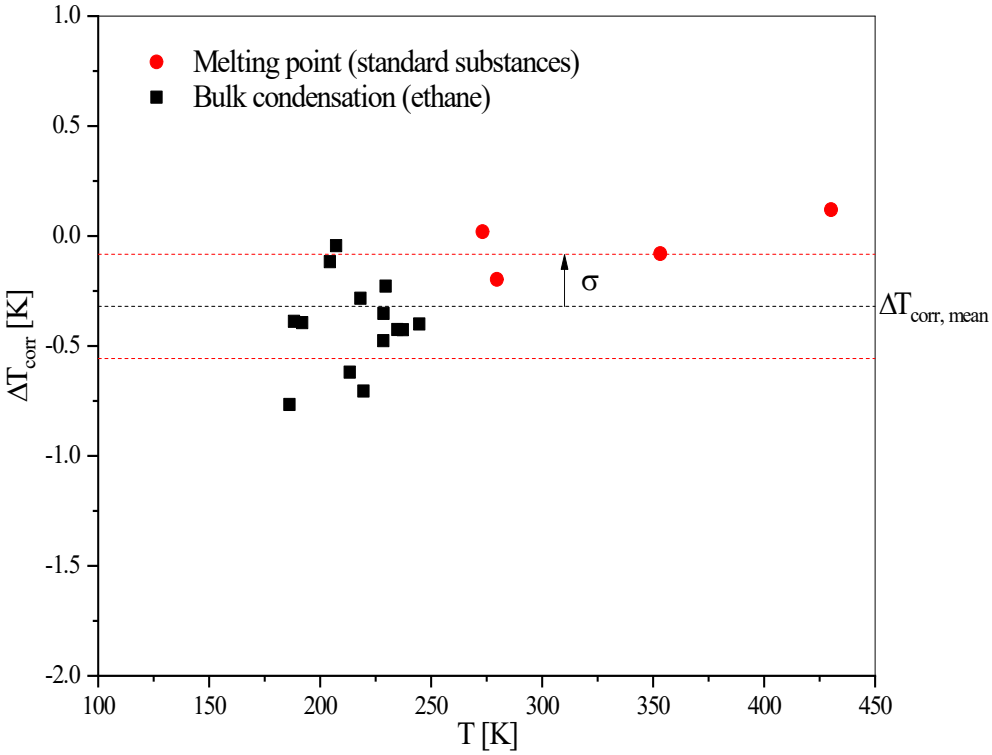

Figure S2. The correction of temperatures for the melting points of standard substances during calibration and bulk ethane condensation during capillary condensation measurements.

Procedure of uncertainty determination for PCP

The procedure to determine the uncertainties of PCP is the same as that adopted in our previous work.[1] The results are given below:

Table S2. Uncertainty determination for T_{Cp} of ethane in MCM-41.

Adsorbent amount, mg	Intercept	Standard error	Intercept + Standard error	Intercept - Standard error	Minimum, K	Maximum, K
92	0.00365	1.70E-05	3.67E-03	3.63E-03	272.705	275.252
150	0.00363	4.82E-06	3.63E-03	3.63E-03	275.116	275.849
210	0.00364	2.08E-05	3.66E-03	3.62E-03	273.164	276.305
Mean					273.662	275.802
T_{Cp} derived directly from three-line approach, K					275.000	
T_{Cp} with uncertainty, K					$275.0^{+0.8}_{-1.3}$	

Table S3. Uncertainty determination for P_{Cp} of ethane in MCM-41.

Adsorbent amount, mg	Intercept	Standard error	Intercept + Standard error	Intercept - Standard error	Minimum, bar	Maximum, bar
92	2.64966	3.12E-02	2.68E+00	2.62E+00	13.715	14.598
150	2.66038	9.46E-03	2.67E+00	2.65E+00	14.167	14.438
210	2.66672	4.22E-02	2.71E+00	2.62E+00	13.798	15.013
Mean					13.893	14.683
P_{Cp} derived directly from three-line approach, bar					14.319	
P_{Cp} with uncertainty, bar					$14.3^{+0.4}_{-0.4}$	

References

1. Yang, H.; Jayaatmaja, K.; Dejam, M.; Tan, S. P.; Adidharma, H. Phase transition and criticality of methane confined in nanopores. Langmuir **2022**, 38, 2046-2054.