

Supplementary Materials

for

Leveraging Nanocrystal HKUST-1 in Mixed-matrix Membranes for Ethylene/Ethane Separation

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Table S1. Fitting parameters for C₂H₄ and C₂H₆ for membranes at 35 °C.Unit of p = bar; Unit of q = mmol g⁻¹

$$q = \frac{q_{sat} b_1 p}{1 + b_1 p}$$

Sample	gas	$q_{sat,1}$	b_1	R ² value
ODPA-TMPDA	C ₂ H ₄	1.111	1.533	0.9974
	C ₂ H ₆	1.459	0.7410	0.9896
ODPA-TMPDA + 20 wt% HKUST-1	C ₂ H ₄	1.153	3.207	0.9998
	C ₂ H ₆	1.318	1.599	0.9928
6FDA-TMPDA	C ₂ H ₄	1.032	1.698	1
	C ₂ H ₆	0.9732	2.181	0.9999
6FDA-TMPDA + 20 wt% HKUST-1	C ₂ H ₄	1.147	2.588	0.9964
	C ₂ H ₆	1.121	3.231	0.9978

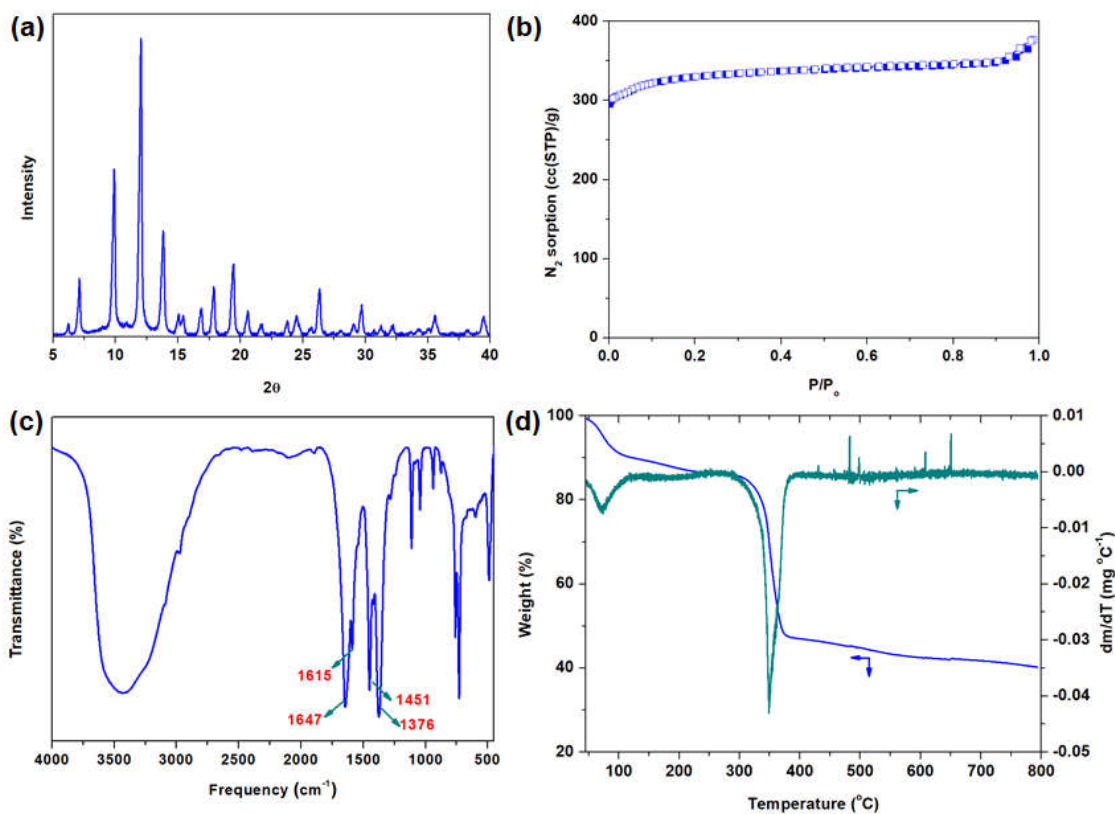


Figure S1. Characterization of nanocrystal HKUST-1, showing (a) X-ray diffraction pattern; (b) N_2 physisorption isotherm at 77 K (open and closed symbols indicate adsorption and desorption branches, respectively); (c) FT-IR spectrum, as well as (d) TGA curves, showing weight loss and dm/dT against temperature, of nanocrystal HKUST-1 from 40 to 800 °C.

Table S2. Porosity properties of nanocrystal HKUST-1 based on N_2 physisorption at 77 K.

$S_{BET}^{[a]}$ (m^2/g)	$S_{LANG}^{[a]}$ (m^2/g)	$S_{micro}^{[b]}$ (m^2/g)	$V_{micro}^{[b]}$ (cc/g)	$V_{total}^{[c]}$ (cc/g)
1125	1464	1087	0.502	0.585

Note: ^[a] P/P_0 range from 0.05 to 0.2 was used to determine the BET and Langmuir surface area; ^[b]t-plot method was used to calculate the micropore surface area and volume, by choosing the P/P_0 range from 0.4 to 0.6; ^[c] $P/P_0 = 0.99$ was used to calculate the total pore volume.

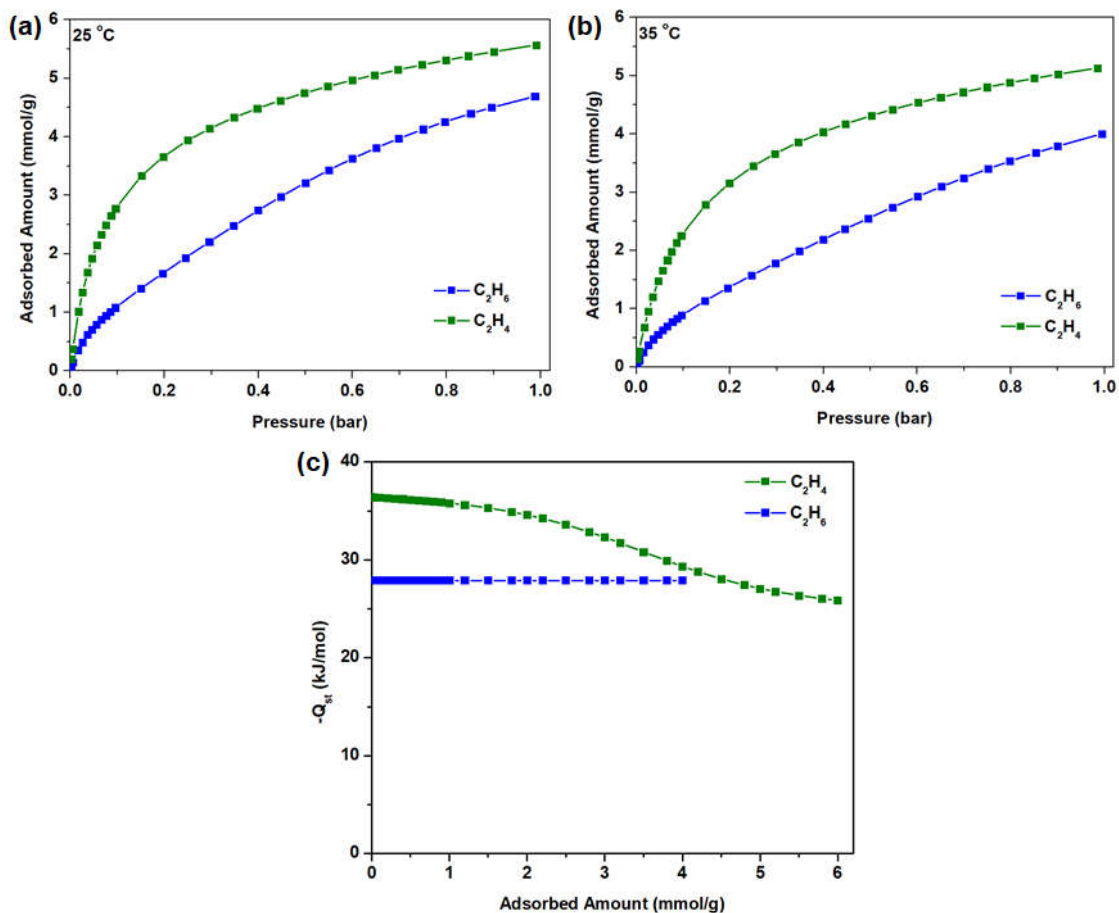


Figure S2. C_2H_4 and C_2H_6 adsorption of HKUST-1 at (a) 25 °C and (b) 35 °C; (c) $-Q_{st}$ of HKUST-1 for C_2H_4 and C_2H_6 .

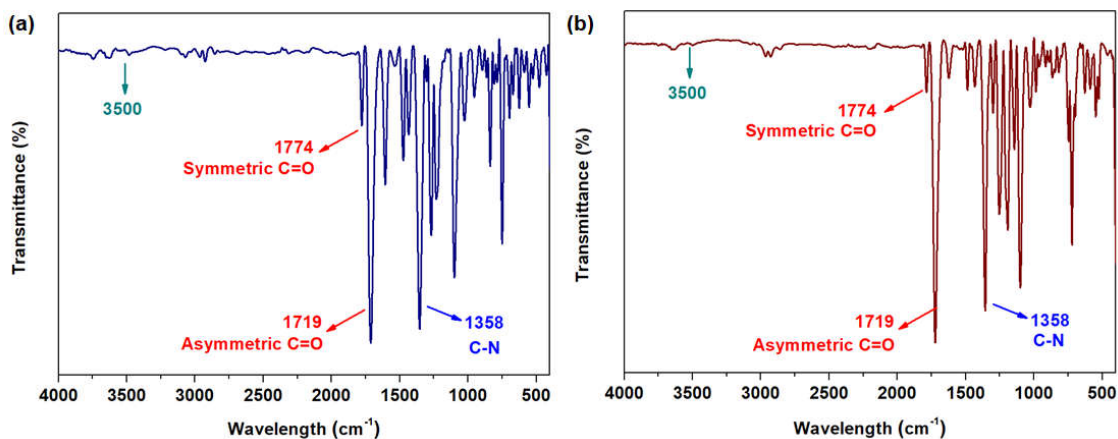


Figure S3. FT-IR spectrum of (a) ODPA-TMPDA and (b) 6FDA-TMPDA polymer.

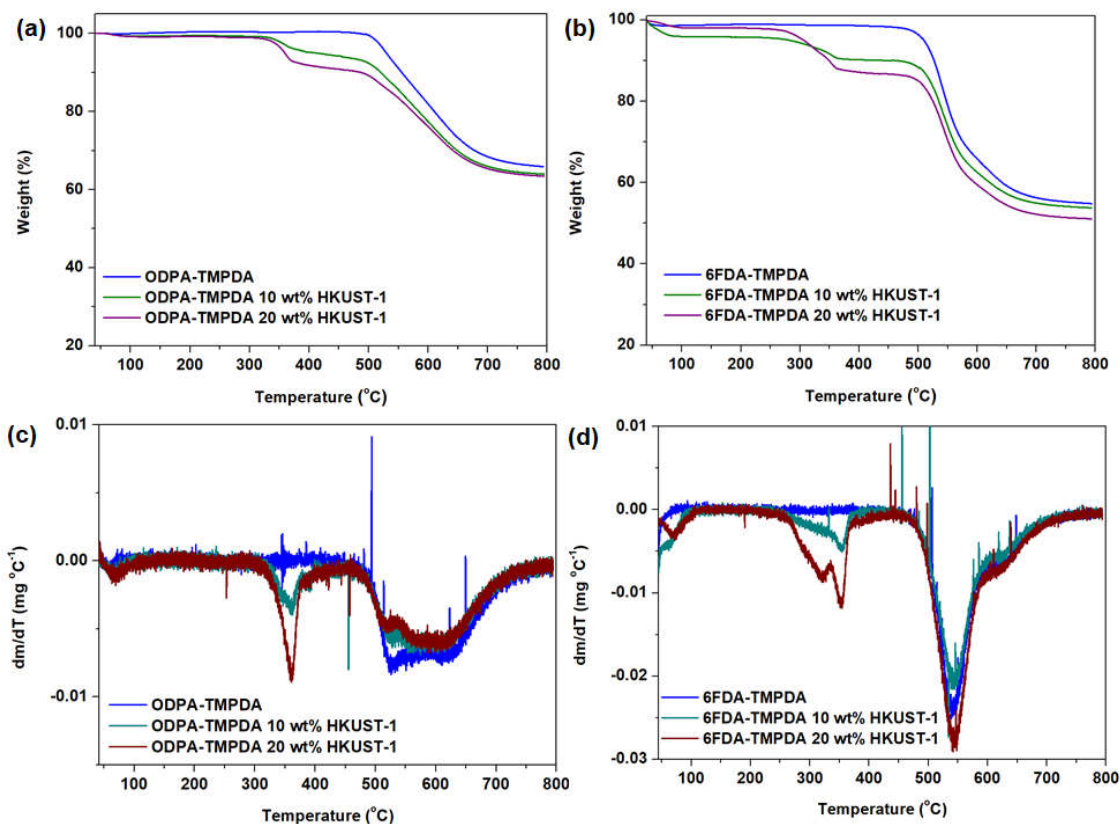


Figure S4. TGA analysis (a, b) weight loss against temperature and (c, d) dm/dT against temperature of 10 wt% and 20 wt% nanocrystal HKUST-1 loading in (a, c) ODP-TMPDA and (b, d) 6FDA-TMPDA polymer.

Table S3. Fitting parameters for C₂H₄ and C₂H₆ for HKUST-1 at 25 and 35 °C.

Unit of p = bar; Unit of q = mmol g⁻¹

$$q = \frac{q_{sat,1} b_1 p}{1 + b_1 p} + \frac{q_{sat,2} b_2 p}{1 + b_2 p}$$

Sample	gas	$q_{sat,1}$	b_1	$q_{sat,2}$	b_2	R^2 value
HKUST-1 (25 °C)	C ₂ H ₄	3.563	1.574	3.498	20.29	0.9998
	C ₂ H ₆	7.208	1.697	-	-	0.9921
HKUST-1 (35 °C)	C ₂ H ₄	3.563	1.145	3.498	12.44	1
	C ₂ H ₆	7.208	1.178	-	-	0.9921