Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

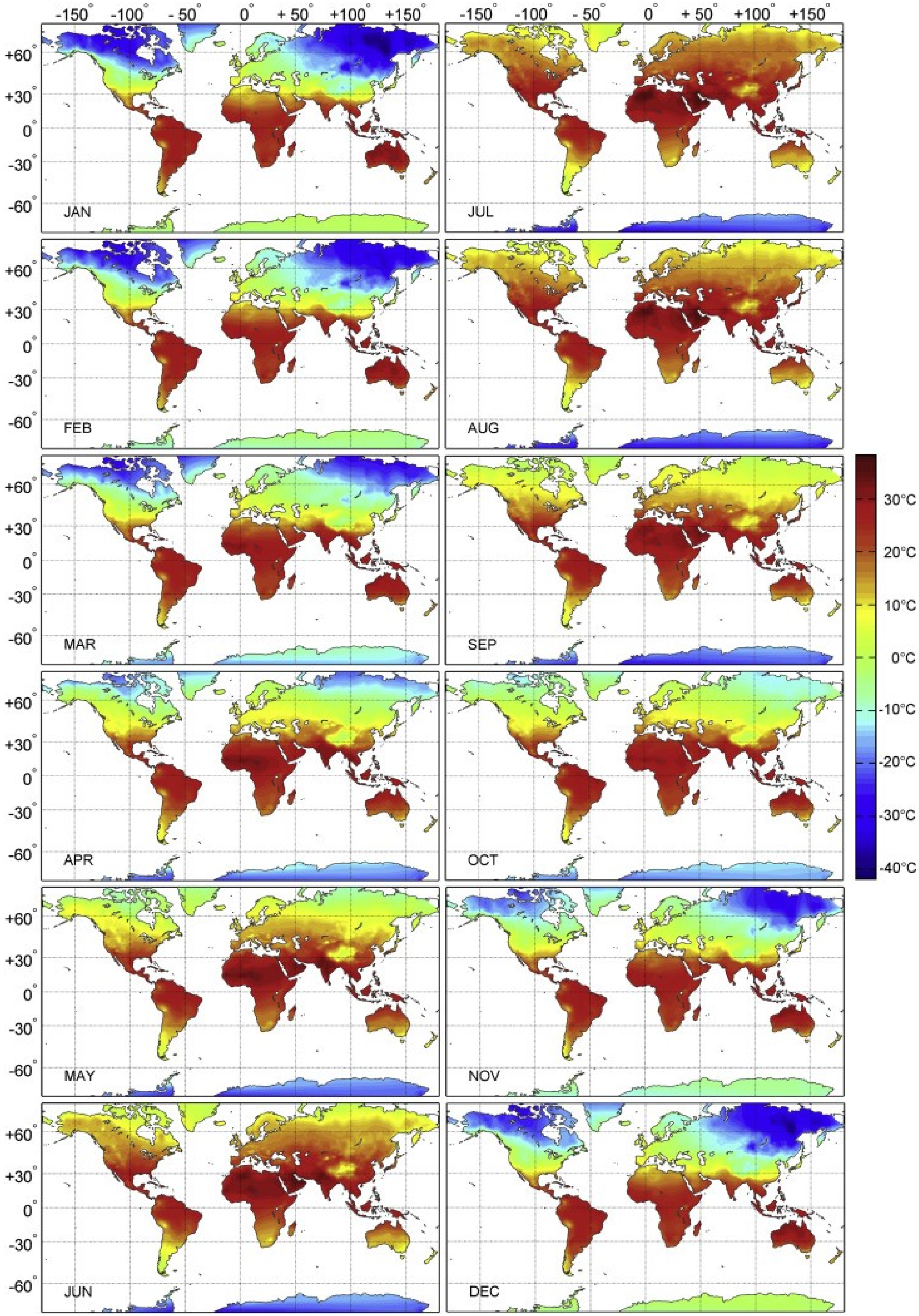
Supporting Information

Ambient and sub-ambient temperature direct air CO_2 capture (DAC) by novel supported in-situ polymerized amines

Akram A. Al-Absi, Anne M. Benneker, Nader Mahinpey*

Department of Chemical and Petroleum Engineering, Schulich School of Engineering, University of Calgary, Calgary, AB, T2N 1N4, Canada

*** Corresponding author:** nader.mahinpey@ucalgary.ca



Supporting Figure S.1 Temporal distribution of mean temperature (°C). Copyright 2016 Elsevier [1]

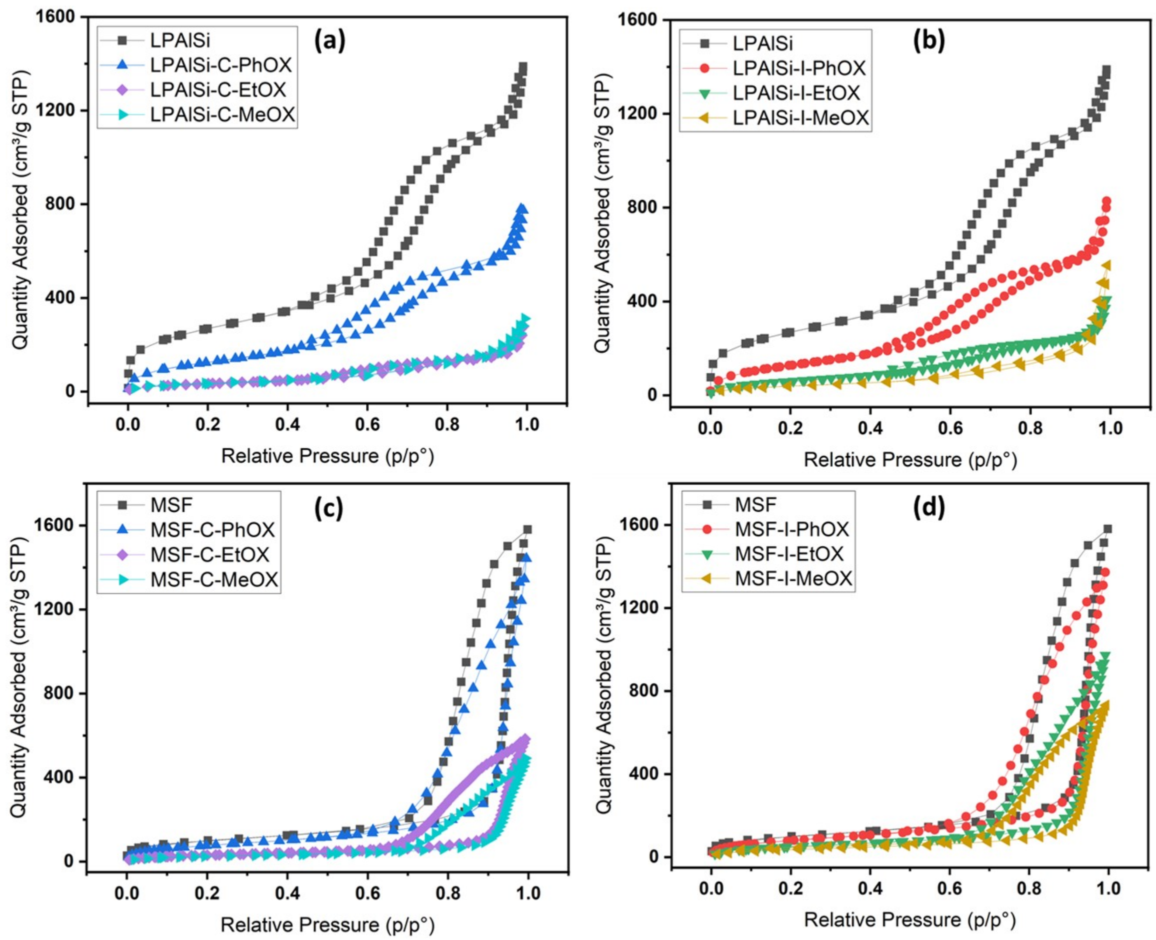


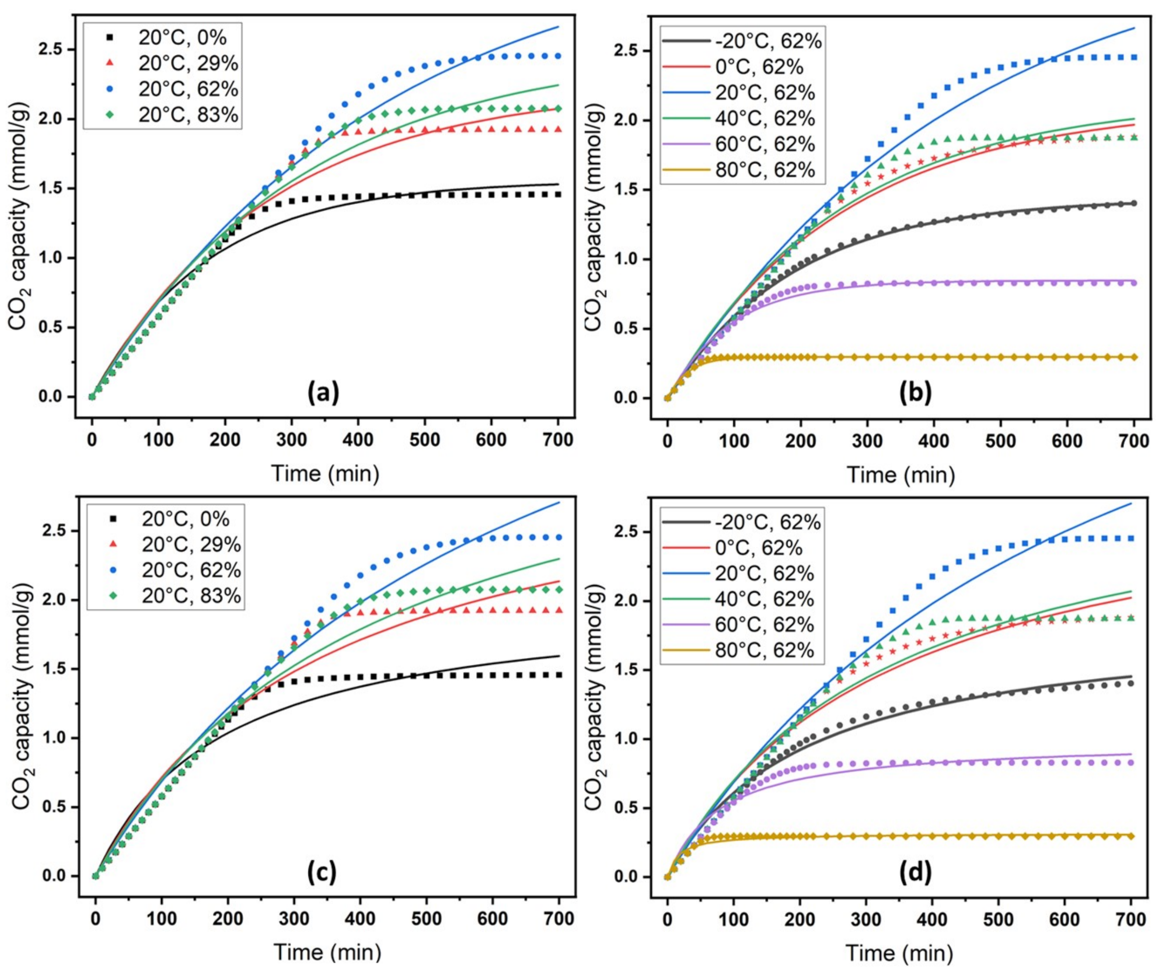
Figure S.2 N_2 adsorption-desorption isotherms at -195.8°C of (a) and (b) LPAlSi based materials, (c) and (d) MSF based materials.

Supporting Table S.1 kinetic parameters for pseudo-1st-order and pseudo-2nd-order models for CO_2 adsorption at different conditions

	First order						
Adsorption conditions	k_1 (min^{-1})	q_e*	R_2	RSS (%)	ARE%	q_{exp}*	Δ q_e (%)
20°C, 0% RH	0.0058	1.56	0.9955	7.8	11.2	1.46	6.9
20°C, 29% RH	0.0038	2.23	0.9941	11.1	12.3	1.92	16.0
20°C, 62% RH	0.0023	3.34	0.9961	10.5	10.1	2.45	35.9
20°C, 83% RH	0.0032	2.51	0.9956	10.0	10.8	2.08	20.7
-20°C, 62% RH	0.0053	1.44	0.9995	2.3	4.5	1.40	2.5
0°C, 62% RH	0.0039	2.11	0.9976	6.6	9.0	1.88	12.1
40°C, 62% RH	0.0038	2.16	0.9955	9.4	11.1	1.87	15.3
60°C, 62% RH	0.0106	0.85	0.9982	3.1	6.6	0.83	2.3
80°C, 62% RH	0.0338	0.30	0.9990	0.9	3.1	0.30	0.7
	Second order						
	k_2 #	q_e*	R_2	RSS %	ARE%	q_{exp}*	Δ q_e (%)

20°C, 0% RH	0.0026	2.03	0.9919	10.4	14.8	1.46	39.3
20°C, 29% RH	0.0009	3.19	0.9916	13.1	14.3	1.92	66.0
20°C, 62% RH	0.0003	5.29	0.9952	11.6	10.9	2.45	115.8
20°C, 83% RH	0.0006	3.71	0.9938	11.8	12.4	2.08	78.6
-20°C, 62% RH	0.0025	1.89	0.9983	4.3	8.0	1.40	34.6
0°C, 62% RH	0.0010	2.99	0.9959	8.7	11.3	1.88	58.9
40°C, 62% RH	0.0010	3.07	0.9932	11.5	13.2	1.87	64.2
60°C, 62% RH	0.0128	0.99	0.9940	5.6	12.0	0.83	19.5
80°C, 62% RH	0.1876	0.32	0.9955	1.9	7.2	0.30	6.8

* mmolCO_2/g, # (g/mmol CO_2/min).



Supporting Figure S.3 Experimental CO_2 adsorption data versus first (a, b) and second order kinetics models (c, d): (a, c) at different temperatures, (b, d) at different relative humidities.

Supporting Table S.2 Langmuir and Freundlich isotherms' parameters for MSF-C-EtOX and LPAlSi-C-EtOX at different temperatures.

	parameter	MSF-C-EtOX				
Model	**Temperature**	**-20 °C**	**0 °C**	**20 °C**	**40 °C**	**60 °C**
Langmuir	q_m (mmol/g)	1.18	1.33	1.85	2.47	2.02
	K_L ($mbar^{-1}$)	16.91	4.83	5.85	5.20	1.38
	RSS %	**9.7**	**13.1**	**11.7**	**9.3**	**8.7**
	ARE%	**7.2**	**9.2**	**6.5**	**3.6**	**6.5**
Freundlich	n	12.53	13.59	12.54	18.03	9.89
	K_F ($mmol/g(mbar)^{(-1/n)}$)	0.74	0.87	1.16	1.82	1.10
	RSS %	**2.8**	**2.9**	**14.5**	**16.8**	**20.8**
	ARE%	**2.1**	**2.0**	**10.9**	**6.4**	**20.1**
	LPAlSi-C-EtOX					
Langmuir	q_m (mmol/g)	1.92	1.07	1.88	2.54	2.46
	K_L ($mbar^{-1}$)	0.02	2.95	0.12	4.64	0.33
	RSS %	**16.1**	**11.6**	**20.2**	**13.7**	**12.8**
	ARE%	**10.6**	**10.0**	**10.1**	**5.2**	**7.0**
Freundlich	BT (J.g/mmol^2)	8.769	26.503	15.889	21.106	10.943
	K_F ($mmol/g(mbar)^{(-1/n)}$)	2	773	356	4015300	44
	RSS %	**11.1**	**5.0**	**9.2**	**10.1**	**13.0**
	ARE%	**3.0**	**4.0**	**3.5**	**3.6**	**16.5**

References

1 M. Mourshed, *Renewable energy*, 2016, **94**, 55–71.