Supplementary Information:

Cost-effective CO_2 capture based on *in silico* screening of zeolites and process optimization

M. M. Faruque Hasan,[1] Eric L. First,[1] and Christodoulos A. Floudas[*]

Department of Chemical and Biological Engineering, Princeton University

Princeton, NJ, 08544, USA

Contents

[1] These authors have contributed equally.

[*] Author to whom all correspondence should be addressed; Tel: (609) 258-4595; Fax: (609) 258-0211; E-mail: floudas@titan.princeton.edu.

Micropore diffusion of CO_2 and N_2 in zeolites

Table S1: Analysis of mass transfer control in selected zeolites. Micropore diffusivities are calculated for CO_2 and N_2 in selected zeolites using molecular dynamics simulations, and micropore resistances are calculated by eqn (9) in the main text. Macropore resistance is 2.49×10^{-2} s, from eqn (8) in the main text.

	Micropore diffusivity (cm^2/s)		Micropore resistance (s)		Macropore/micropore resistance ratio	
Zeolite	CO_2	N_2	CO_2	N_2	CO_2	N_2
AFG	1.60×10^{-8}	2.00×10^{-9}	8.42×10^{-12}	1.48×10^{-9}	2.96×10^{9}	1.68×10^{7}
AFX	1.00×10^{-10}	1.00×10^{-10}	2.89×10^{-9}	7.68×10^{-8}	8.63×10^{6}	3.24×10^{5}
AHT	8.80×10^{-8}	3.00×10^{-9}	7.56×10^{-13}	1.13×10^{-8}	3.29×10^{10}	2.21×10^{6}
ANA	1.00×10^{-9}	1.00×10^{-9}	2.87×10^{-8}	1.75×10^{-8}	8.68×10^{5}	1.42×10^{6}
AST	4.00×10^{-9}	2.00×10^{-9}	1.87×10^{-10}	1.64×10^{-9}	1.33×10^{8}	1.52×10^{7}
BCT	4.27×10^{-6}	4.73×10^{-7}	9.05×10^{-11}	9.82×10^{-9}	2.75×10^{8}	2.54×10^{6}
DAC	1.00×10^{-10}	1.00×10^{-10}	1.09×10^{-9}	6.22×10^{-8}	2.29×10^{7}	4.00×10^{5}
FAR	8.00×10^{-9}	1.00×10^{-10}	4.47×10^{-11}	3.60×10^{-8}	5.57×10^{8}	6.93×10^{5}
FRA	4.00×10^{-9}	1.00×10^{-9}	5.30×10^{-11}	3.19×10^{-9}	4.70×10^{8}	7.80×10^{6}
GIS	1.00×10^{-10}	1.00×10^{-10}	4.32×10^{-10}	5.21×10^{-8}	5.76×10^{7}	4.78×10^{5}
GIU	2.50×10^{-8}	1.00×10^{-10}	9.58×10^{-12}	3.12×10^{-8}	2.60×10^{9}	7.98×10^{5}
JBW	1.00×10^{-10}	1.00×10^{-10}	4.53×10^{-10}	8.79×10^{-8}	5.50×10^{7}	2.84×10^{5}
LOS	6.60×10^{-8}	1.00×10^{-9}	8.14×10^{-13}	2.79×10^{-9}	3.06×10^{10}	8.95×10^{6}
MAR	5.35×10^{-7}	1.00×10^{-9}	8.80×10^{-13}	2.55×10^{-9}	2.83×10^{10}	9.78×10^{6}
MFI	5.12×10^{-5}	1.58×10^{-4}	1.37×10^{-14}	8.14×10^{-14}	1.81×10^{12}	3.06×10^{11}
MSO	2.30×10^{-8}	1.00×10^{-10}	2.11×10^{-11}	4.06×10^{-8}	1.18×10^{9}	6.14×10^{5}
MTN	2.00×10^{-9}	1.00×10^{-9}	4.28×10^{-10}	4.55×10^{-9}	5.83×10^{7}	5.48×10^{6}
MVY	3.00×10^{-9}	1.96×10^{-6}	2.27×10^{-11}	7.89×10^{-11}	1.10×10^{9}	3.16×10^{8}
NON	3.00×10^{-9}	6.00×10^{-9}	1.68×10^{-10}	8.00×10^{-10}	1.48×10^{8}	3.12×10^{7}
SGT	5.00×10^{-9}	2.00×10^{-9}	9.66×10^{-11}	1.37×10^{-9}	2.58×10^{8}	1.82×10^{7}
SIV	1.00×10^{-10}	1.00×10^{-10}	7.83×10^{-10}	7.00×10^{-8}	3.18×10^{7}	3.56×10^{5}
SOD	1.00×10^{-8}	1.00×10^{-9}	3.60×10^{-11}	2.07×10^{-9}	6.93×10^{8}	1.20×10^{7}
WEI	1.00×10^{-10}	1.00×10^{-10}	3.81×10^{-9}	6.90×10^{-7}	6.53×10^{6}	3.61×10^{4}

Optimal process conditions and costs details

Table S2: Optimal purity, recovery, and cost breakdown for different zeolites. The feed is considered to be 1 kmol/s mixture of 14% CO_2 and 86% N_2. Material cost is computed considering \$2/kg of zeolite. Costs include both CO_2 capture and compression. Purity, recovery, and energy penalty are at optimal cost. Energy penalty is the total energy required for separation, which is the sum of energy consumed by the feed compressor, purge vacuum pump, and vacuum pump for CO_2 recovery. The symbol * next to total cost indicates that purity and/or recovery constraints were not satisfied. For these cases, we report the solution found closest to feasible based on $MIN\sqrt{(0.90-Pu)^2+(0.90-Re)^2}$.

Zeolite	Purity (%)	Recovery (%)	Energy penalty (kWh/ton captured)	Annualized investment cost (\$/yr)	Operating cost (\$/yr)	Material cost (\$/yr)	Total cost (\$/ton captured)
ABW	90.0	91.7	151.73	2,037,607	2,507,948	216,960	26.84
AFG	90.2	90.7	234.87	2,531,091	3,578,914	260,633	35.91
AFN	90.2	90.0	199.19	2,436,006	3,126,006	253,138	32.78
AFX	90.0	90.0	215.46	2,500,722	3,221,354	349,302	34.22
AHT	90.0	91.5	124.32	1,834,905	2,111,399	245,398	23.63
ANA	11.2	2.5	1354.00	3,074,707	16,159,226	2,576,789	122.94*
AST	70.0	72.5	223.75	2,236,933	3,228,416	258,364	32.26*
ATN	89.5	82.6	213.47	2,827,156	3,282,942	654,455	38.13*
AWO	92.0	90.8	164.27	2,012,198	2,609,639	191,895	27.13
BCT	0.2	0.0	804.37	1,213,527	9,577,250	587,198	64.13*
BIK	93.8	90.0	169.68	2,098,183	2,583,588	337,543	28.29
CGF	90.1	90.5	210.65	2,332,301	3,229,208	260,269	32.82
CHA	90.0	90.0	208.20	2,464,853	3,177,808	315,588	33.59
DAC	90.4	91.6	196.20	2,646,627	3,106,511	445,765	34.94
DFT	90.0	90.0	239.24	3,007,169	3,754,768	510,730	40.99
EAB	90.0	90.0	191.03	3,199,209	3,021,596	1,056,843	41.02
EON	90.0	90.0	223.97	2,403,643	3,383,436	269,654	34.14
ERI	90.1	91.3	179.26	2,204,757	2,847,474	225,191	29.75
FAR	90.0	90.0	233.72	3,216,946	3,903,270	233,851	41.45
FAU	47.3	36.5	293.02	2,889,409	4,141,293	672,923	43.42*
FRA	90.2	88.9	246.09	4,290,961	4,127,270	600,098	50.83*

GIS	90.0	90.9	159.39	2,397,742	2,731,782	289,759	30.55
GIU	90.0	90.0	220.15	2,684,860	3,346,817	422,565	36.38
GOO	90.0	90.0	188.87	2,356,454	2,965,301	357,429	32.01
IHW	90.0	90.0	188.95	2,312,687	3,006,939	226,496	31.26
ITR	90.2	85.4	217.79	3,005,169	3,553,528	168,181	37.92*
ITW	90.3	92.0	170.95	2,223,643	2,745,253	245,451	29.39
JBW	90.0	90.0	191.43	2,920,772	3,031,674	805,259	38.09
LEV	90.0	91.4	207.65	2,598,334	3,261,798	363,971	35.08
LOS	90.2	91.0	261.26	2,577,308	3,810,488	169,893	36.96
LTA	90.0	77.7	235.30	3,307,726	3,797,283	262,293	41.53*
LTF	90.1	90.0	174.11	2,203,716	2,785,270	259,770	29.59
MAR	86.5	36.9	420.94	3,390,072	5,548,828	410,747	52.70*
MEL	90.0	90.0	215.54	2,316,525	3,304,784	203,122	32.83
MFI	93.2	92.0	214.06	2,410,319	3,199,028	335,086	33.51
MON	90.0	90.0	202.76	2,316,525	3,304,784	203,122	34.34
MOR	98.8	90.2	276.71	2,266,299	3,988,288	104,644	35.85
MOZ	90.1	92.6	181.21	2,376,336	2,835,194	435,689	31.83
MSO	88.0	81.3	207.91	2,289,997	3,176,511	251,469	32.23*
MTN	85.7	73.7	226.27	2,615,471	3,335,086	565,398	36.73*
MVY	95.3	96.6	156.07	1,965,583	2,431,483	346,991	26.74
NAB	94.0	91.2	161.42	1,924,667	2,566,704	123,025	26.01
NON	89.9	79.5	224.58	2,253,893	3,285,762	257,332	32.68*
OFF	90.2	90.3	173.27	2,209,004	2,761,833	237,551	29.36
RRO	90.2	90.0	154.06	2,278,216	2,516,574	470,999	29.68
RWR	90.1	90.4	168.41	2,181,757	2,758,220	229,884	29.14
RWY	86.4	82.2	248.21	4,725,418	4,610,099	581,216	55.90*
SAO	69.9	70.4	192.04	2,625,293	2,884,852	730,621	35.18*
SGT	89.9	48.7	353.21	3,146,377	4,813,174	210,250	46.05*
SIV	90.0	90.0	191.30	2,397,156	3,098,296	277,978	32.54
SOD	71.3	63.8	298.30	2,816,703	4,236,908	472,748	42.42*
TOL	57.3	74.6	182.09	3,143,793	3,106,329	533,459	38.24*
TON	90.8	90.4	159.32	2,227,743	2,574,352	329,495	28.93
VNI	90.1	90.6	167.60	2,087,030	2,685,697	213,899	28.11
WEI	90.0	90.0	146.95	2,083,016	2,349,450	408,643	27.29
ZON	90.0	90.0	211.08	2,387,004	3,274,738	209,359	33.09
13X	91.5	91.5	206.30	2,211,417	3,169,525	265,974	31.83

Table S3: Optimal conditions for the 4-step adsorption process for CO_2 capture using different zeolites. The feed is considered to be 1 kmol/s mixture of 14% CO_2 and 86% N_2. The pressurization time is fixed to be 20 s.

		Column	Adsorption step		Blowdown step		Evacuation step	
Zeolite	Number of columns	Length (m)	pressure (bar)	duration (s)	pressure (bar)	duration (s)	pressure (bar)	duration (s)
ABW	2	1.00	2.34	31.88	0.48	50.77	0.02	69.97
AFG	2	1.00	2.58	25.80	0.26	61.18	0.01	78.05
AFN	2	1.00	2.04	20.00	0.24	24.66	0.01	45.49
AFX	2	1.00	1.91	20.00	0.19	32.20	0.01	70.11
AHT	2	1.00	2.01	33.73	0.65	49.26	0.03	74.45
ANA	2	4.82	1.01	37.26	0.89	67.05	0.26	90.14
AST	2	1.00	2.79	20.00	0.61	38.49	0.01	75.27
ATN	2	1.00	1.00	36.79	0.10	100.00	0.01	100.00
AWO	2	1.00	2.20	50.00	0.35	55.13	0.02	100.00
BCT	1	1.02	1.05	21.75	0.37	28.21	0.01	70.01
BIK	2	1.00	2.00	25.00	0.20	45.00	0.02	90.00
CGF	2	1.00	2.84	26.18	0.44	70.23	0.01	89.98
CHA	2	1.00	1.91	25.00	0.23	39.51	0.01	76.21
DAC	2	1.00	1.00	50.00	0.12	67.71	0.01	100.00
DFT	2	1.00	1.36	33.03	0.10	100.00	0.01	91.66
EAB	2	1.00	1.00	20.00	0.12	90.69	0.01	94.74
EON	2	1.00	2.86	26.72	0.36	73.06	0.01	100.00
ERI	2	1.00	3.08	27.25	0.45	66.54	0.02	87.79
FAR	1	1.00	3.49	20.00	0.45	34.09	0.01	100.00
FAU	2	2.62	2.84	21.34	0.94	42.55	0.01	82.48
FRA	1	1.00	1.25	20.00	0.10	20.00	0.01	100.00
GIS	2	1.00	1.56	35.85	0.22	53.77	0.02	63.21
GIU	2	1.00	1.74	21.06	0.20	45.00	0.01	79.09
GOO	2	1.00	2.74	20.00	0.47	82.46	0.01	86.44
IHW	2	1.00	3.67	20.00	0.48	61.86	0.02	75.45
ITR	1	1.00	4.46	20.00	0.62	20.00	0.01	100.00
ITW	2	1.00	2.80	30.22	0.32	72.66	0.03	98.63

JBW	2	1.00	1.00	28.99	0.11	100.00	0.01	100.00
LEV	2	1.00	2.23	20.00	0.29	58.46	0.01	74.67
LOS	2	1.00	3.04	22.25	0.25	20.00	0.01	60.31
LTA	1	1.00	2.54	20.00	0.30	20.00	0.01	82.11
LTF	2	1.00	2.82	29.76	0.47	82.75	0.02	100.00
MAR	1	1.00	1.58	20.00	0.10	20.00	0.01	78.44
MEL	2	1.00	3.53	23.42	0.47	59.49	0.01	76.19
MFI	2	1.00	2.00	25.00	0.20	45.00	0.01	88.69
MON	2	1.42	8.47	40.14	0.75	43.26	0.04	81.73
MOR	2	1.04	5.66	34.68	0.28	59.50	0.01	95.97
MOZ	2	1.00	1.67	28.73	0.29	74.22	0.01	100.00
MSO	2	1.00	3.11	20.00	0.49	59.70	0.01	67.12
MTN	2	1.00	1.99	20.00	0.29	100.00	0.01	100.00
MVY	2	1.03	1.94	23.66	0.38	39.43	0.01	82.20
NAB	2	1.08	5.86	20.26	0.61	35.83	0.05	68.59
NON	2	1.00	2.93	20.00	0.38	47.45	0.01	73.38
OFF	2	1.00	2.91	30.16	0.36	72.20	0.03	100.00
RRO	2	1.00	1.00	45.38	0.25	71.59	0.01	90.99
RWR	2	1.00	1.41	50.00	0.29	38.88	0.01	63.97
RWY	1	1.35	1.00	35.25	0.10	23.87	0.01	82.75
SAO	2	1.00	1.54	20.00	0.41	100.00	0.01	100.00
SGT	1	1.00	3.48	20.00	0.22	20.00	0.01	96.07
SIV	2	1.00	2.00	44.63	0.26	100.00	0.01	100.00
SOD	2	1.00	2.38	20.00	0.33	100.00	0.01	100.00
TOL	1	1.00	1.23	20.00	0.48	20.00	0.01	79.96
TON	2	1.00	2.92	20.00	0.39	72.43	0.03	92.80
VNI	2	1.00	3.32	24.79	0.59	63.06	0.02	79.91
WEI	2	1.03	1.91	20.47	0.39	43.32	0.01	80.74
ZON	2	1.00	3.66	24.49	0.39	68.00	0.02	87.65
13X	2	1.04	2.88	30.50	0.52	89.09	0.01	100.00

Zeolites for CO_2 capture

ABW

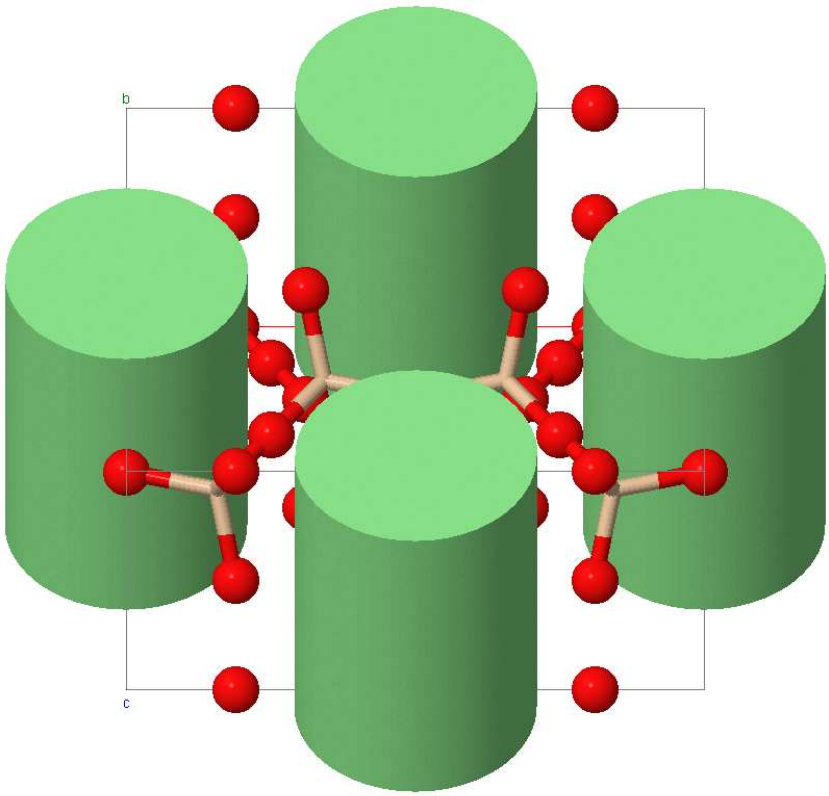

Figure S1: Main pore system of ABW from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S4: Physical properties for ABW.

Property	Value
Pore limiting diamater, PLD [Å]	4.1
Largest cavity diameter, LCD [Å]	4.1
Solid density [kg m^{-3}]	1755

Table S5: Adsorption and geometric properties for ABW.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01490	0.00057
Heat of adsorption at 298 K [kJ mol^{-1}]	32.5	15.3
Accessible volume [cm^3 g^{-1}]	0.204	0.338
Accessible surface area [m^2 g^{-1}]	1324	3074

Table S6: Performance metrics for ABW.

Property	Value
Shape selectivity	–
Size selectivity	0.40
Adsorption selectivity	26.25
Minimum parasitic energy [kJ/kg CO_2]	915.51
Purity [%] at minimum parasitic energy	88.41
Cost [$/ton of CO_2 captured and compressed]	26.84
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	91.71
Energy penalty [kWh/ton CO_2 captured] at optimum cost	151.73

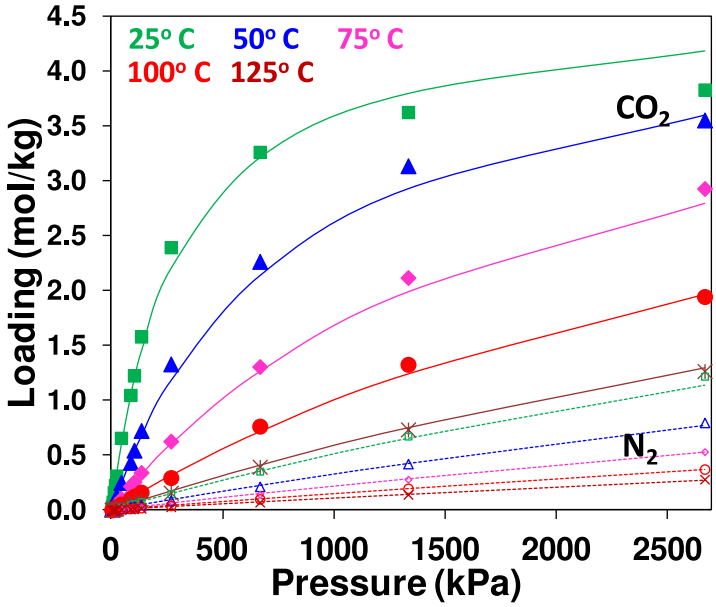

Figure S2: Adsorption isotherms of ABW. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S7: Dual-site Langmuir isotherm parameters for ABW.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.59	2.57
b^o [m^3 mol^{-1}]	9.00×10^{-8}	0
ΔU [kJ mol^{-1}]	28.49	7.21
Site 2		
q^{sat} [mol kg^{-1}]	4.59	4.59
b^o [m^3 mol^{-1}]	9.00×10^{-6}	1.00×10^{-6}
ΔU [kJ mol^{-1}]	0	13.48

AFG

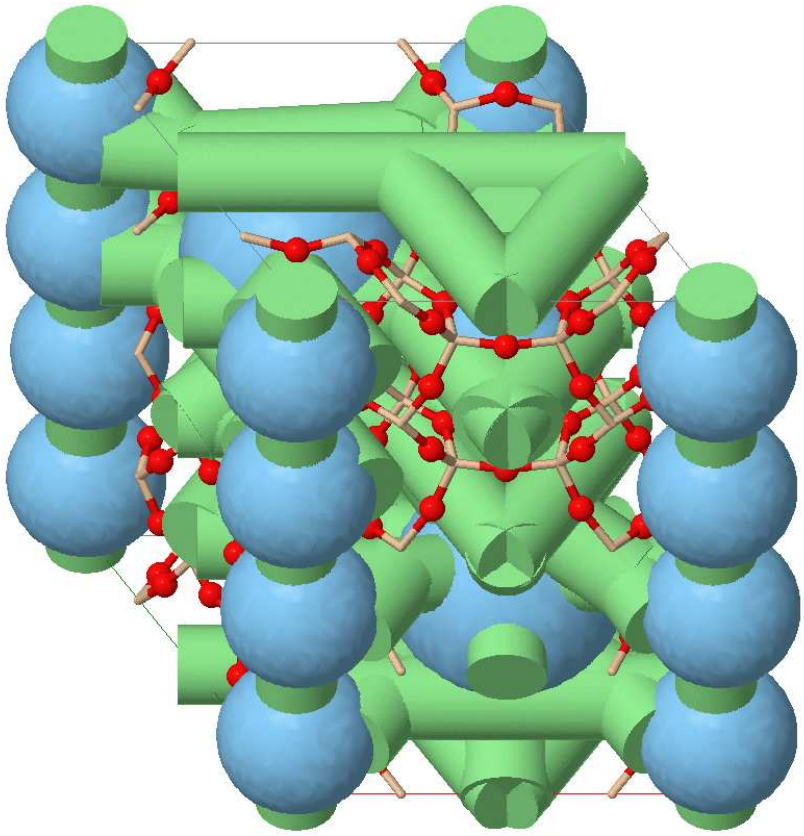

Figure S3: Main pore system of AFG from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S8: Physical properties for AFG.

Property	Value
Pore limiting diamater, PLD [Å]	2.7
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1689

Table S9: Adsorption and geometric properties for AFG.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.02154	0.00098
Heat of adsorption at 298 K [kJ mol^{-1}]	27.8	14.6
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S10: Performance metrics for AFG.

Property	Value
Shape selectivity	0.31
Size selectivity	–
Adsorption selectivity	22.00
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	35.91
Purity [%] at optimum cost	90.21
Recovery [%] at optimum cost	90.69
Energy penalty [kWh/ton CO_2 captured] at optimum cost	234.87

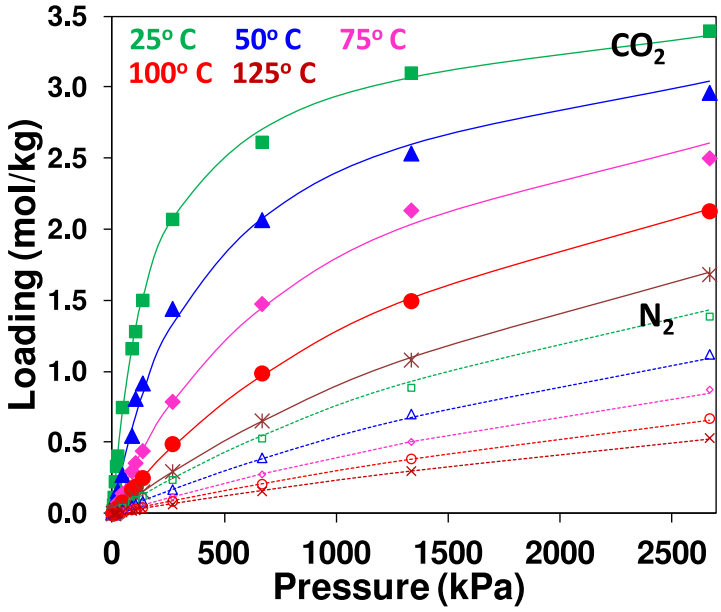

Figure S4: Adsorption isotherms of AFG. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S11: Dual-site Langmuir isotherm parameters for AFG.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.08	4.08
b^o [m^3 mol^{-1}]	1.79×10^{-4}	9.00×10^{-6}
ΔU [kJ mol^{-1}]	0	10.50
Site 2		
q^{sat} [mol kg^{-1}]	3.64	0.04
b^o [m^3 mol^{-1}]	2.20×10^{-7}	3.00×10^{-6}
ΔU [kJ mol^{-1}]	27.51	16.93

AFN

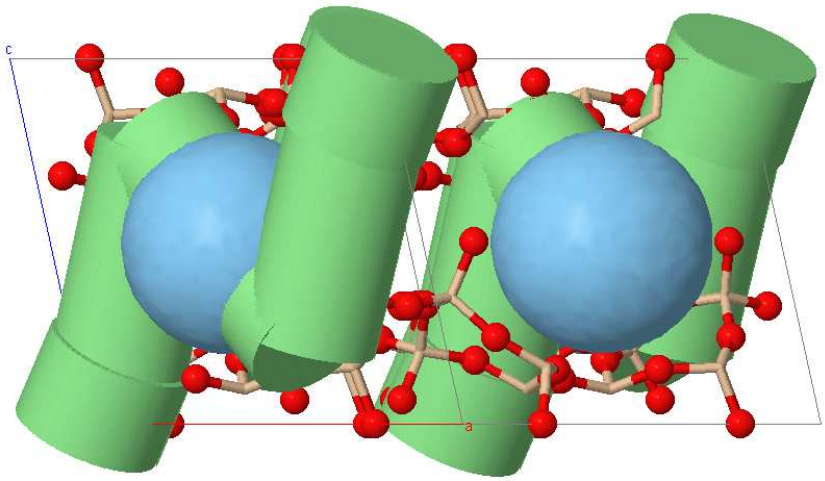

Figure S5: Main pore system of AFN from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S12: Physical properties for AFN.

Property	Value
Pore limiting diamater, PLD [Å]	3.7
Largest cavity diameter, LCD [Å]	5.9
Solid density [kg m^{-3}]	1736

Table S13: Adsorption and geometric properties for AFN.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01702	0.00061
Heat of adsorption at 298 K [kJ mol^{-1}]	27.3	15.0
Accessible volume [cm^3 g^{-1}]	0.245	0.289
Accessible surface area [m^2 g^{-1}]	748	925

Table S14: Performance metrics for AFN.

Property	Value
Shape selectivity	–
Size selectivity	0.15
Adsorption selectivity	27.68
Minimum parasitic energy [kJ/kg CO_2]	1123.68
Purity [%] at minimum parasitic energy	79.83
Cost [$/ton of CO_2 captured and compressed]	32.78
Purity [%] at optimum cost	90.15
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	199.19

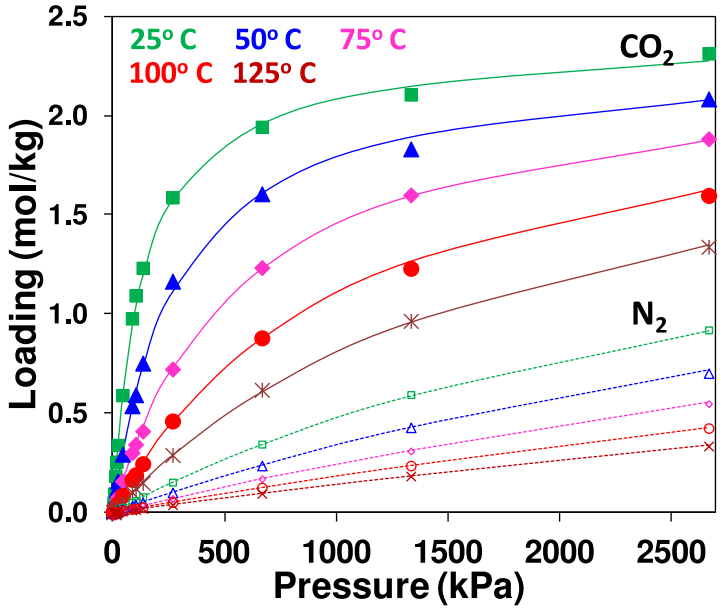

Figure S6: Adsorption isotherms of AFN. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S15: Dual-site Langmuir isotherm parameters for AFN.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.78	2.27
b^o [m^3 mol^{-1}]	0	8.00×10^{-6}
ΔU [kJ mol^{-1}]	50.00	11.06
Site 2		
q^{sat} [mol kg^{-1}]	2.27	2.78
b^o [m^3 mol^{-1}]	1.00×10^{-6}	0
ΔU [kJ mol^{-1}]	23.82	50.00

AFX

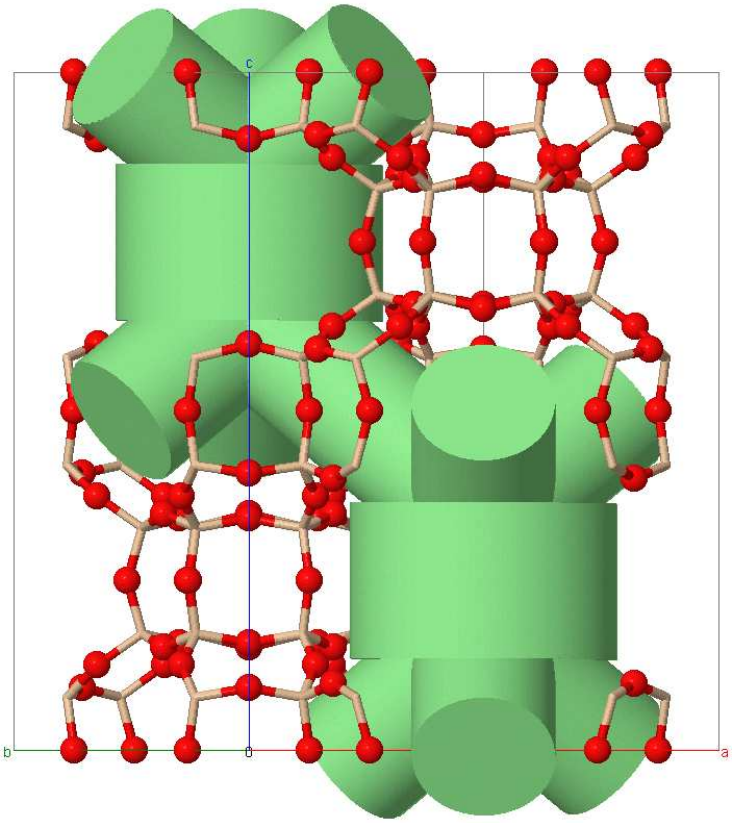

Figure S7: Main pore system of AFX from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S16: Physical properties for AFX.

Property	Value
Pore limiting diamater, PLD [Å]	4.1
Largest cavity diameter, LCD [Å]	7.8
Solid density [kg m^{-3}]	1502

Table S17: Adsorption and geometric properties for AFX.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.02607	0.00098
Heat of adsorption at 298 K [kJ mol^{-1}]	27.0	11.8
Accessible volume [cm^3 g^{-1}]	0.382	0.388
Accessible surface area [m^2 g^{-1}]	3326	4586

Table S18: Performance metrics for AFX.

Property	Value
Shape selectivity	–
Size selectivity	0.01
Adsorption selectivity	26.52
Minimum parasitic energy [kJ/kg CO_2]	1207.60
Purity [%] at minimum parasitic energy	72.76
Cost [$/ton of CO_2 captured and compressed]	34.22
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	215.46

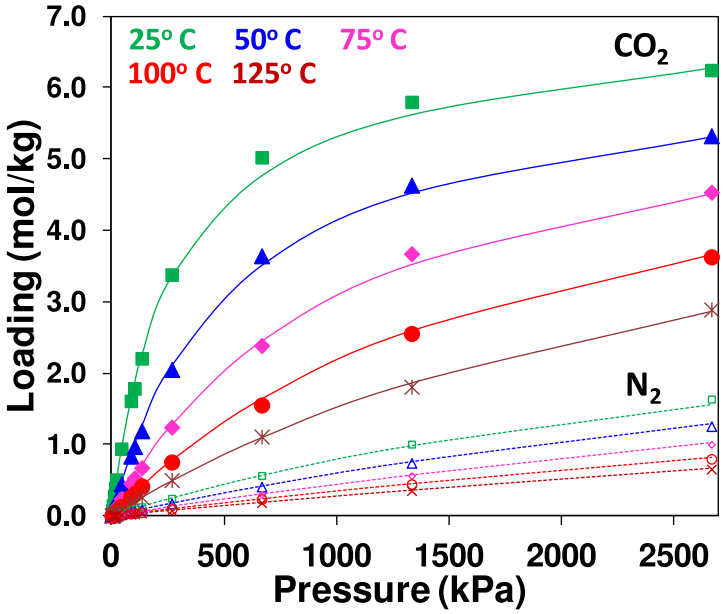

Figure S8: Adsorption isotherms of AFX. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S19: Dual-site Langmuir isotherm parameters for AFX.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	7.50	4.68
b^o [m^3 mol^{-1}]	0	1.20×10^{-5}
ΔU [kJ mol^{-1}]	50.00	9.33
Site 2		
q^{sat} [mol kg^{-1}]	6.19	7.50
b^o [m^3 mol^{-1}]	1.00×10^{-6}	0
ΔU [kJ mol^{-1}]	22.41	50.00

AHT

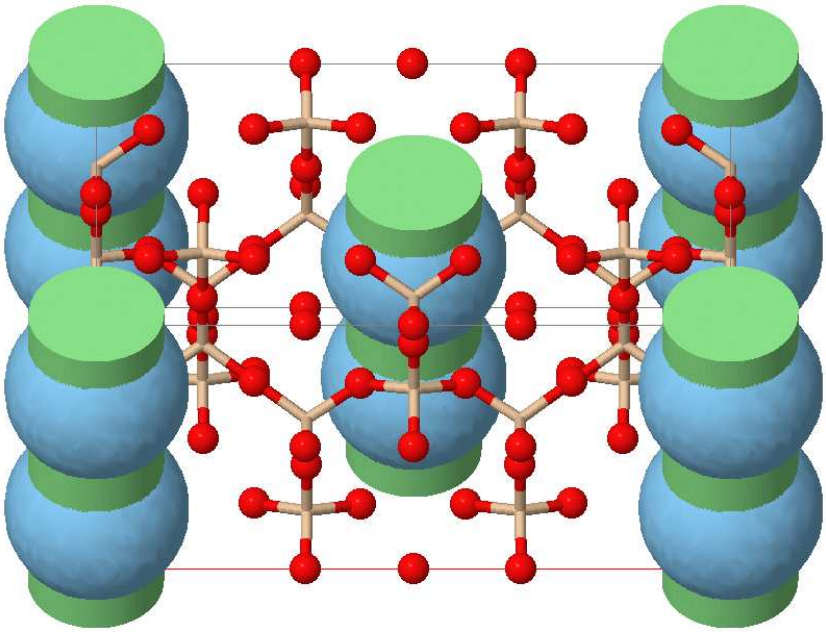

Figure S9: Main pore system of AHT from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S20: Physical properties for AHT.

Property	Value
Pore limiting diamater, PLD [Å]	3.4
Largest cavity diameter, LCD [Å]	4.6
Solid density [kg m^{-3}]	1917

Table S21: Adsorption and geometric properties for AHT.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.06093	0.00012
Heat of adsorption at 298 K [kJ mol^{-1}]	37.0	14.0
Accessible volume [cm^3 g^{-1}]	–	0.214
Accessible surface area [m^2 g^{-1}]	–	406

Table S22: Performance metrics for AHT.

Property	Value
Shape selectivity	0.01
Size selectivity	1.00
Adsorption selectivity	505.3
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	23.63
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	91.51
Energy penalty [kWh/ton CO_2 captured] at optimum cost	124.32

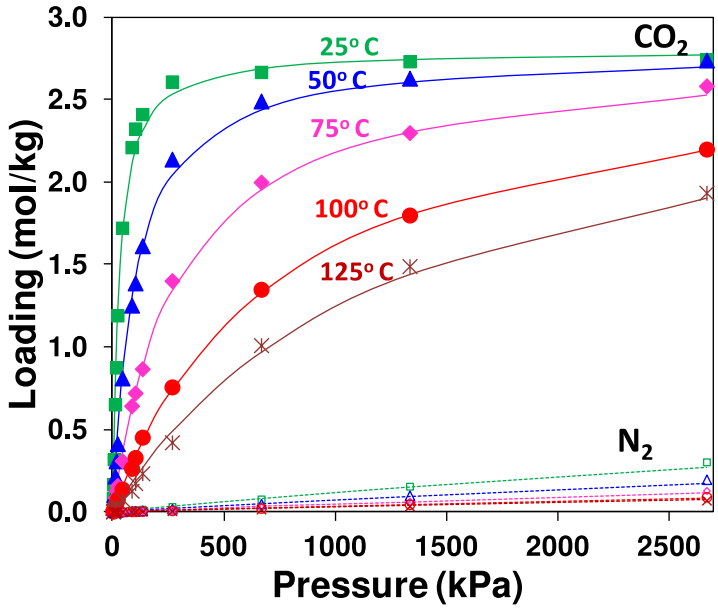

Figure S10: Adsorption isotherms of AHT. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S23: Dual-site Langmuir isotherm parameters for AHT.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	1.93	3.29
b^o [m^3 mol^{-1}]	0	6.30×10^{-7}
ΔU [kJ mol^{-1}]	0	12.30
Site 2		
q^{sat} [mol kg^{-1}]	3.29	0
b^o [m^3 mol^{-1}]	6.00×10^{-8}	0
ΔU [kJ mol^{-1}]	33.79	50.00

ANA

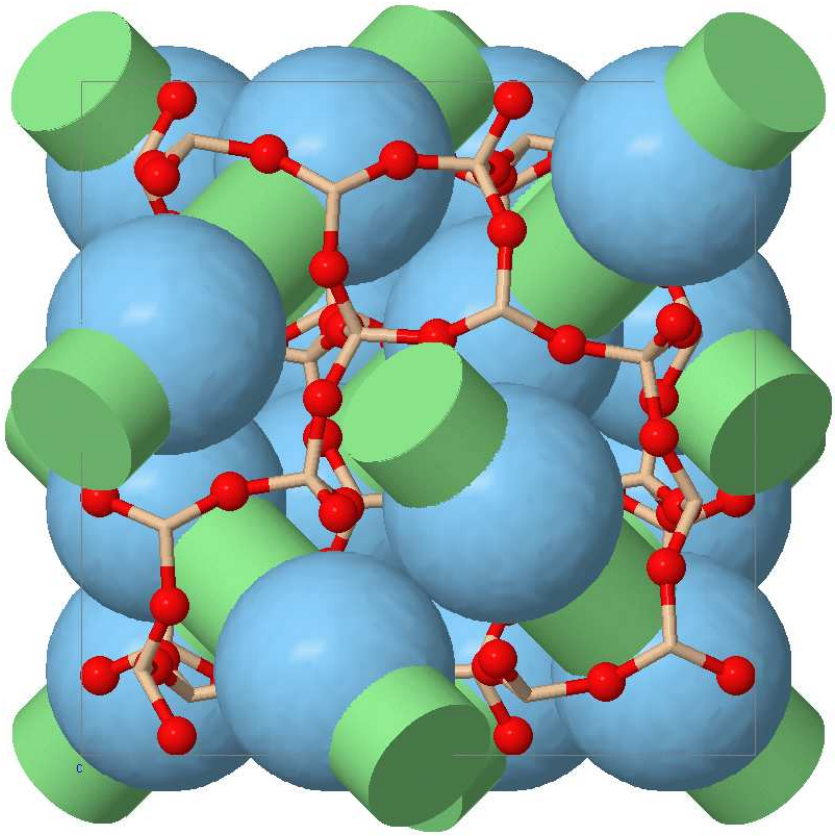

Figure S11: Main pore system of ANA from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S24: Physical properties for ANA.

Property	Value
Pore limiting diamater, PLD [Å]	3.0
Largest cavity diameter, LCD [Å]	4.9
Solid density [kg m^{-3}]	1918

Table S25: Adsorption and geometric properties for ANA.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00011	0.00018
Heat of adsorption at 298 K [kJ mol^{-1}]	30.7	18.7
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S26: Performance metrics for ANA.

Property	Value
Shape selectivity	0.44
Size selectivity	–
Adsorption selectivity	0.63
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	122.94
Purity [%] at optimum cost	11.24
Recovery [%] at optimum cost	2.49
Energy penalty [kWh/ton CO_2 captured] at optimum cost	1354.00

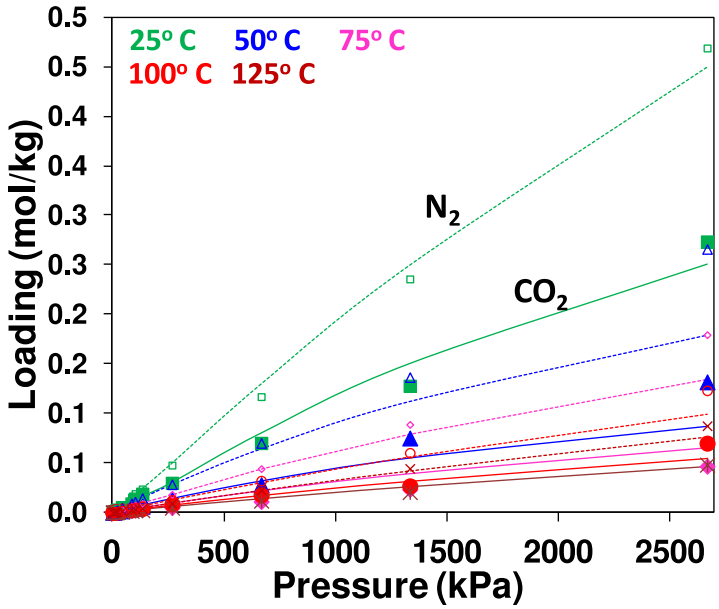

Figure S12: Adsorption isotherms of ANA. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S27: Dual-site Langmuir isotherm parameters for ANA.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	0.33	0.33
b^o [m^3 mol^{-1}]	0	1.00×10^{-5}
ΔU [kJ mol^{-1}]	50.00	10.45
Site 2		
q^{sat} [mol kg^{-1}]	0.33	0.33
b^o [m^3 mol^{-1}]	3.10×10^{-5}	2.90×10^{-7}
ΔU [kJ mol^{-1}]	6.46	19.58

AST

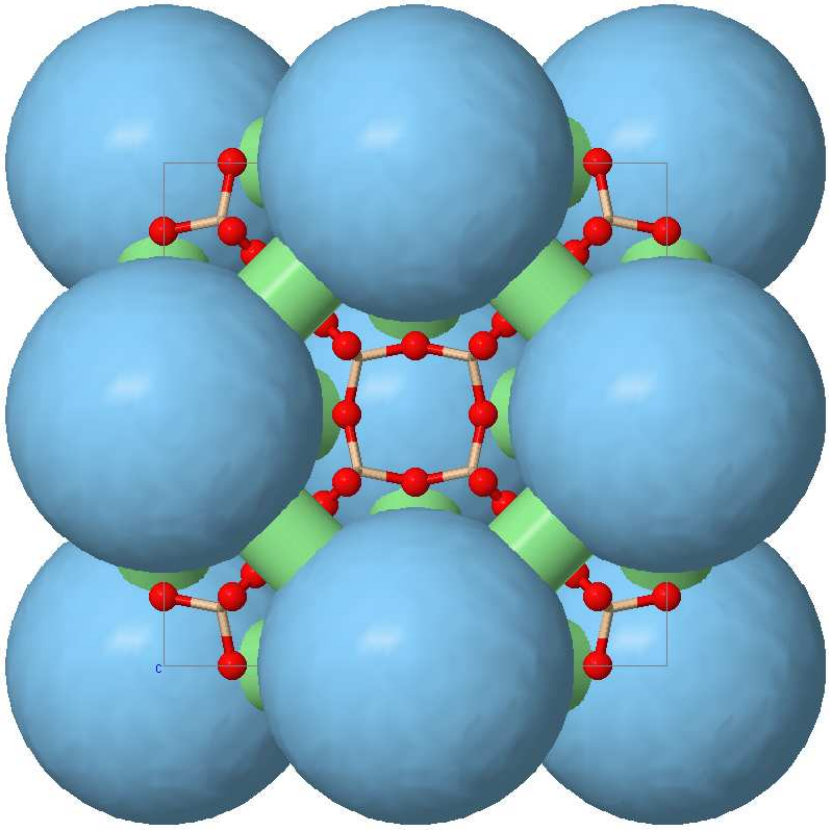

Figure S13: Main pore system of AST from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S28: Physical properties for AST.

Property	Value
Pore limiting diamater, PLD [Å]	2.5
Largest cavity diameter, LCD [Å]	8.6
Solid density [kg m^{-3}]	1578

Table S29: Adsorption and geometric properties for AST.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00356	0.00081
Heat of adsorption at 298 K [kJ mol^{-1}]	2.5	15.1
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S30: Performance metrics for AST.

Property	Value
Shape selectivity	0.14
Size selectivity	–
Adsorption selectivity	4.39
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	32.26
Purity [%] at optimum cost	69.97
Recovery [%] at optimum cost	72.46
Energy penalty [kWh/ton CO_2 captured] at optimum cost	223.75

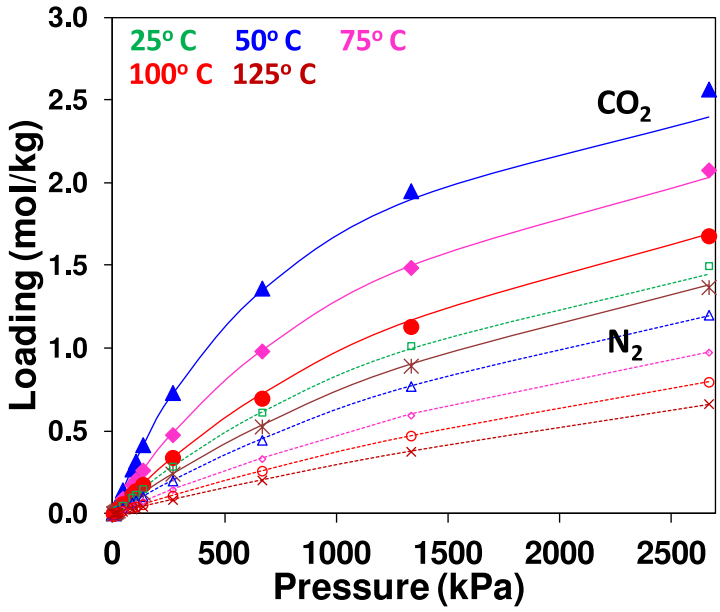

Figure S14: Adsorption isotherms of AST. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S31: Dual-site Langmuir isotherm parameters for AST.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.08	3.08
b^o [m^3 mol^{-1}]	3.00×10^{-6}	1.80×10^{-5}
ΔU [kJ mol^{-1}]	9.66	9.92
Site 2		
q^{sat} [mol kg^{-1}]	3.08	0.04
b^o [m^3 mol^{-1}]	9.00×10^{-6}	1.81×10^{-4}
ΔU [kJ mol^{-1}]	15.58	0

ATN

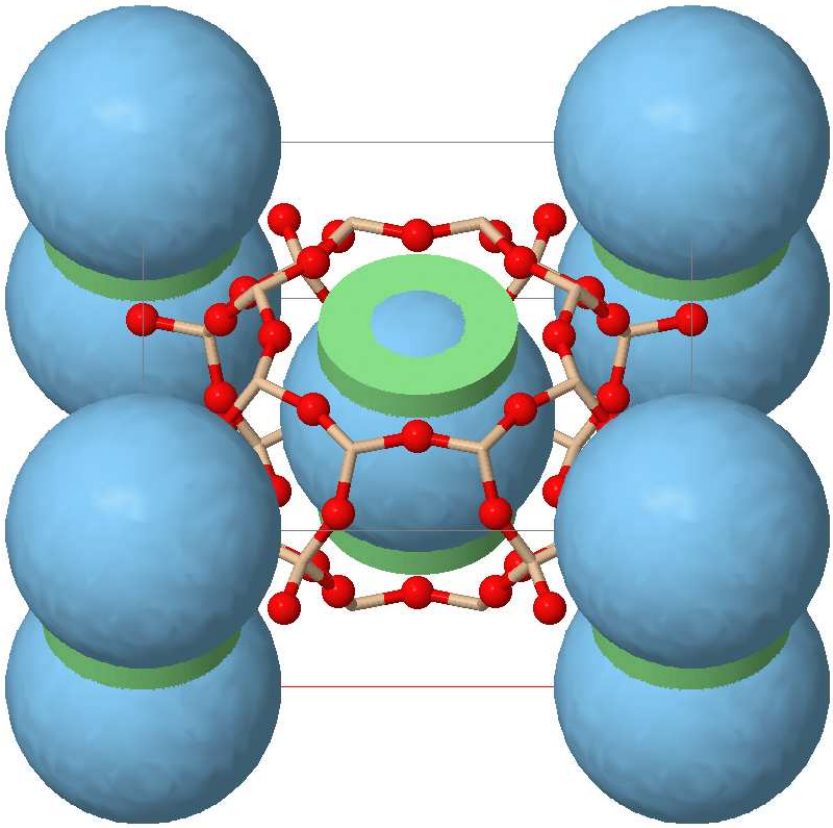

Figure S15: Main pore system of ATN from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S32: Physical properties for ATN.

Property	Value
Pore limiting diamater, PLD [Å]	4.7
Largest cavity diameter, LCD [Å]	6.6
Solid density [kg m^{-3}]	1778

Table S33: Adsorption and geometric properties for ATN.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.09238	0.00122
Heat of adsorption at 298 K [kJ mol^{-1}]	35.9	15.9
Accessible volume [cm^3 g^{-1}]	0.238	0.316
Accessible surface area [m^2 g^{-1}]	985	1602

Table S34: Performance metrics for ATN.

Property	Value
Shape selectivity	–
Size selectivity	0.25
Adsorption selectivity	75.69
Minimum parasitic energy [kJ/kg CO_2]	853.40
Purity [%] at minimum parasitic energy	88.73
Cost [$/ton of CO_2 captured and compressed]	38.13
Purity [%] at optimum cost	89.52
Recovery [%] at optimum cost	82.60
Energy penalty [kWh/ton CO_2 captured] at optimum cost	213.47

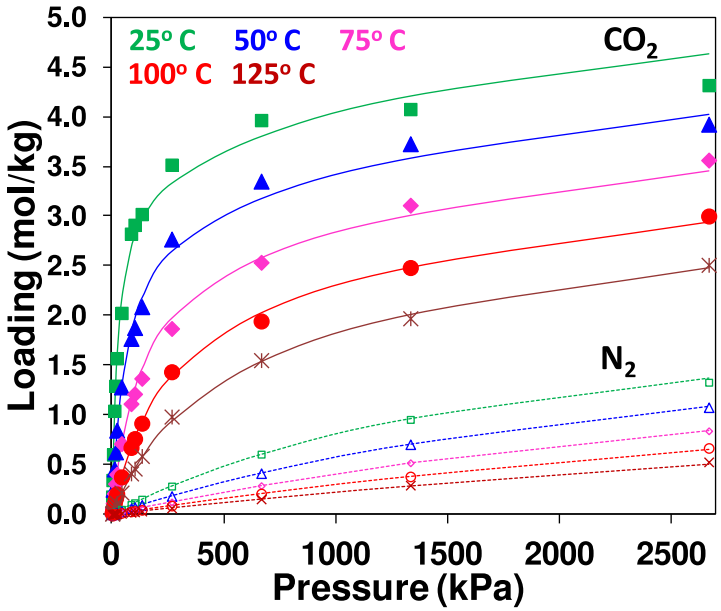

Figure S16: Adsorption isotherms of ATN. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S35: Dual-site Langmuir isotherm parameters for ATN.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	5.18	4.30
b^o [m^3 mol^{-1}]	5.00×10^{-6}	4.00×10^{-6}
ΔU [kJ mol^{-1}]	11.88	12.87
Site 2		
q^{sat} [mol kg^{-1}]	5.18	0
b^o [m^3 mol^{-1}]	5.30×10^{-7}	9.00×10^{-6}
ΔU [kJ mol^{-1}]	29.02	20.43

AWO

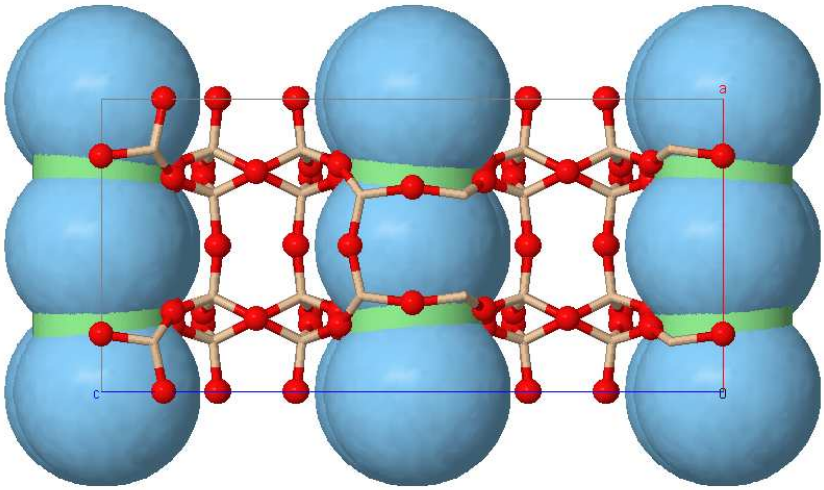

Figure S17: Main pore system of AWO from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S36: Physical properties for AWO.

Property	Value
Pore limiting diamater, PLD [Å]	4.3
Largest cavity diameter, LCD [Å]	5.8
Solid density [kg m^{-3}]	1819

Table S37: Adsorption and geometric properties for AWO.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.05281	0.00080
Heat of adsorption at 298 K [kJ mol^{-1}]	32.4	17.4
Accessible volume [cm^3 g^{-1}]	0.178	0.227
Accessible surface area [m^2 g^{-1}]	1150	1180

Table S38: Performance metrics for AWO.

Property	Value
Shape selectivity	–
Size selectivity	0.22
Adsorption selectivity	65.87
Minimum parasitic energy [kJ/kg CO_2]	866.85
Purity [%] at minimum parasitic energy	88.78
Cost [$/ton of CO_2 captured and compressed]	27.13
Purity [%] at optimum cost	92.01
Recovery [%] at optimum cost	90.81
Energy penalty [kWh/ton CO_2 captured] at optimum cost	164.27

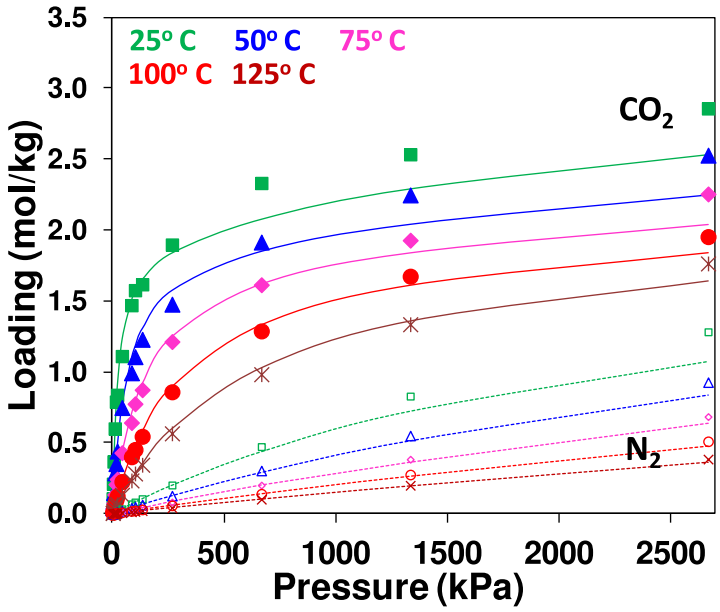

Figure S18: Adsorption isotherms of AWO. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S39: Dual-site Langmuir isotherm parameters for AWO.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.92	2.76
b^o [m^3 mol^{-1}]	2.00×10^{-6}	2.00×10^{-6}
ΔU [kJ mol^{-1}]	24.69	15.20
Site 2		
q^{sat} [mol kg^{-1}]	3.43	0
b^o [m^3 mol^{-1}]	0	0
ΔU [kJ mol^{-1}]	28.90	27.46

BCT

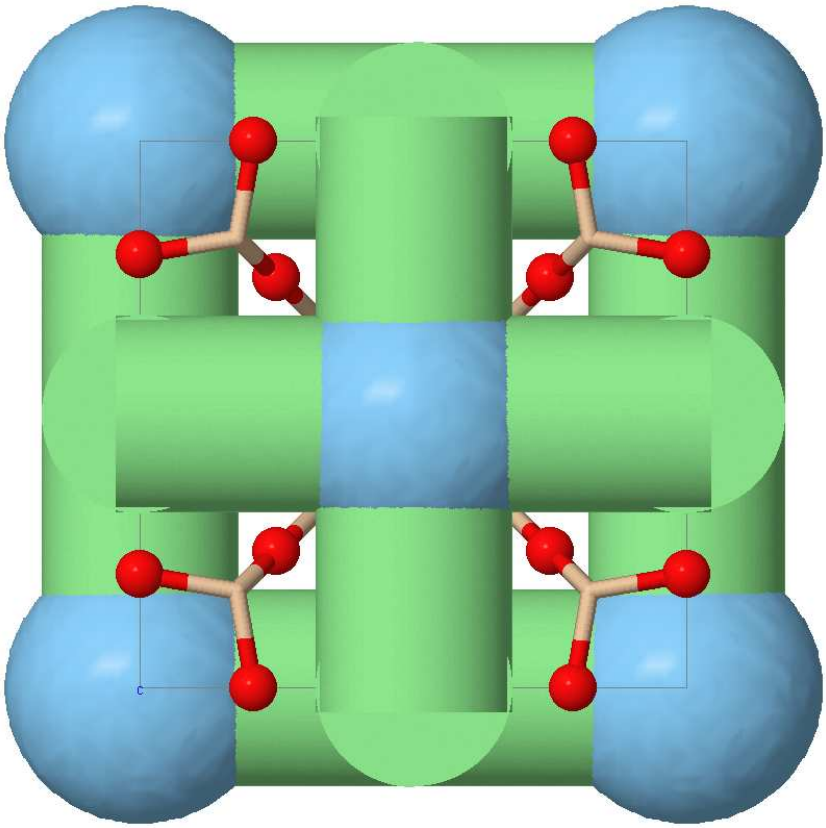

Figure S19: Main pore system of BCT from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S40: Physical properties for BCT.

Property	Value
Pore limiting diamater, PLD [Å]	3.2
Largest cavity diameter, LCD [Å]	4.4
Solid density [kg m^{-3}]	1895

Table S41: Adsorption and geometric properties for BCT.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00001	0.00000
Heat of adsorption at 298 K [kJ mol^{-1}]	2.5	2.5
Accessible volume [cm^3 g^{-1}]	–	0.320
Accessible surface area [m^2 g^{-1}]	–	2711

Table S42: Performance metrics for BCT.

Property	Value
Shape selectivity	0.14
Size selectivity	1.00
Adsorption selectivity	12.00
Minimum parasitic energy [kJ/kg CO_2]	3984634.94
Purity [%] at minimum parasitic energy	51.26
Cost [$/ton of CO_2 captured and compressed]	64.20
Purity [%] at optimum cost	0.15
Recovery [%] at optimum cost	0.02
Energy penalty [kWh/ton CO_2 captured] at optimum cost	804.37

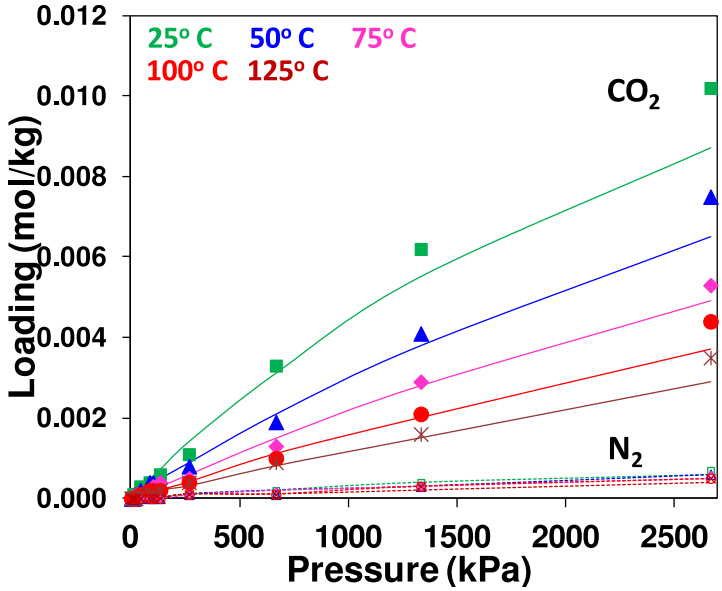

Figure S20: Adsorption isotherms of BCT. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S43: Dual-site Langmuir isotherm parameters for BCT.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	0.01	0.01
b^o [m^3 mol^{-1}]	7.00×10^{-6}	0
ΔU [kJ mol^{-1}]	11.68	13.21
Site 2		
q^{sat} [mol kg^{-1}]	0.01	0.01
b^o [m^3 mol^{-1}]	3.00×10^{-6}	2.30×10^{-5}
ΔU [kJ mol^{-1}]	11.67	2.72

BIK

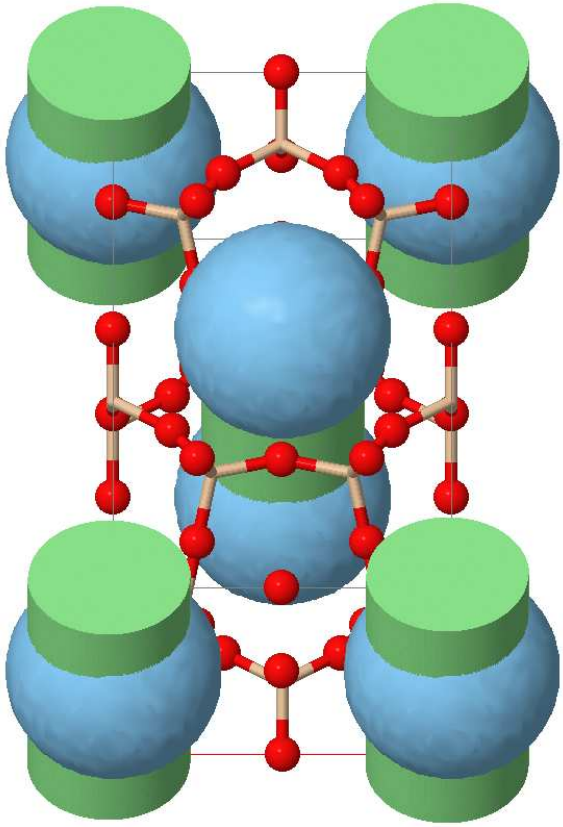

Figure S21: Main pore system of BIK from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S44: Physical properties for BIK.

Property	Value
Pore limiting diamater, PLD [Å]	3.6
Largest cavity diameter, LCD [Å]	4.8
Solid density [kg m^{-3}]	1862

Table S45: Adsorption and geometric properties for BIK.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.05365	0.00042
Heat of adsorption at 298 K [kJ mol^{-1}]	34.1	16.5
Accessible volume [cm^3 g^{-1}]	0.166	0.166
Accessible surface area [m^2 g^{-1}]	1043	1043

Table S46: Performance metrics for BIK.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	127.7
Minimum parasitic energy [kJ/kg CO_2]	899.44
Purity [%] at minimum parasitic energy	90.70
Cost [$/ton of CO_2 captured and compressed]	28.29
Purity [%] at optimum cost	93.79
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	169.68

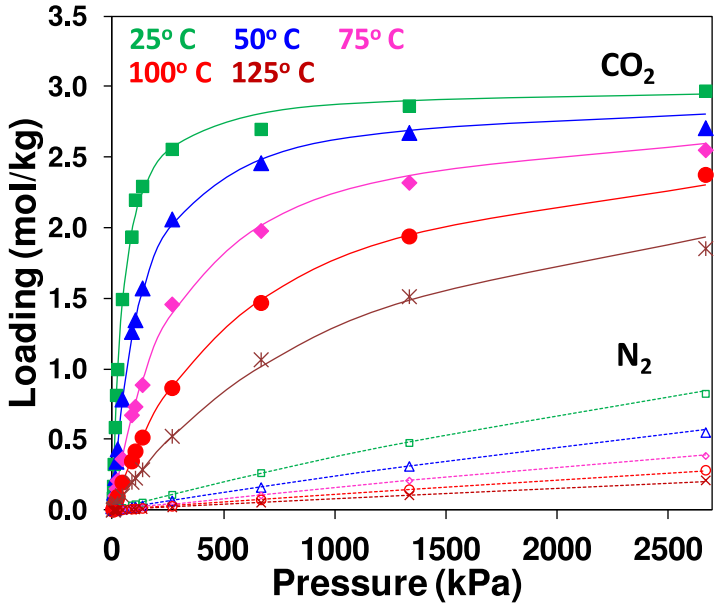

Figure S22: Adsorption isotherms of BIK. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S47: Dual-site Langmuir isotherm parameters for BIK.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.31	3.47
b^o [m^3 mol^{-1}]	0	1.00×10^{-6}
ΔU [kJ mol^{-1}]	0	13.43
Site 2		
q^{sat} [mol kg^{-1}]	3.57	0
b^o [m^3 mol^{-1}]	2.60×10^{-7}	2.50×10^{-7}
ΔU [kJ mol^{-1}]	30.03	25.94

CGF

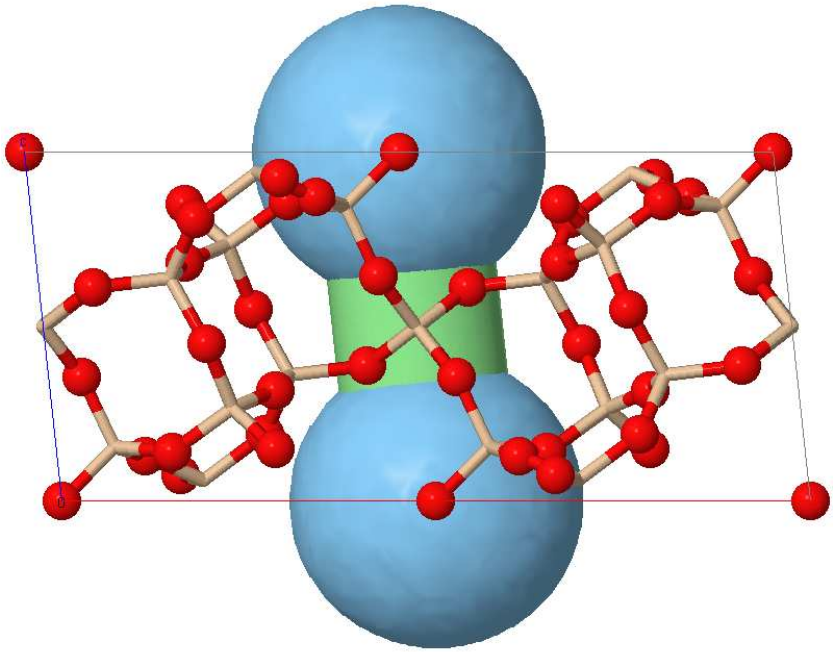

Figure S23: Main pore system of CGF from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S48: Physical properties for CGF.

Property	Value
Pore limiting diamater, PLD [Å]	3.5
Largest cavity diameter, LCD [Å]	6.4
Solid density [kg m^{-3}]	1896

Table S49: Adsorption and geometric properties for CGF.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01311	0.00069
Heat of adsorption at 298 K [kJ mol^{-1}]	26.7	15.6
Accessible volume [cm^3 g^{-1}]	0.057	0.166
Accessible surface area [m^2 g^{-1}]	215	886

Table S50: Performance metrics for CGF.

Property	Value
Shape selectivity	–
Size selectivity	0.66
Adsorption selectivity	18.88
Minimum parasitic energy [kJ/kg CO_2]	1372.73
Purity [%] at minimum parasitic energy	76.50
Cost [$/ton of CO_2 captured and compressed]	32.82
Purity [%] at optimum cost	90.05
Recovery [%] at optimum cost	90.46
Energy penalty [kWh/ton CO_2 captured] at optimum cost	210.65

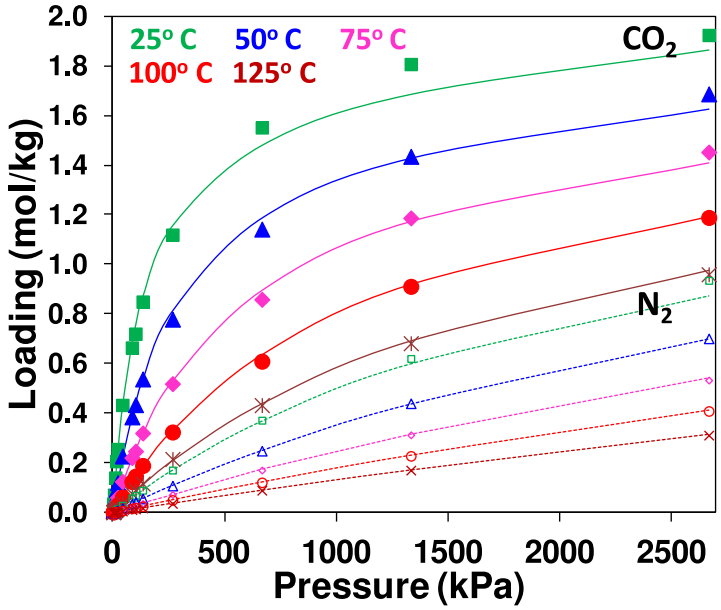

Figure S24: Adsorption isotherms of CGF. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S51: Dual-site Langmuir isotherm parameters for CGF.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.31	2.31
b^o [m^3 mol^{-1}]	2.00×10^{-8}	4.00×10^{-6}
ΔU [kJ mol^{-1}]	24.15	13.21
Site 2		
q^{sat} [mol kg^{-1}]	1.54	0.13
b^o [m^3 mol^{-1}]	1.00×10^{-6}	0
ΔU [kJ mol^{-1}]	24.06	47.67

CHA

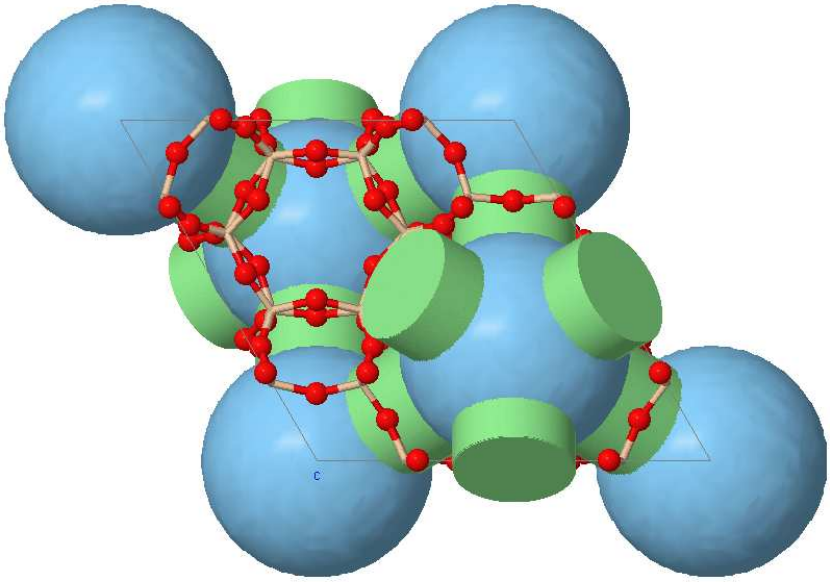

Figure S25: Main pore system of CHA from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S52: Physical properties for CHA.

Property	Value
Pore limiting diamater, PLD [Å]	4.2
Largest cavity diameter, LCD [Å]	8.0
Solid density [kg m^{-3}]	1502

Table S53: Adsorption and geometric properties for CHA.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01689	0.00103
Heat of adsorption at 298 K [kJ mol^{-1}]	26.5	12.3
Accessible volume [cm^3 g^{-1}]	0.402	0.402
Accessible surface area [m^2 g^{-1}]	1568	1568

Table S54: Performance metrics for CHA.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	16.39
Minimum parasitic energy [kJ/kg CO_2]	1587.04
Purity [%] at minimum parasitic energy	61.43
Cost [$/ton of CO_2 captured and compressed]	33.59
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	208.20

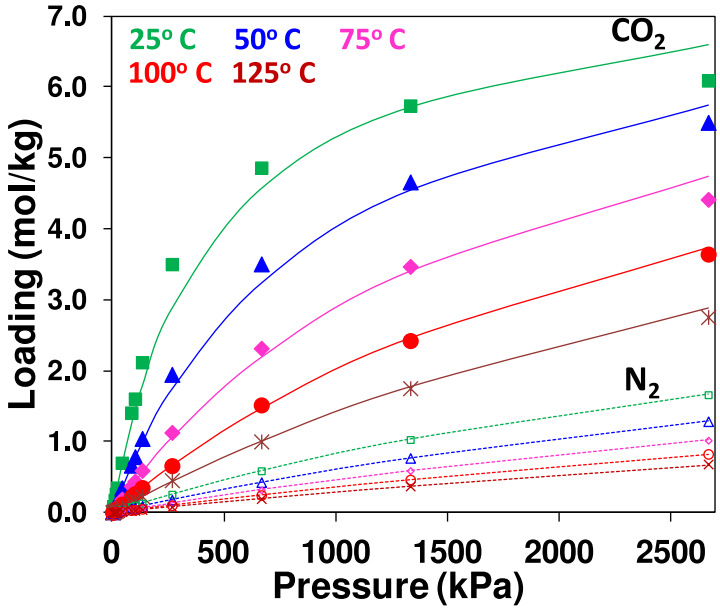

Figure S26: Adsorption isotherms of CHA. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S55: Dual-site Langmuir isotherm parameters for CHA.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	7.31	5.02
b^o [m^3 mol^{-1}]	8.30×10^{-5}	1.30×10^{-5}
ΔU [kJ mol^{-1}]	0	9.13
Site 2		
q^{sat} [mol kg^{-1}]	7.31	0.32
b^o [m^3 mol^{-1}]	1.00×10^{-6}	1.29×10^{-4}
ΔU [kJ mol^{-1}]	21.03	0

DAC

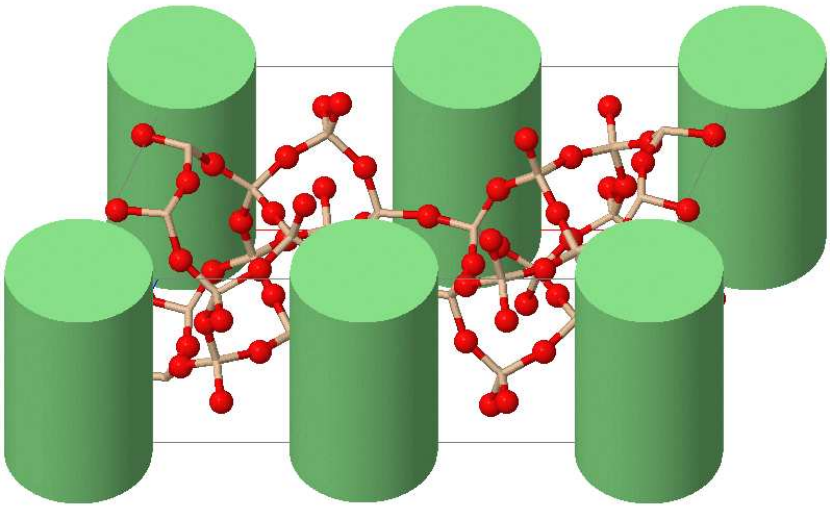

Figure S27: Main pore system of DAC from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S56: Physical properties for DAC.

Property	Value
Pore limiting diamater, PLD [Å]	4.8
Largest cavity diameter, LCD [Å]	5.8
Solid density [kg m^{-3}]	1741

Table S57: Adsorption and geometric properties for DAC.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.08167	0.00143
Heat of adsorption at 298 K [kJ mol^{-1}]	31.3	15.9
Accessible volume [cm^3 g^{-1}]	0.308	0.308
Accessible surface area [m^2 g^{-1}]	1639	1639

Table S58: Performance metrics for DAC.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	57.11
Minimum parasitic energy [kJ/kg CO_2]	841.70
Purity [%] at minimum parasitic energy	86.84
Cost [$/ton of CO_2 captured and compressed]	34.94
Purity [%] at optimum cost	90.36
Recovery [%] at optimum cost	91.57
Energy penalty [kWh/ton CO_2 captured] at optimum cost	196.20

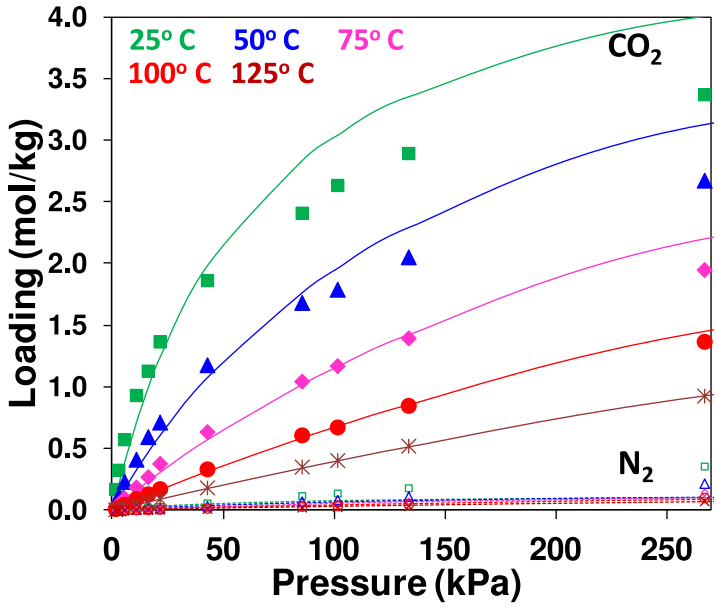

Figure S28: Adsorption isotherms of DAC. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S59: Dual-site Langmuir isotherm parameters for DAC.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	5.09	5.38
b^o [m^3 mol^{-1}]	1.00×10^{-6}	2.00×10^{-6}
ΔU [kJ mol^{-1}]	25.56	14.97
Site 2		
q^{sat} [mol kg^{-1}]	5.38	0
b^o [m^3 mol^{-1}]	0	0
ΔU [kJ mol^{-1}]	29.65	28.72

DFT

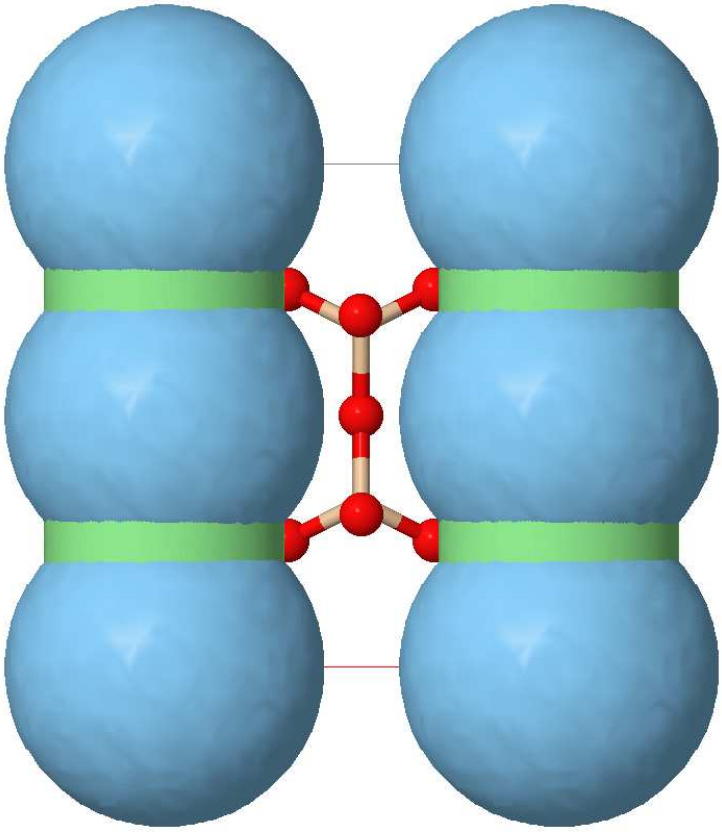

Figure S29: Main pore system of DFT from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S60: Physical properties for DFT.

Property	Value
Pore limiting diamater, PLD [Å]	4.3
Largest cavity diameter, LCD [Å]	5.7
Solid density [kg m^{-3}]	1767

Table S61: Adsorption and geometric properties for DFT.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.08991	0.00140
Heat of adsorption at 298 K [kJ mol^{-1}]	36.8	18.6
Accessible volume [cm^3 g^{-1}]	0.331	0.331
Accessible surface area [m^2 g^{-1}]	1775	1775

Table S62: Performance metrics for DFT.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	64.27
Minimum parasitic energy [kJ/kg CO_2]	887.36
Purity [%] at minimum parasitic energy	86.55
Cost [$/ton of CO_2 captured and compressed]	40.99
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	239.24

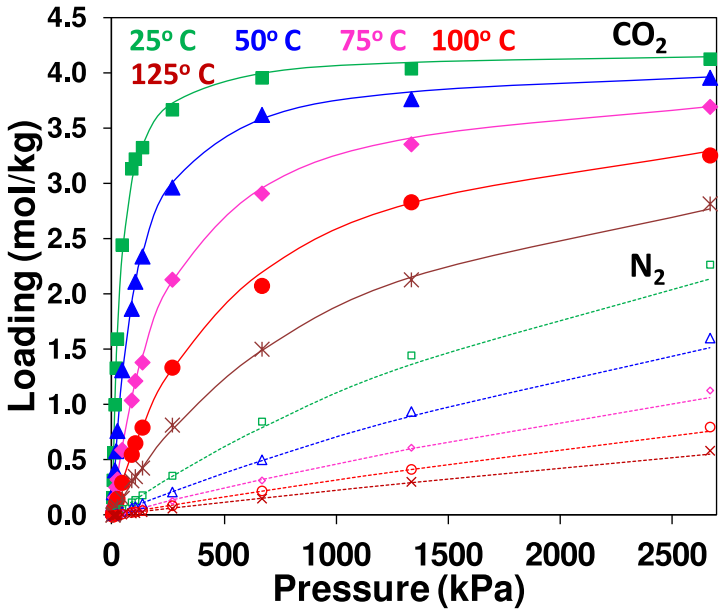

Figure S30: Adsorption isotherms of DFT. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S63: Dual-site Langmuir isotherm parameters for DFT.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.74	4.95
b^o [m^3 mol^{-1}]	0	2.00×10^{-6}
ΔU [kJ mol^{-1}]	0	14.86
Site 2		
q^{sat} [mol kg^{-1}]	4.95	0
b^o [m^3 mol^{-1}]	1.60×10^{-7}	1.50×10^{-7}
ΔU [kJ mol^{-1}]	31.95	27.82

EAB

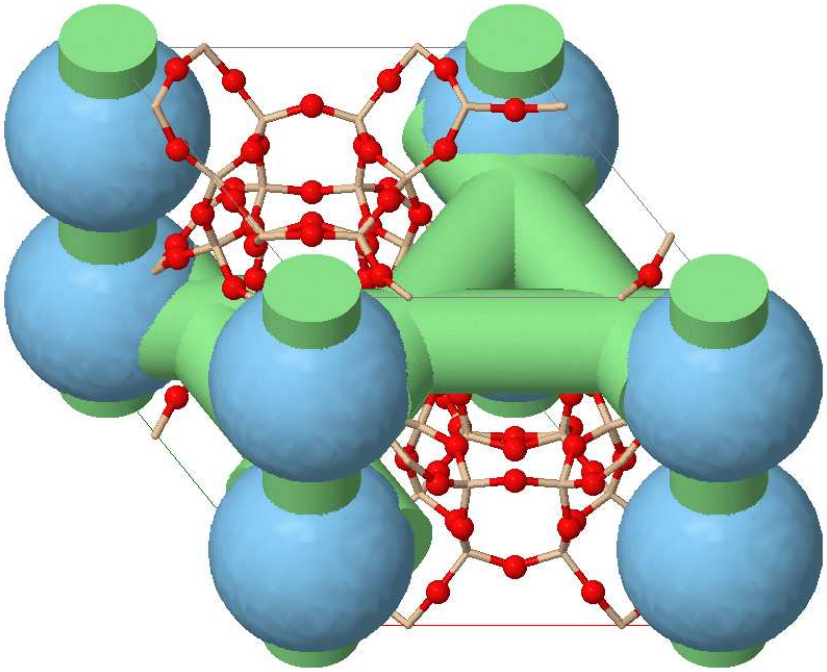

Figure S31: Main pore system of EAB from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S64: Physical properties for EAB.

Property	Value
Pore limiting diamater, PLD [Å]	3.4
Largest cavity diameter, LCD [Å]	7.4
Solid density [kg m^{-3}]	1592

Table S65: Adsorption and geometric properties for EAB.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01636	0.00061
Heat of adsorption at 298 K [kJ mol^{-1}]	29.0	11.5
Accessible volume [cm^3 g^{-1}]	–	0.260
Accessible surface area [m^2 g^{-1}]	–	1745

Table S66: Performance metrics for EAB.

Property	Value
Shape selectivity	–
Size selectivity	1.00
Adsorption selectivity	26.62
Minimum parasitic energy [kJ/kg CO_2]	1224.72
Purity [%] at minimum parasitic energy	70.03
Cost [$/ton of CO_2 captured and compressed]	41.02
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	191.03

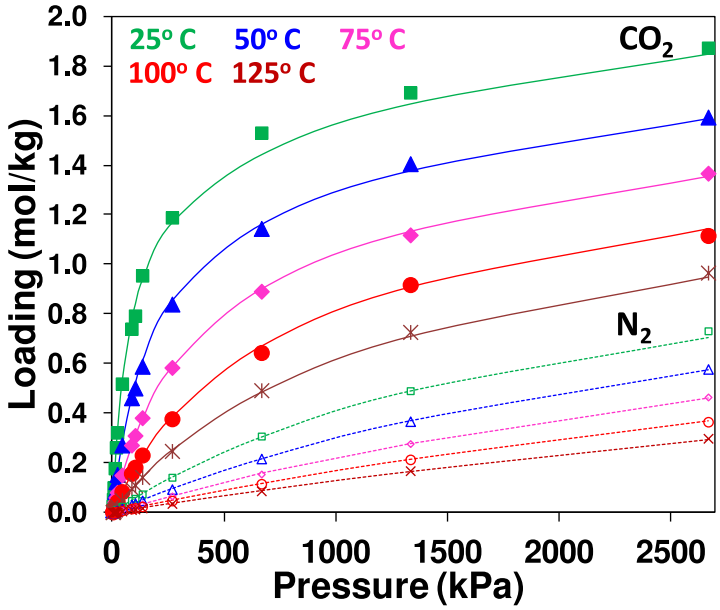

Figure S32: Adsorption isotherms of EAB. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S67: Dual-site Langmuir isotherm parameters for EAB.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.25	2.25
b^o [m^3 mol^{-1}]	2.00×10^{-6}	7.00×10^{-6}
ΔU [kJ mol^{-1}]	13.61	11.40
Site 2		
q^{sat} [mol kg^{-1}]	2.25	0
b^o [m^3 mol^{-1}]	7.60×10^{-7}	4.00×10^{-6}
ΔU [kJ mol^{-1}]	25.38	20.14

EON

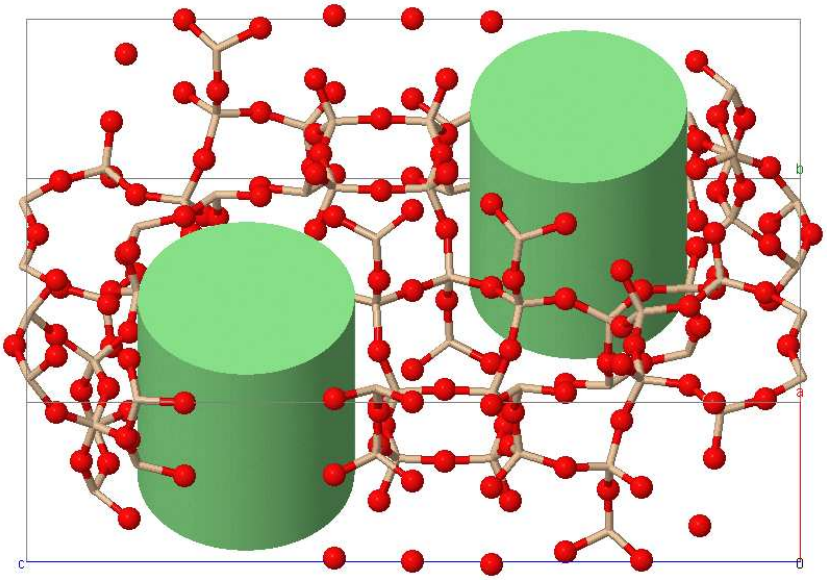

Figure S33: Main pore system of EON from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S68: Physical properties for EON.

Property	Value
Pore limiting diamater, PLD [Å]	7.3
Largest cavity diameter, LCD [Å]	7.3
Solid density [kg m^{-3}]	1680

Table S69: Adsorption and geometric properties for EON.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01372	0.00101
Heat of adsorption at 298 K [kJ mol^{-1}]	26.9	14.6
Accessible volume [cm^3 g^{-1}]	0.122	0.236
Accessible surface area [m^2 g^{-1}]	577	1140

Table S70: Performance metrics for EON.

Property	Value
Shape selectivity	–
Size selectivity	0.48
Adsorption selectivity	13.64
Minimum parasitic energy [kJ/kg CO_2]	948.99
Purity [%] at minimum parasitic energy	84.08
Cost [$/ton of CO_2 captured and compressed]	34.14
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	223.97

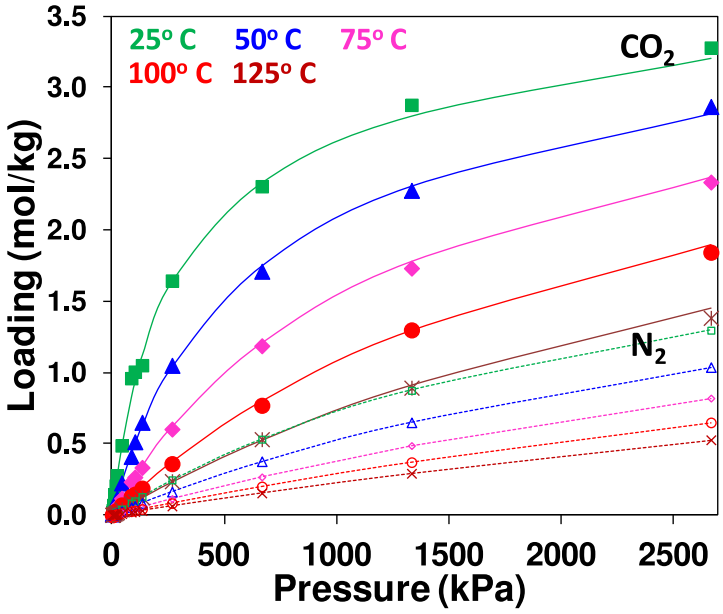

Figure S34: Adsorption isotherms of EON. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S71: Dual-site Langmuir isotherm parameters for EON.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.94	3.94
b^o [m^3 mol^{-1}]	3.00×10^{-6}	7.00×10^{-6}
ΔU [kJ mol^{-1}]	12.27	11.25
Site 2		
q^{sat} [mol kg^{-1}]	2.64	0.16
b^o [m^3 mol^{-1}]	6.00×10^{-7}	0
ΔU [kJ mol^{-1}]	24.57	43.26

ERI

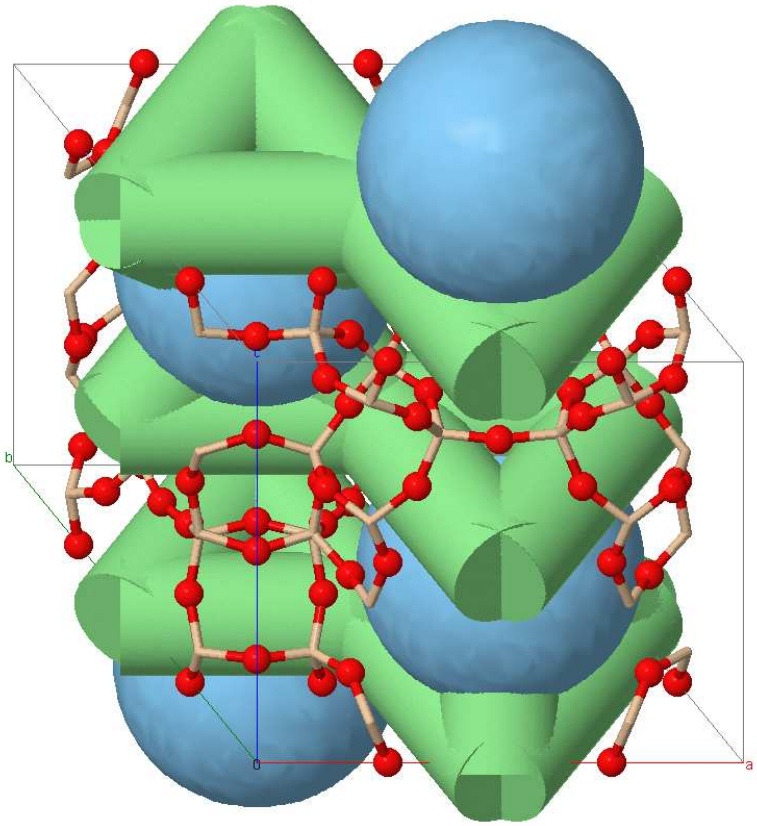

Figure S35: Main pore system of ERI from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S72: Physical properties for ERI.

Property	Value
Pore limiting diamater, PLD [Å]	3.3
Largest cavity diameter, LCD [Å]	7.7
Solid density [kg m^{-3}]	1604

Table S73: Adsorption and geometric properties for ERI.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01211	0.00088
Heat of adsorption at 298 K [kJ mol^{-1}]	25.2	12.3
Accessible volume [cm^3 g^{-1}]	–	0.328
Accessible surface area [m^2 g^{-1}]	–	817

Table S74: Performance metrics for ERI.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	13.82
Minimum parasitic energy [kJ/kg CO_2]	1779.39
Purity [%] at minimum parasitic energy	57.78
Cost [$/ton of CO_2 captured and compressed]	29.75
Purity [%] at optimum cost	90.06
Recovery [%] at optimum cost	91.31
Energy penalty [kWh/ton CO_2 captured] at optimum cost	179.26

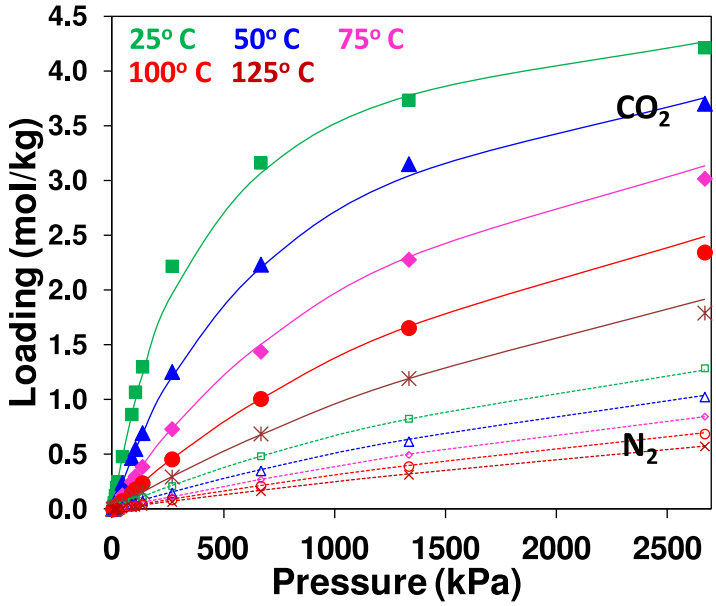

Figure S36: Adsorption isotherms of ERI. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S75: Dual-site Langmuir isotherm parameters for ERI.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.65	2.81
b^o [m^3 mol^{-1}]	0	2.30×10^{-5}
ΔU [kJ mol^{-1}]	3.61	8.70
Site 2		
q^{sat} [mol kg^{-1}]	4.90	0
b^o [m^3 mol^{-1}]	2.00×10^{-6}	0
ΔU [kJ mol^{-1}]	20.20	50.00

FAR

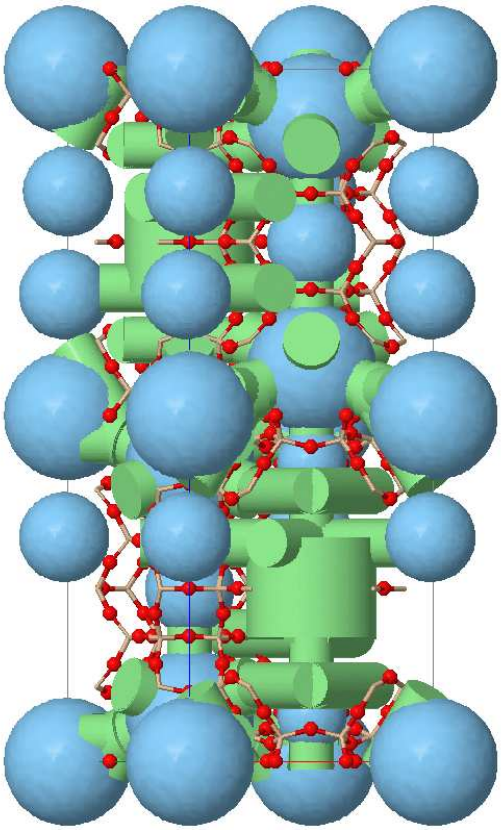

Figure S37: Main pore system of FAR from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S76: Physical properties for FAR.

Property	Value
Pore limiting diamater, PLD [Å]	2.7
Largest cavity diameter, LCD [Å]	6.7
Solid density [kg m^{-3}]	1705

Table S77: Adsorption and geometric properties for FAR.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00804	0.00080
Heat of adsorption at 298 K [kJ mol^{-1}]	26.5	15.2
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S78: Performance metrics for FAR.

Property	Value
Shape selectivity	0.34
Size selectivity	–
Adsorption selectivity	10.01
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	41.45
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	233.72

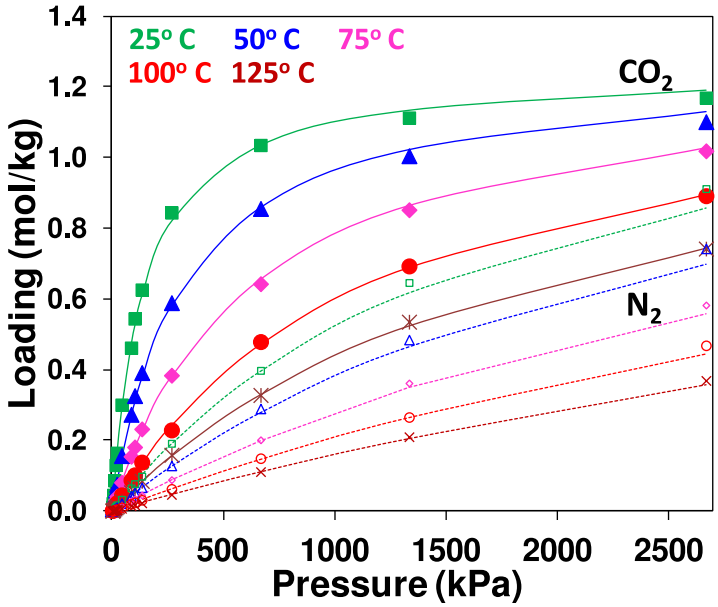

Figure S38: Adsorption isotherms of FAR. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S79: Dual-site Langmuir isotherm parameters for FAR.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	1.40	1.40
b^o [m^3 mol^{-1}]	0	1.00×10^{-5}
ΔU [kJ mol^{-1}]	0	12.28
Site 2		
q^{sat} [mol kg^{-1}]	1.40	0
b^o [m^3 mol^{-1}]	2.00×10^{-6}	8.00×10^{-8}
ΔU [kJ mol^{-1}]	22.75	24.89

FAU

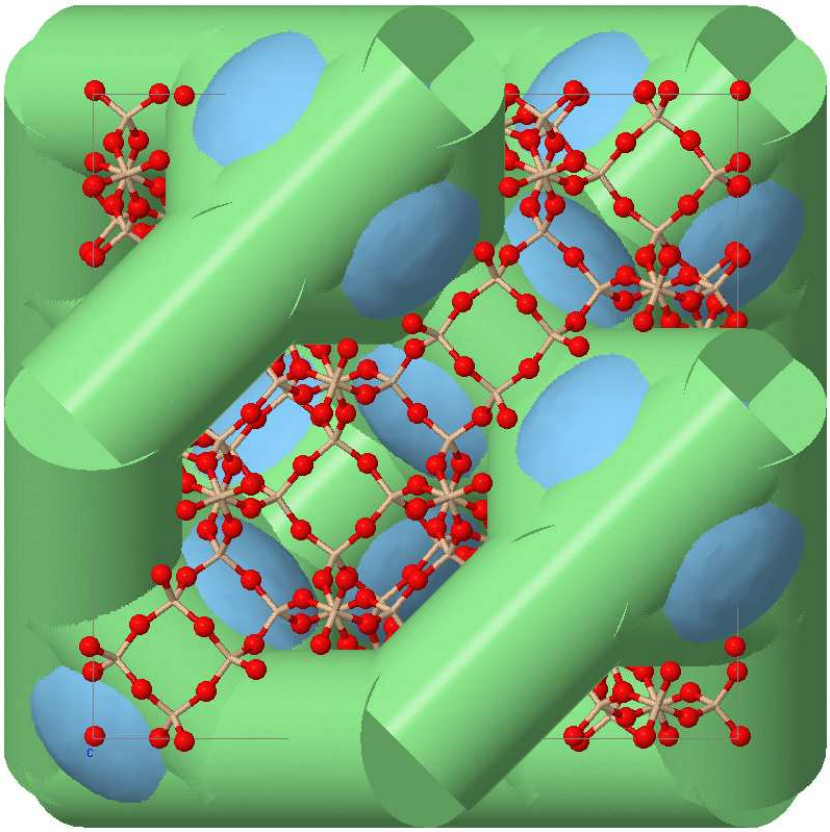

Figure S39: Main pore system of FAU from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S80: Physical properties for FAU.

Property	Value
Pore limiting diamater, PLD [Å]	6.7
Largest cavity diameter, LCD [Å]	11.9
Solid density [kg m^{-3}]	1328

Table S81: Adsorption and geometric properties for FAU.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00291	0.00055
Heat of adsorption at 298 K [kJ mol^{-1}]	19.6	8.5
Accessible volume [cm^3 g^{-1}]	0.402	0.402
Accessible surface area [m^2 g^{-1}]	1190	1190

Table S82: Performance metrics for FAU.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	5.29
Minimum parasitic energy [kJ/kg CO_2]	3794.76
Purity [%] at minimum parasitic energy	37.54
Cost [$/ton of CO_2 captured and compressed]	43.42
Purity [%] at optimum cost	47.26
Recovery [%] at optimum cost	36.49
Energy penalty [kWh/ton CO_2 captured] at optimum cost	293.02

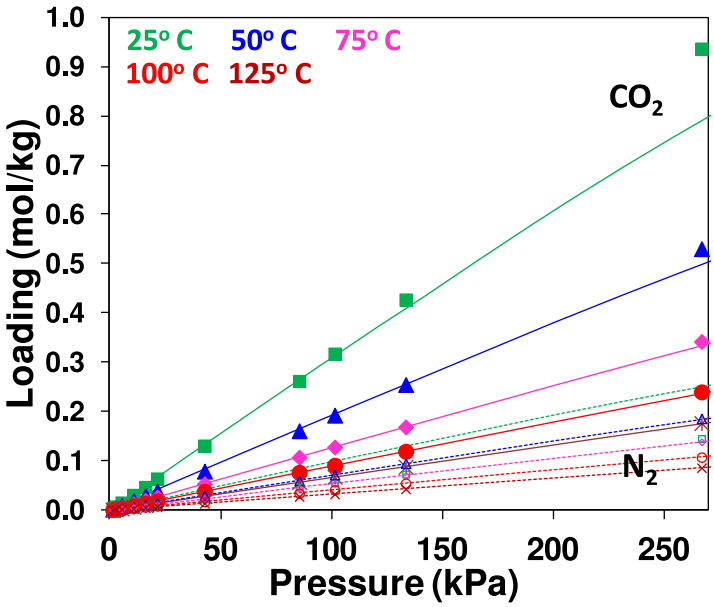

Figure S40: Adsorption isotherms of FAU. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S83: Dual-site Langmuir isotherm parameters for FAU.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	7.33	7.33
b^o [m^3 mol^{-1}]	3.40×10^{-7}	1.20×10^{-5}
ΔU [kJ mol^{-1}]	17.95	8.32
Site 2		
q^{sat} [mol kg^{-1}]	7.33	0.14
b^o [m^3 mol^{-1}]	1.20×10^{-5}	0
ΔU [kJ mol^{-1}]	9.61	11.27

FRA

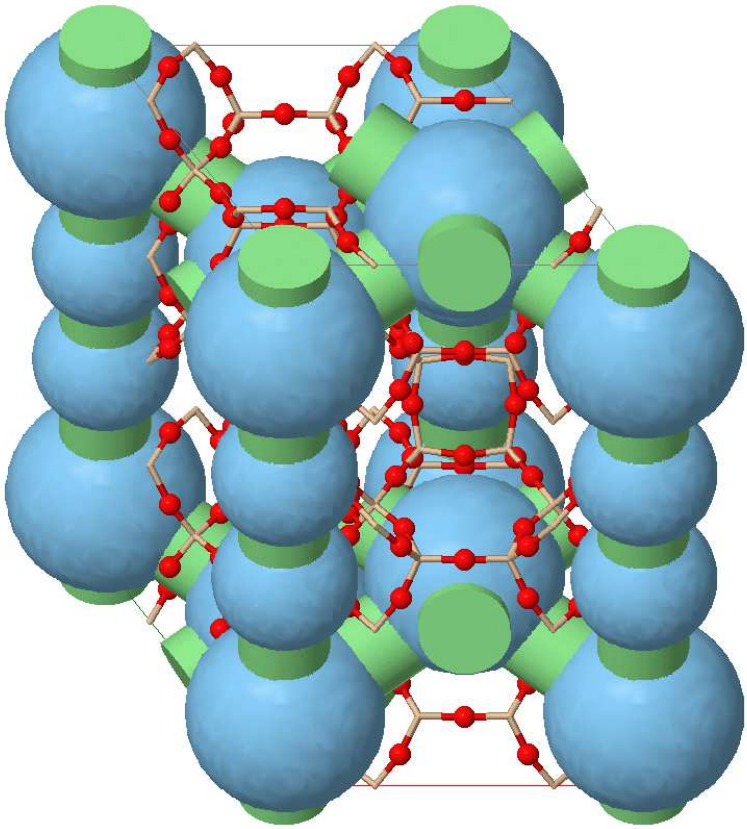

Figure S41: Main pore system of FRA from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S84: Physical properties for FRA.

Property	Value
Pore limiting diamater, PLD [Å]	3.3
Largest cavity diameter, LCD [Å]	7.3
Solid density [kg m^{-3}]	1561

Table S85: Adsorption and geometric properties for FRA.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.02215	0.00147
Heat of adsorption at 298 K [kJ mol^{-1}]	24.7	15.1
Accessible volume [cm^3 g^{-1}]	–	0.290
Accessible surface area [m^2 g^{-1}]	–	1383

Table S86: Performance metrics for FRA.

Property	Value
Shape selectivity	0.05
Size selectivity	1.00
Adsorption selectivity	15.07
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	50.83
Purity [%] at optimum cost	90.20
Recovery [%] at optimum cost	88.88
Energy penalty [kWh/ton CO_2 captured] at optimum cost	246.09

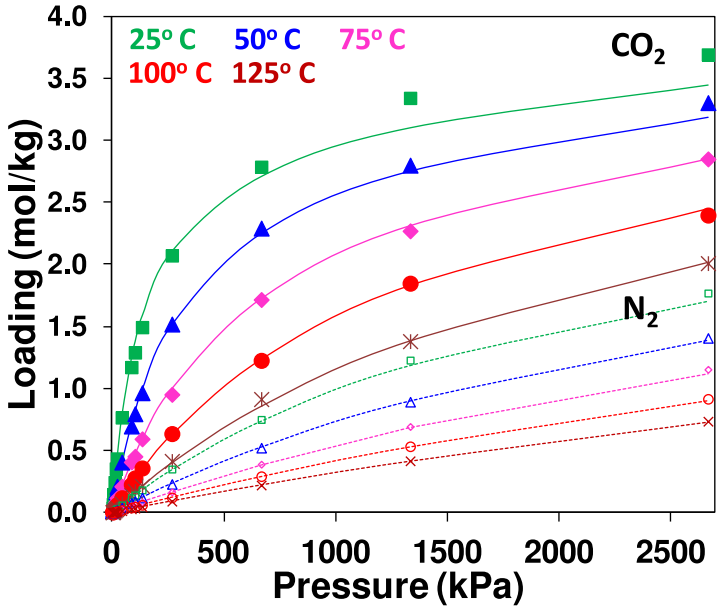

Figure S42: Adsorption isotherms of FRA. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S87: Dual-site Langmuir isotherm parameters for FRA.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.43	4.43
b^o [m^3 mol^{-1}]	3.00×10^{-6}	1.00×10^{-5}
ΔU [kJ mol^{-1}]	11.78	10.93
Site 2		
q^{sat} [mol kg^{-1}]	4.43	0
b^o [m^3 mol^{-1}]	7.20×10^{-7}	2.50×10^{-7}
ΔU [kJ mol^{-1}]	24.45	25.79

GIS

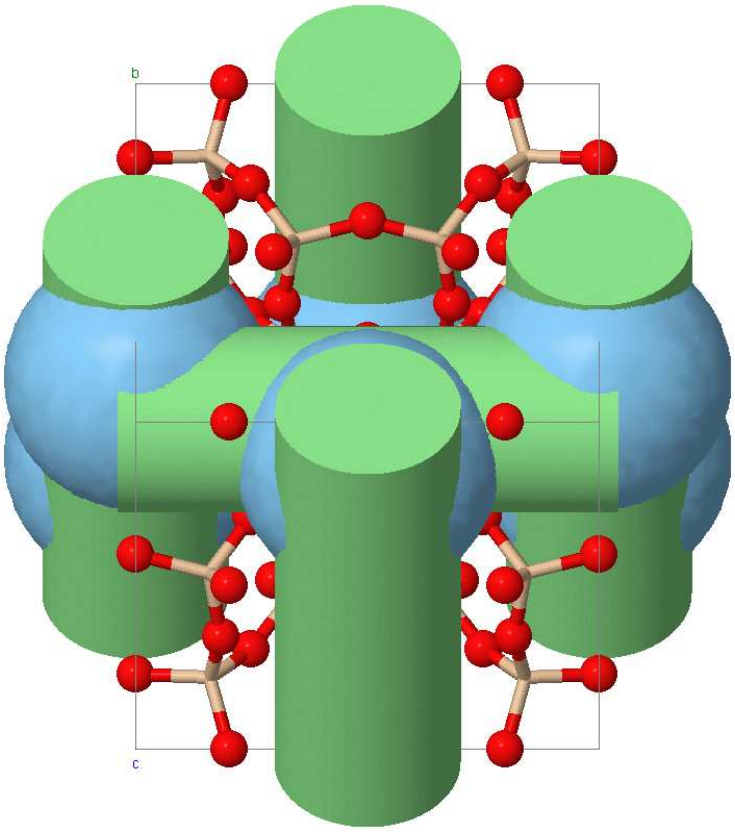

Figure S43: Main pore system of GIS from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S88: Physical properties for GIS.

Property	Value
Pore limiting diamater, PLD [Å]	3.9
Largest cavity diameter, LCD [Å]	5.6
Solid density [kg m^{-3}]	1636

Table S89: Adsorption and geometric properties for GIS.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.14461	0.00120
Heat of adsorption at 298 K [kJ mol^{-1}]	33.7	15.6
Accessible volume [cm^3 g^{-1}]	0.376	0.376
Accessible surface area [m^2 g^{-1}]	1255	1255

Table S90: Performance metrics for GIS.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	120.9
Minimum parasitic energy [kJ/kg CO_2]	793.66
Purity [%] at minimum parasitic energy	89.68
Cost [$/ton of CO_2 captured and compressed]	30.55
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.89
Energy penalty [kWh/ton CO_2 captured] at optimum cost	159.39

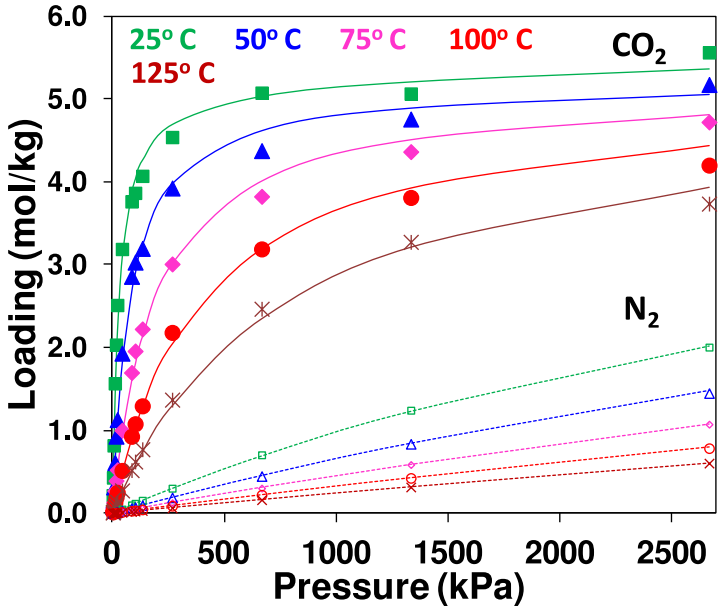

Figure S44: Adsorption isotherms of GIS. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S91: Dual-site Langmuir isotherm parameters for GIS.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	6.68	6.33
b^o [m^3 mol^{-1}]	0	3.00×10^{-6}
ΔU [kJ mol^{-1}]	50.00	12.52
Site 2		
q^{sat} [mol kg^{-1}]	5.15	0.02
b^o [m^3 mol^{-1}]	5.20×10^{-7}	7.20×10^{-5}
ΔU [kJ mol^{-1}]	29.79	0

GIU

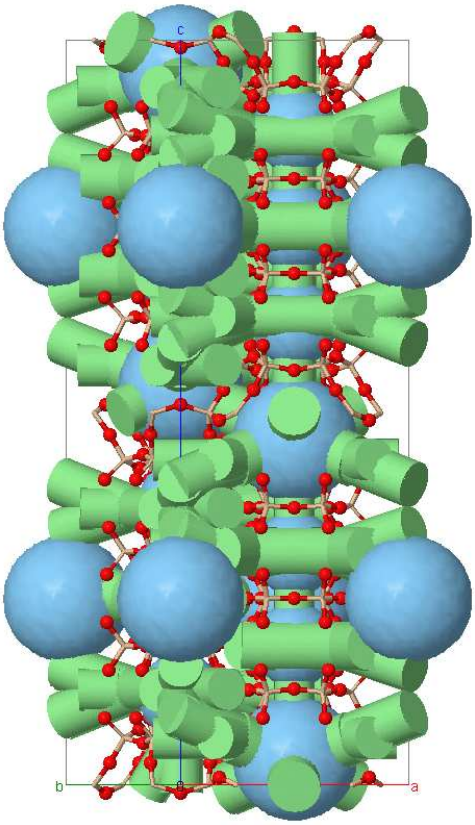

Figure S45: Main pore system of GIU from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S92: Physical properties for GIU.

Property	Value
Pore limiting diamater, PLD [Å]	2.9
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1709

Table S93: Adsorption and geometric properties for GIU.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01382	0.00106
Heat of adsorption at 298 K [kJ mol^{-1}]	27.4	15.5
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S94: Performance metrics for GIU.

Property	Value
Shape selectivity	0.19
Size selectivity	–
Adsorption selectivity	13.02
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	36.38
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	220.15

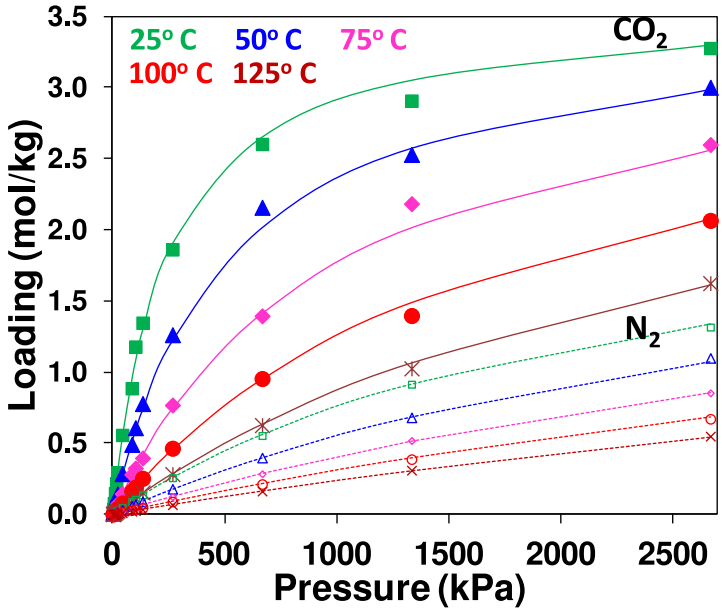

Figure S46: Adsorption isotherms of GIU. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S95: Dual-site Langmuir isotherm parameters for GIU.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.35	2.50
b^o [m^3 mol^{-1}]	0	1.20×10^{-5}
ΔU [kJ mol^{-1}]	28.82	11.17
Site 2		
q^{sat} [mol kg^{-1}]	3.63	0
b^o [m^3 mol^{-1}]	1.00×10^{-6}	9.50×10^{-5}
ΔU [kJ mol^{-1}]	22.45	0

GOO

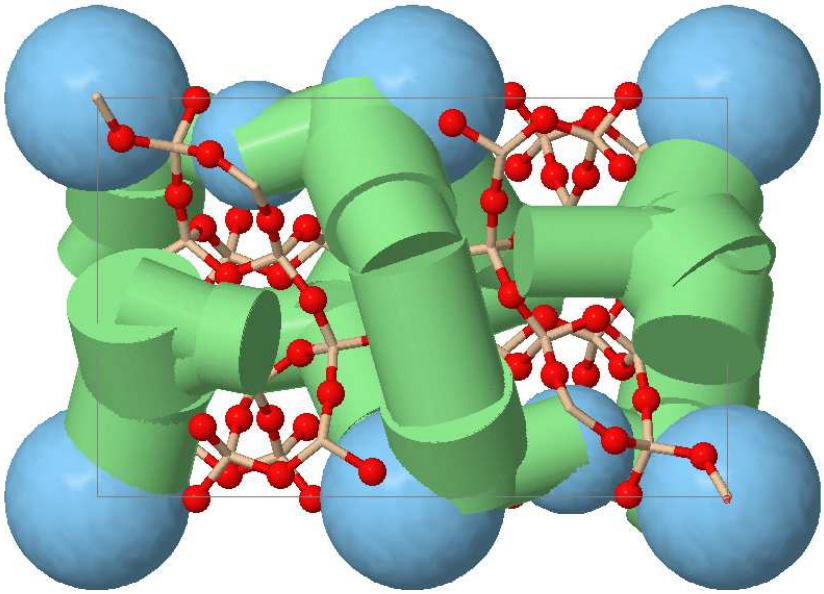

Figure S47: Main pore system of GOO from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S96: Physical properties for GOO.

Property	Value
Pore limiting diamater, PLD [Å]	3.6
Largest cavity diameter, LCD [Å]	5.1
Solid density [kg m^{-3}]	1892

Table S97: Adsorption and geometric properties for GOO.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00531	0.00044
Heat of adsorption at 298 K [kJ mol^{-1}]	28.9	16.7
Accessible volume [cm^3 g^{-1}]	0.092	0.181
Accessible surface area [m^2 g^{-1}]	426	918

Table S98: Performance metrics for GOO.

Property	Value
Shape selectivity	–
Size selectivity	0.49
Adsorption selectivity	12.02
Minimum parasitic energy [kJ/kg CO_2]	1276.35
Purity [%] at minimum parasitic energy	78.49
Cost [$/ton of CO_2 captured and compressed]	32.01
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	188.87

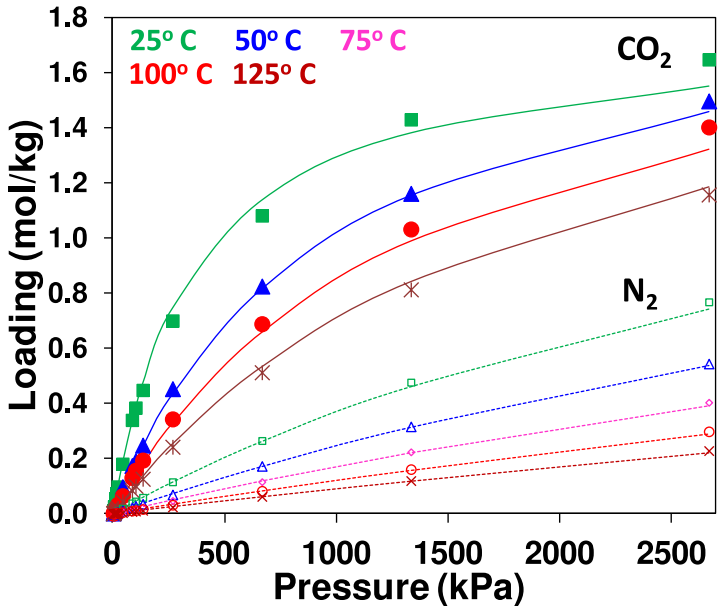

Figure S48: Adsorption isotherms of GOO. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S99: Dual-site Langmuir isotherm parameters for GOO.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	1.98	1.98
b^o [m^3 mol^{-1}]	2.70×10^{-7}	3.00×10^{-6}
ΔU [kJ mol^{-1}]	10.67	12.84
Site 2		
q^{sat} [mol kg^{-1}]	1.98	0
b^o [m^3 mol^{-1}]	4.80×10^{-5}	0
ΔU [kJ mol^{-1}]	11.99	50.00

IHW

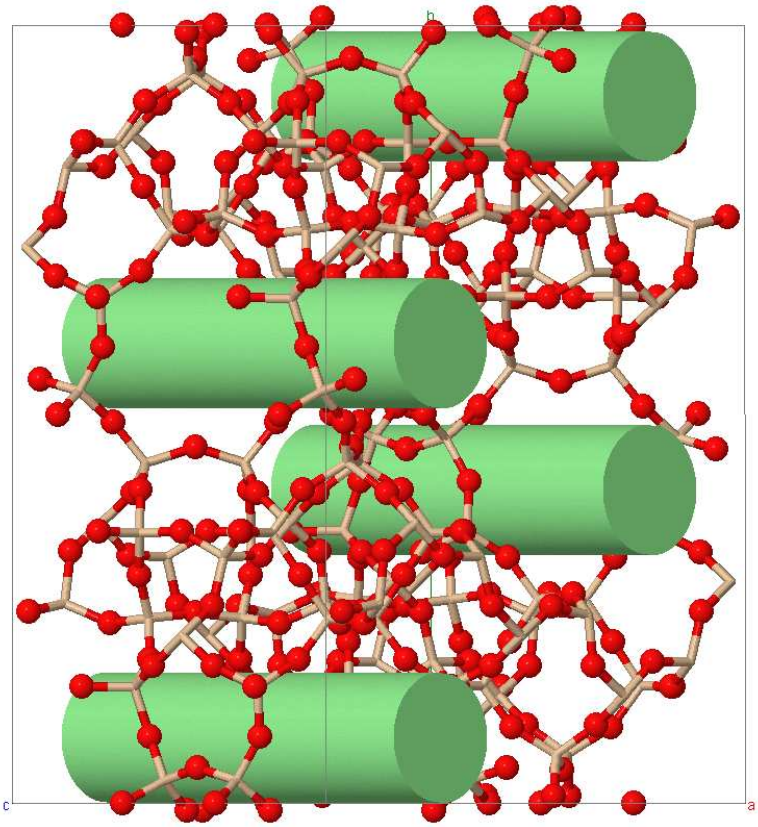

Figure S49: Main pore system of IHW from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S100: Physical properties for IHW.

Property	Value
Pore limiting diamater, PLD [Å]	4.0
Largest cavity diameter, LCD [Å]	6.2
Solid density [kg m^{-3}]	1843

Table S101: Adsorption and geometric properties for IHW.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00956	0.00069
Heat of adsorption at 298 K [kJ mol^{-1}]	26.8	13.0
Accessible volume [cm^3 g^{-1}]	0.074	0.156
Accessible surface area [m^2 g^{-1}]	620	1174

Table S102: Performance metrics for IHW.

Property	Value
Shape selectivity	–
Size selectivity	0.52
Adsorption selectivity	13.94
Minimum parasitic energy [kJ/kg CO_2]	1995.29
Purity [%] at minimum parasitic energy	57.23
Cost [$/ton of CO_2 captured and compressed]	31.26
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	188.95

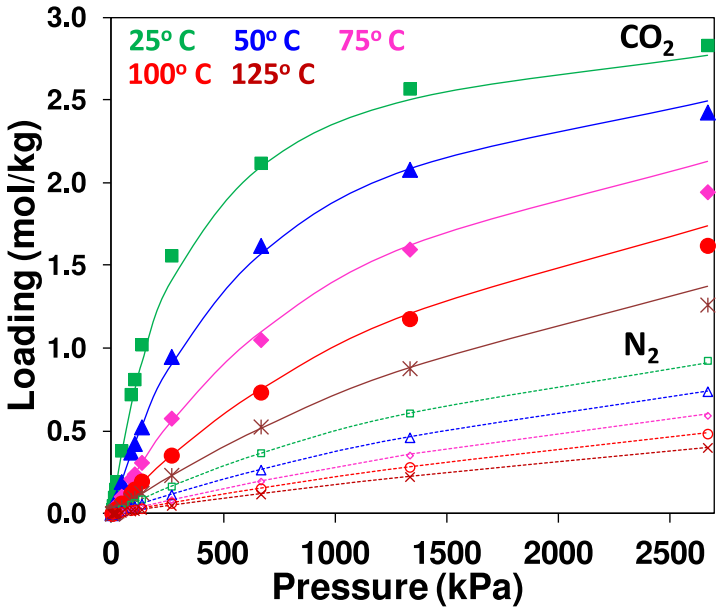

Figure S50: Adsorption isotherms of IHW. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S103: Dual-site Langmuir isotherm parameters for IHW.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.40	1.83
b^o [m^3 mol^{-1}]	0	1.90×10^{-5}
ΔU [kJ mol^{-1}]	2.05	9.61
Site 2		
q^{sat} [mol kg^{-1}]	3.10	0.06
b^o [m^3 mol^{-1}]	2.00×10^{-6}	0
ΔU [kJ mol^{-1}]	20.30	50.00

ITR

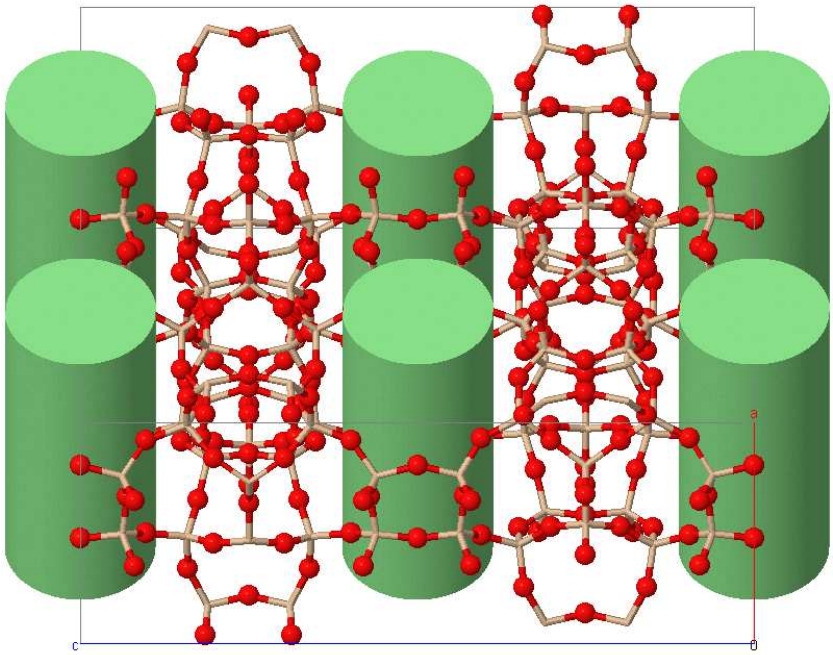

Figure S51: Main pore system of ITR from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S104: Physical properties for ITR.

Property	Value
Pore limiting diamater, PLD [Å]	5.6
Largest cavity diameter, LCD [Å]	6.5
Solid density [kg m^{-3}]	1731

Table S105: Adsorption and geometric properties for ITR.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00844	0.00066
Heat of adsorption at 298 K [kJ mol^{-1}]	24.8	12.9
Accessible volume [cm^3 g^{-1}]	0.167	0.206
Accessible surface area [m^2 g^{-1}]	1678	2016

Table S106: Performance metrics for ITR.

Property	Value
Shape selectivity	–
Size selectivity	0.19
Adsorption selectivity	12.84
Minimum parasitic energy [kJ/kg CO_2]	1936.74
Purity [%] at minimum parasitic energy	56.76
Cost [$/ton of CO_2 captured and compressed]	37.92
Purity [%] at optimum cost	90.18
Recovery [%] at optimum cost	85.40
Energy penalty [kWh/ton CO_2 captured] at optimum cost	217.79

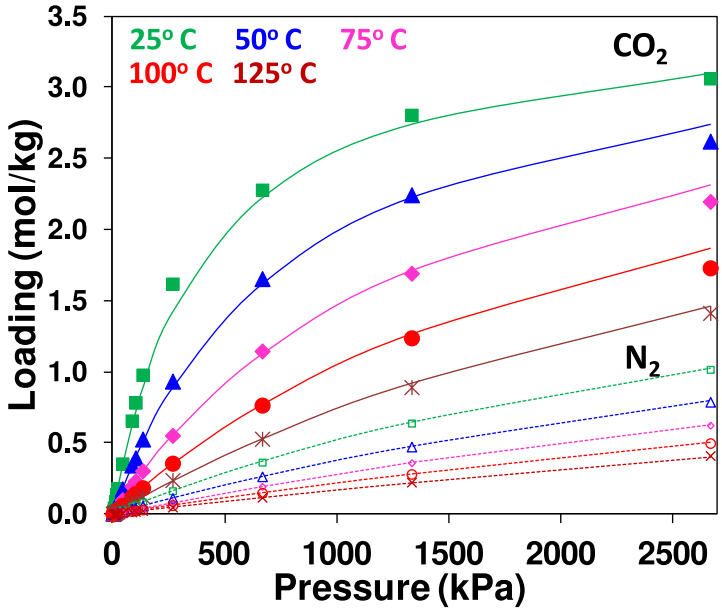

Figure S52: Adsorption isotherms of ITR. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S107: Dual-site Langmuir isotherm parameters for ITR.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.66	2.49
b^o [m^3 mol^{-1}]	0	1.20×10^{-5}
ΔU [kJ mol^{-1}]	17.34	9.89
Site 2		
q^{sat} [mol kg^{-1}]	3.57	0
b^o [m^3 mol^{-1}]	2.00×10^{-6}	0
ΔU [kJ mol^{-1}]	19.36	50.00

ITW

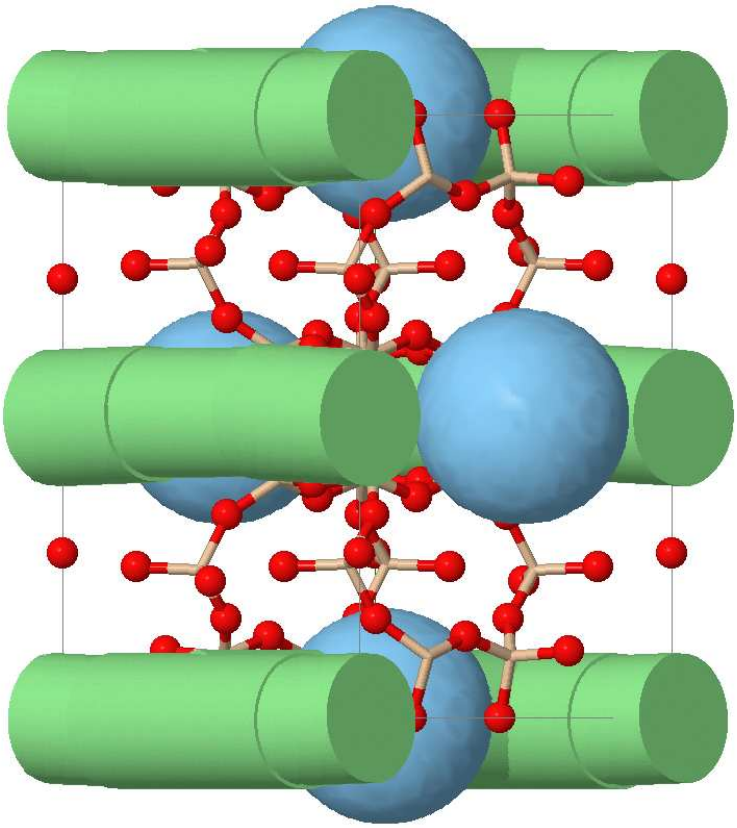

Figure S53: Main pore system of ITW from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S108: Physical properties for ITW.

Property	Value
Pore limiting diamater, PLD [Å]	3.4
Largest cavity diameter, LCD [Å]	5.4
Solid density [kg m^{-3}]	1768

Table S109: Adsorption and geometric properties for ITW.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.03854	0.00099
Heat of adsorption at 298 K [kJ mol^{-1}]	30.5	15.2
Accessible volume [cm^3 g^{-1}]	–	0.311
Accessible surface area [m^2 g^{-1}]	–	997

Table S110: Performance metrics for ITW.

Property	Value
Shape selectivity	–
Size selectivity	1.00
Adsorption selectivity	39.10
Minimum parasitic energy [kJ/kg CO_2]	1095.99
Purity [%] at minimum parasitic energy	78.19
Cost [$/ton of CO_2 captured and compressed]	29.39
Purity [%] at optimum cost	90.25
Recovery [%] at optimum cost	92.03
Energy penalty [kWh/ton CO_2 captured] at optimum cost	170.95

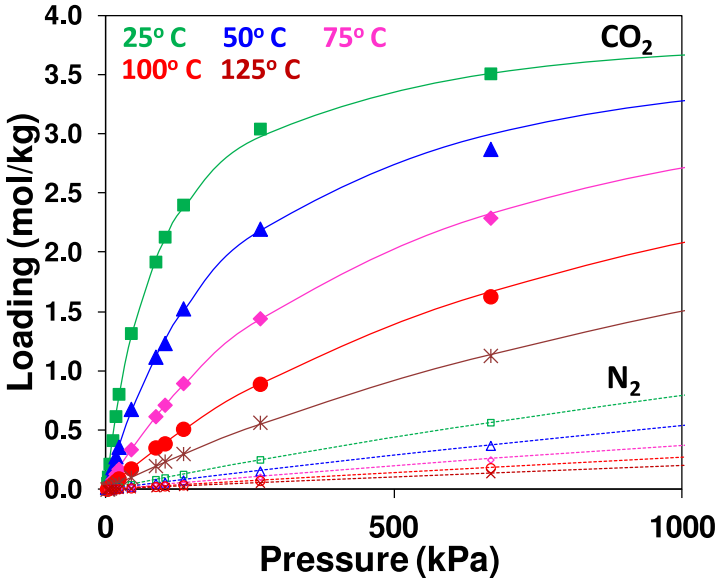

Figure S54: Adsorption isotherms of ITW. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S111: Dual-site Langmuir isotherm parameters for ITW.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	5.08	3.75
b^o [m^3 mol^{-1}]	0	4.00×10^{-6}
ΔU [kJ mol^{-1}]	2.77	12.47
Site 2		
q^{sat} [mol kg^{-1}]	3.98	0
b^o [m^3 mol^{-1}]	8.10×10^{-7}	0
ΔU [kJ mol^{-1}]	25.83	44.94

JBW

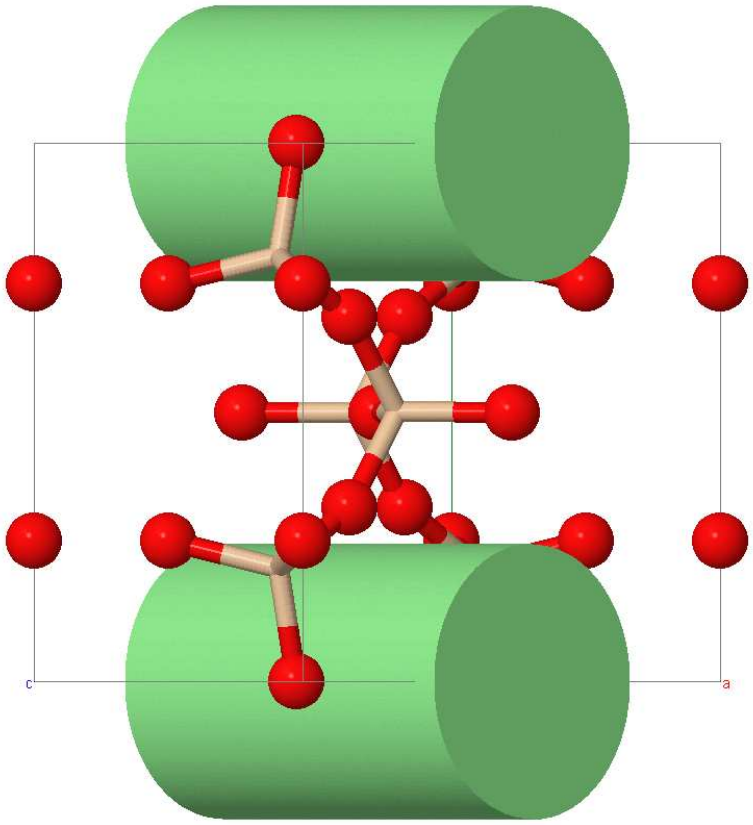

Figure S55: Main pore system of JBW from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S112: Physical properties for JBW.

Property	Value
Pore limiting diamater, PLD [Å]	3.8
Largest cavity diameter, LCD [Å]	3.8
Solid density [kg m^{-3}]	1874

Table S113: Adsorption and geometric properties for JBW.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.11442	0.00059
Heat of adsorption at 298 K [kJ mol^{-1}]	38.7	17.5
Accessible volume [cm^3 g^{-1}]	0.112	0.112
Accessible surface area [m^2 g^{-1}]	834	834

Table S114: Performance metrics for JBW.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	194.4
Minimum parasitic energy [kJ/kg CO_2]	746.47
Purity [%] at minimum parasitic energy	95.19
Cost [$/ton of CO_2 captured and compressed]	38.09
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	191.43

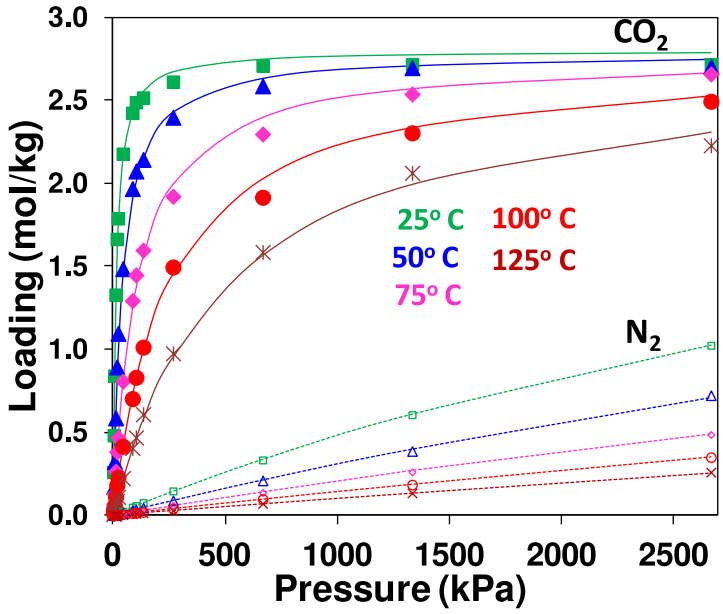

Figure S56: Adsorption isotherms of JBW. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S115: Dual-site Langmuir isotherm parameters for JBW.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.26	3.26
b^o [m^3 mol^{-1}]	0	2.00×10^{-6}
ΔU [kJ mol^{-1}]	1.47	13.76
Site 2		
q^{sat} [mol kg^{-1}]	3.19	0
b^o [m^3 mol^{-1}]	2.30×10^{-7}	6.00×10^{-8}
ΔU [kJ mol^{-1}]	33.50	31.74

LEV

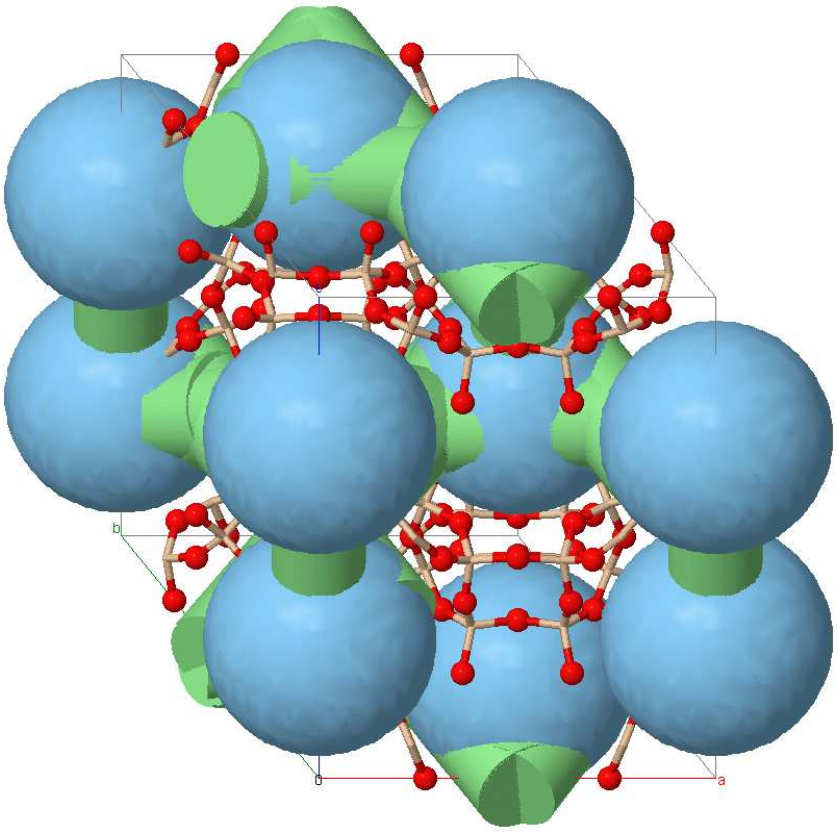

Figure S57: Main pore system of LEV from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S116: Physical properties for LEV.

Property	Value
Pore limiting diamater, PLD [Å]	3.4
Largest cavity diameter, LCD [Å]	7.7
Solid density [kg m^{-3}]	1589

Table S117: Adsorption and geometric properties for LEV.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01731	0.00095
Heat of adsorption at 298 K [kJ mol^{-1}]	28.1	13.4
Accessible volume [cm^3 g^{-1}]	–	0.356
Accessible surface area [m^2 g^{-1}]	–	1721

Table S118: Performance metrics for LEV.

Property	Value
Shape selectivity	–
Size selectivity	1.00
Adsorption selectivity	18.20
Minimum parasitic energy [kJ/kg CO_2]	1471.22
Purity [%] at minimum parasitic energy	63.65
Cost [$/ton of CO_2 captured and compressed]	35.08
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	91.41
Energy penalty [kWh/ton CO_2 captured] at optimum cost	207.65

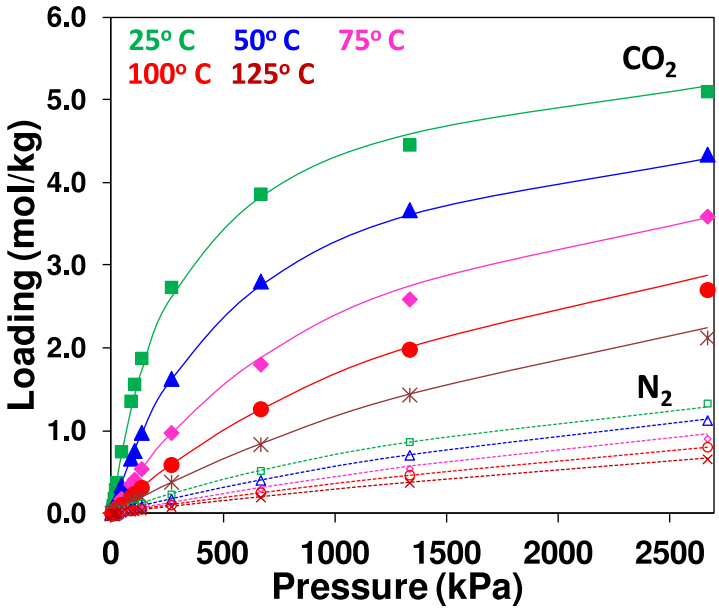

Figure S58: Adsorption isotherms of LEV. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S119: Dual-site Langmuir isotherm parameters for LEV.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	6.13	3.13
b^o [m^3 mol^{-1}]	0	2.90×10^{-5}
ΔU [kJ mol^{-1}]	50.00	8.07
Site 2		
q^{sat} [mol kg^{-1}]	5.04	0
b^o [m^3 mol^{-1}]	1.00×10^{-6}	0
ΔU [kJ mol^{-1}]	22.02	48.71

LOS

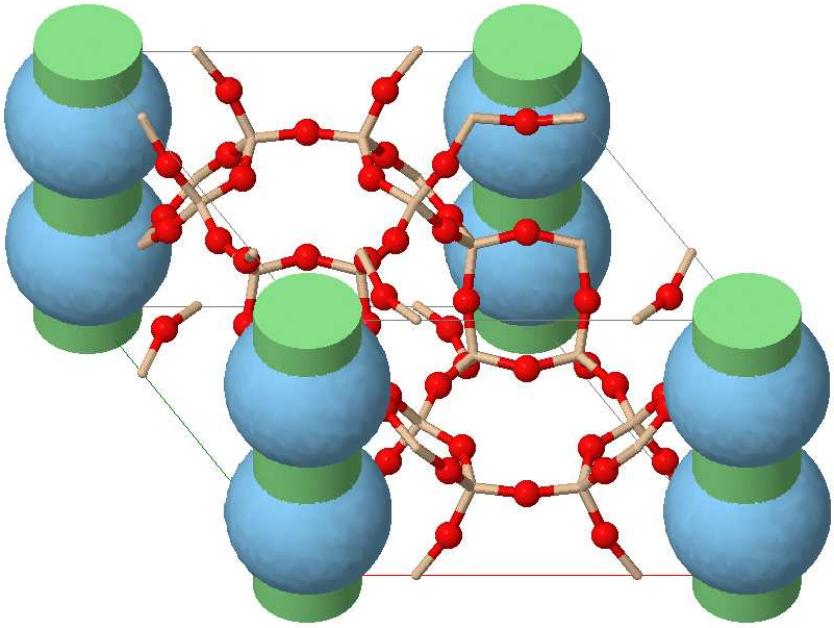

Figure S59: Main pore system of LOS from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S120: Physical properties for LOS.

Property	Value
Pore limiting diamater, PLD [Å]	3.1
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1682

Table S121: Adsorption and geometric properties for LOS.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.07158	0.00138
Heat of adsorption at 298 K [kJ mol^{-1}]	31.9	16.8
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S122: Performance metrics for LOS.

Property	Value
Shape selectivity	0.38
Size selectivity	–
Adsorption selectivity	51.69
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	36.96
Purity [%] at optimum cost	90.19
Recovery [%] at optimum cost	91.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	261.26

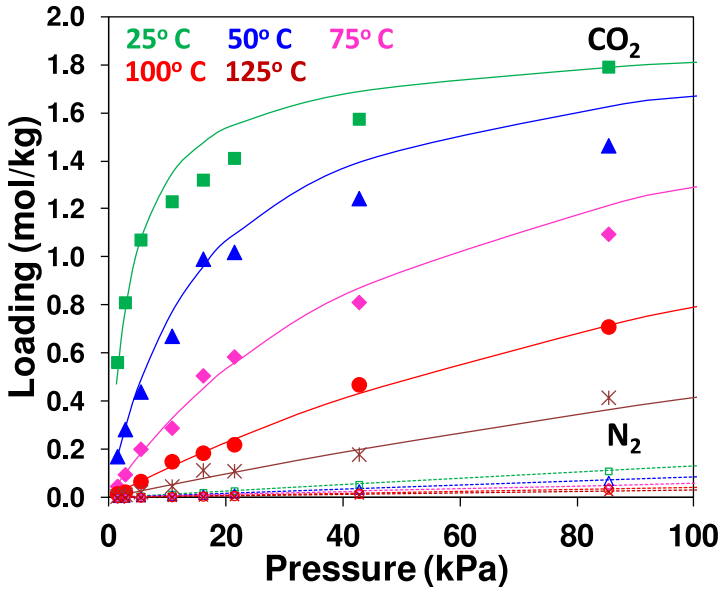

Figure S60: Adsorption isotherms of LOS. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S123: Dual-site Langmuir isotherm parameters for LOS.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.36	3.36
b^o [m^3 mol^{-1}]	1.00×10^{-6}	8.00×10^{-6}
ΔU [kJ mol^{-1}]	15.38	12.04
Site 2		
q^{sat} [mol kg^{-1}]	3.36	0
b^o [m^3 mol^{-1}]	1.00×10^{-8}	0
ΔU [kJ mol^{-1}]	42.17	45.23

LTA

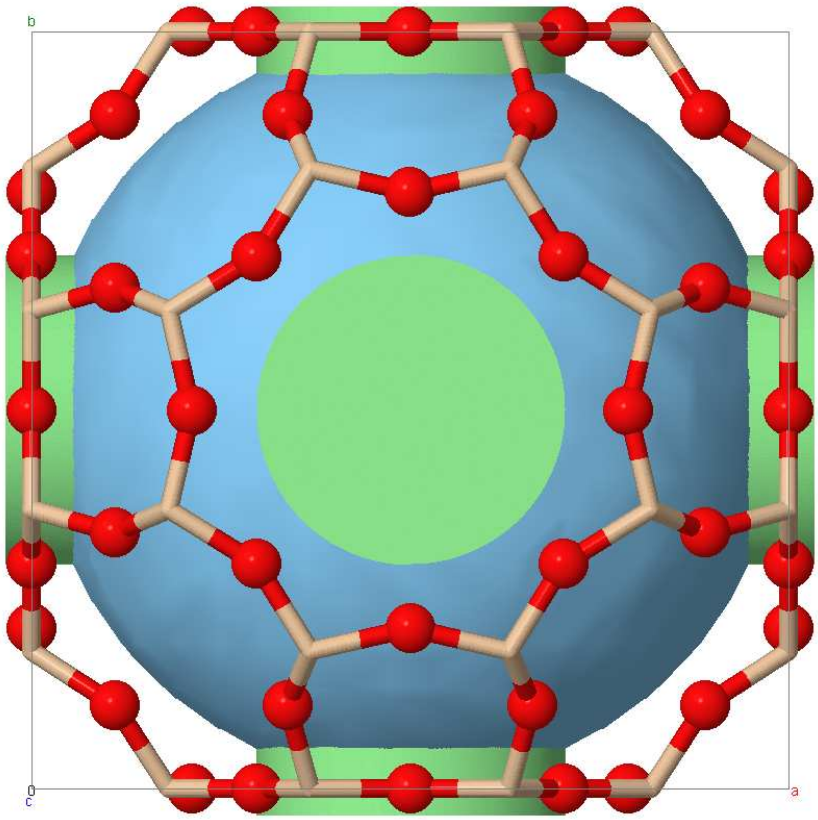

Figure S61: Main pore system of LTA from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S124: Physical properties for LTA.

Property	Value
Pore limiting diamater, PLD [Å]	4.9
Largest cavity diameter, LCD [Å]	11.7
Solid density [kg m^{-3}]	1414

Table S125: Adsorption and geometric properties for LTA.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00716	0.00093
Heat of adsorption at 298 K [kJ mol^{-1}]	24.3	11.5
Accessible volume [cm^3 g^{-1}]	0.369	0.369
Accessible surface area [m^2 g^{-1}]	1198	1198

Table S126: Performance metrics for LTA.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	7.69
Minimum parasitic energy [kJ/kg CO_2]	2464.34
Purity [%] at minimum parasitic energy	47.52
Cost [$/ton of CO_2 captured and compressed]	41.53
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	77.66
Energy penalty [kWh/ton CO_2 captured] at optimum cost	235.30

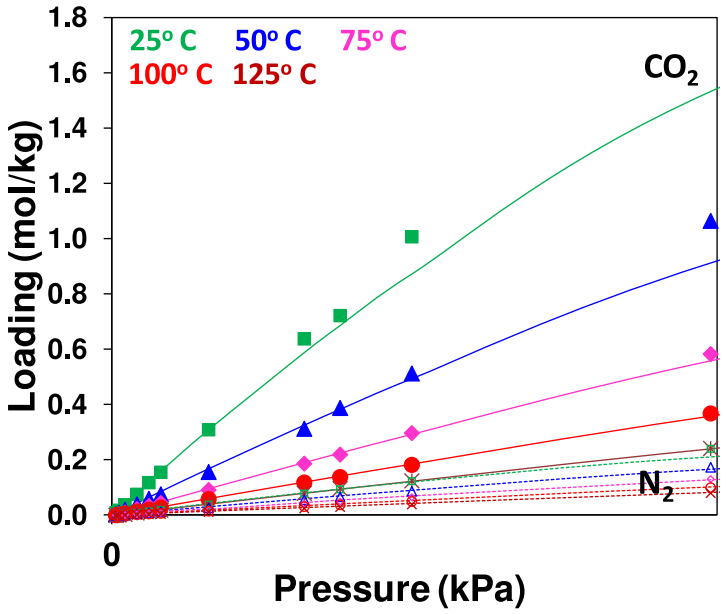

Figure S62: Adsorption isotherms of LTA. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S127: Dual-site Langmuir isotherm parameters for LTA.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	7.20	7.20
b^o [m^3 mol^{-1}]	2.00×10^{-6}	1.00×10^{-5}
ΔU [kJ mol^{-1}]	17.72	8.82
Site 2		
q^{sat} [mol kg^{-1}]	0	0
b^o [m^3 mol^{-1}]	0	0
ΔU [kJ mol^{-1}]	24.46	10.95

LTF

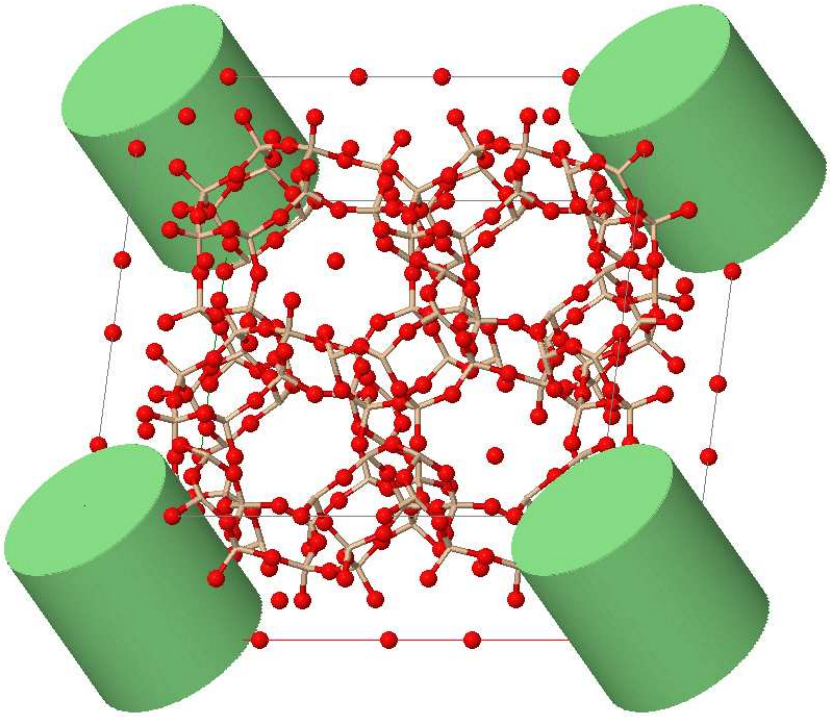

Figure S63: Main pore system of LTF from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S128: Physical properties for LTF.

Property	Value
Pore limiting diamater, PLD [Å]	8.1
Largest cavity diameter, LCD [Å]	8.1
Solid density [kg m^{-3}]	1685

Table S129: Adsorption and geometric properties for LTF.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01941	0.00089
Heat of adsorption at 298 K [kJ mol^{-1}]	29.3	14.5
Accessible volume [cm^3 g^{-1}]	0.251	0.305
Accessible surface area [m^2 g^{-1}]	1225	1839

Table S130: Performance metrics for LTF.

Property	Value
Shape selectivity	–
Size selectivity	0.18
Adsorption selectivity	21.89
Minimum parasitic energy [kJ/kg CO_2]	1370.41
Purity [%] at minimum parasitic energy	70.71
Cost [$/ton of CO_2 captured and compressed]	29.59
Purity [%] at optimum cost	90.05
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	174.11

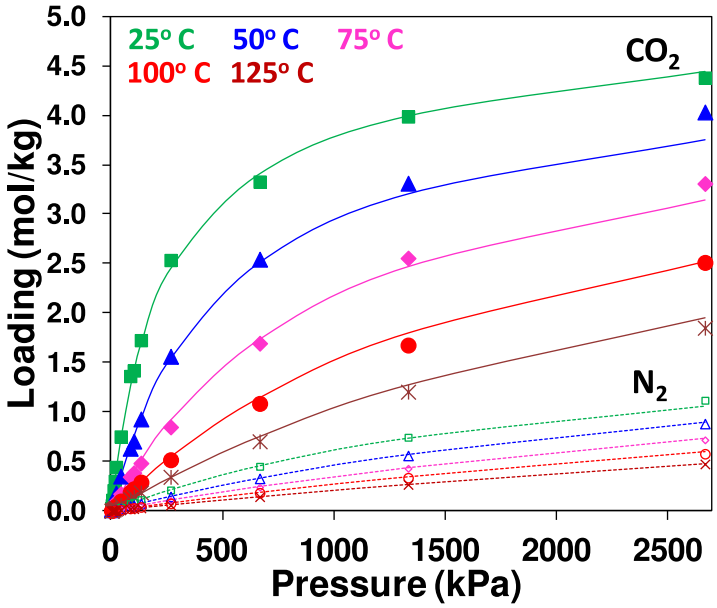

Figure S64: Adsorption isotherms of LTF. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S131: Dual-site Langmuir isotherm parameters for LTF.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	5.26	2.43
b^o [m^3 mol^{-1}]	0	1.20×10^{-5}
ΔU [kJ mol^{-1}]	32.54	10.72
Site 2		
q^{sat} [mol kg^{-1}]	4.07	0.06
b^o [m^3 mol^{-1}]	8.40×10^{-7}	0
ΔU [kJ mol^{-1}]	23.76	43.24

MAR

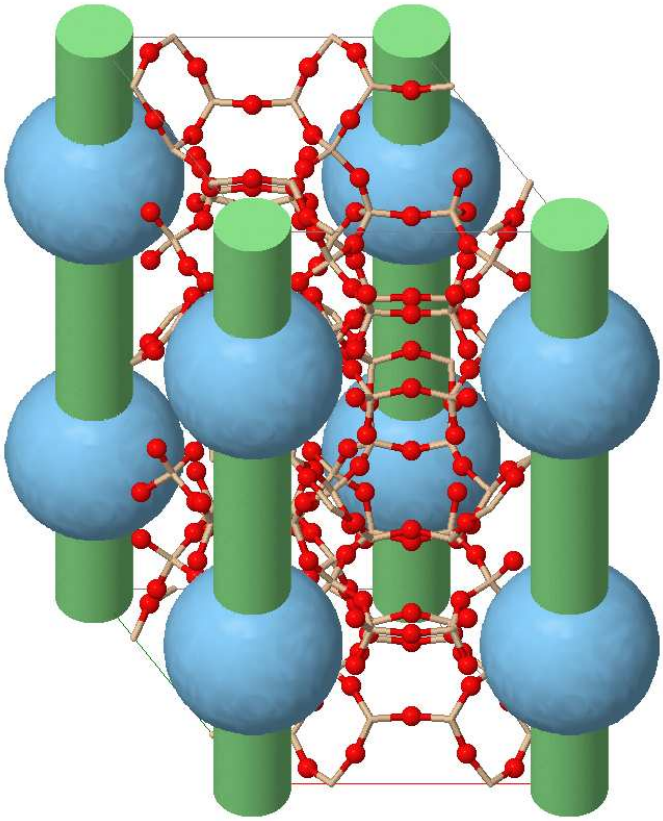

Figure S65: Main pore system of MAR from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S132: Physical properties for MAR.

Property	Value
Pore limiting diamater, PLD [Å]	3.0
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1773

Table S133: Adsorption and geometric properties for MAR.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00725	0.00134
Heat of adsorption at 298 K [kJ mol^{-1}]	28.6	17.1
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S134: Performance metrics for MAR.

Property	Value
Shape selectivity	0.44
Size selectivity	–
Adsorption selectivity	5.40
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	52.70
Purity [%] at optimum cost	86.53
Recovery [%] at optimum cost	36.87
Energy penalty [kWh/ton CO_2 captured] at optimum cost	420.94

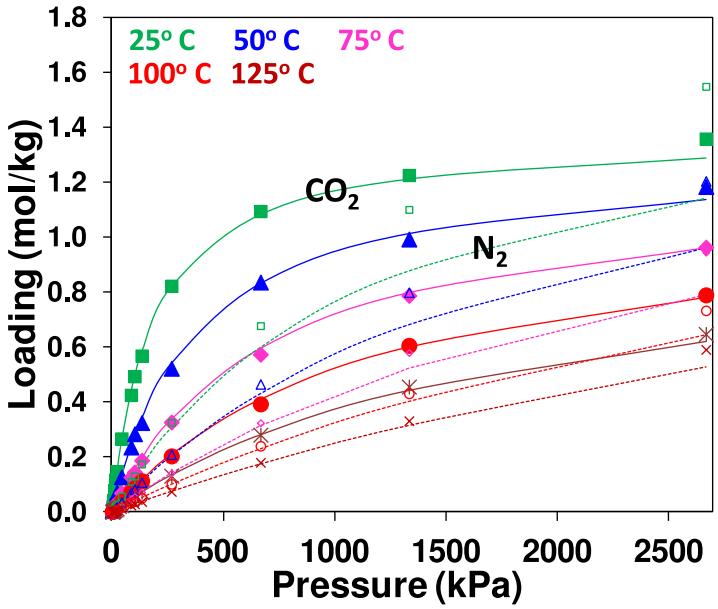

Figure S66: Adsorption isotherms of MAR. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S135: Dual-site Langmuir isotherm parameters for MAR.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	1.20	1.63
b^o [m^3 mol^{-1}]	0	1.20×10^{-5}
ΔU [kJ mol^{-1}]	0.60	12.78
Site 2		
q^{sat} [mol kg^{-1}]	1.63	0
b^o [m^3 mol^{-1}]	1.00×10^{-6}	2.10×10^{-5}
ΔU [kJ mol^{-1}]	22.62	11.47

MEL

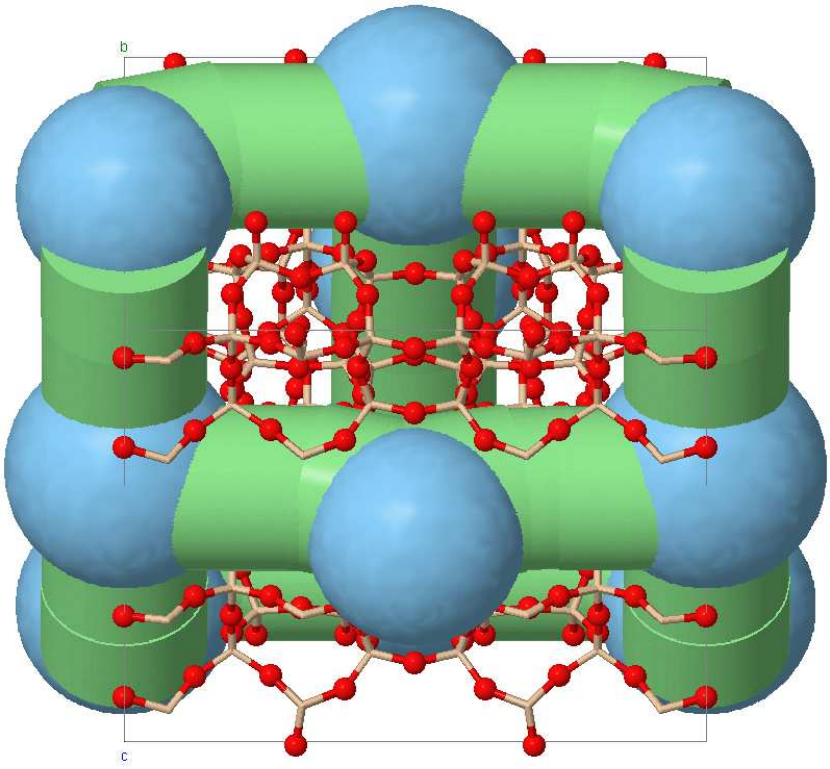

Figure S67: Main pore system of MEL from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S136: Physical properties for MEL.

Property	Value
Pore limiting diamater, PLD [Å]	5.7
Largest cavity diameter, LCD [Å]	8.4
Solid density [kg m^{-3}]	1732

Table S137: Adsorption and geometric properties for MEL.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00935	0.00076
Heat of adsorption at 298 K [kJ mol^{-1}]	24.1	12.0
Accessible volume [cm^3 g^{-1}]	0.224	0.224
Accessible surface area [m^2 g^{-1}]	995	995

Table S138: Performance metrics for MEL.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	12.31
Minimum parasitic energy [kJ/kg CO_2]	1948.91
Purity [%] at minimum parasitic energy	55.56
Cost [$/ton of CO_2 captured and compressed]	32.83
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	215.54

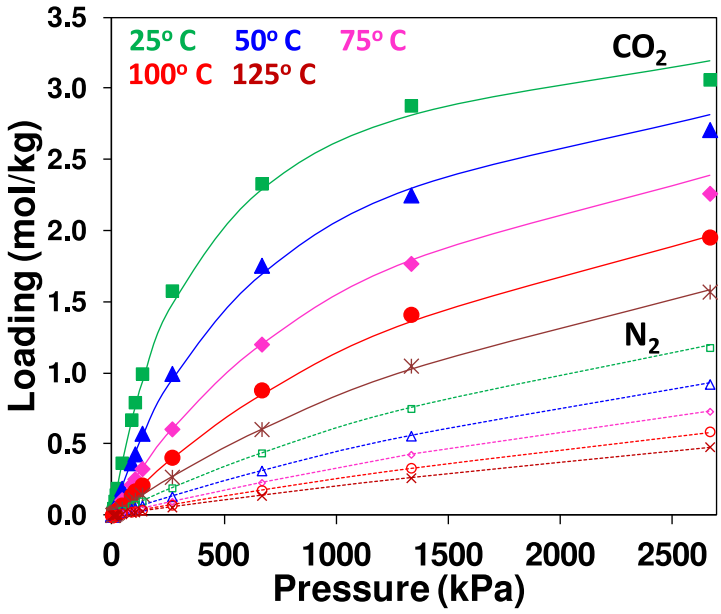

Figure S68: Adsorption isotherms of MEL. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S139: Dual-site Langmuir isotherm parameters for MEL.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.68	3.12
b^o [m^3 mol^{-1}]	6.30×10^{-5}	1.30×10^{-5}
ΔU [kJ mol^{-1}]	0	9.55
Site 2		
q^{sat} [mol kg^{-1}]	3.68	0
b^o [m^3 mol^{-1}]	3.00×10^{-6}	3.50×10^{-5}
ΔU [kJ mol^{-1}]	18.95	5.93

MFI

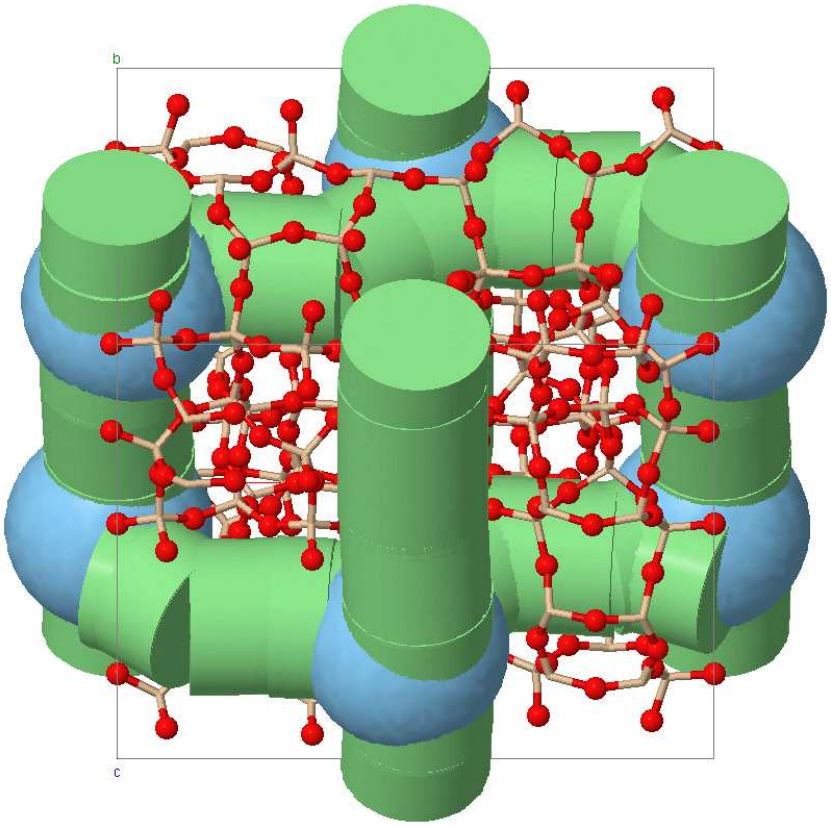

Figure S69: Main pore system of MFI from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S140: Physical properties for MFI.

Property	Value
Pore limiting diamater, PLD [Å]	5.0
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1838

Table S141: Adsorption and geometric properties for MFI.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01302	0.00071
Heat of adsorption at 298 K [kJ mol^{-1}]	26.5	14.4
Accessible volume [cm^3 g^{-1}]	0.193	0.193
Accessible surface area [m^2 g^{-1}]	1007	1007

Table S142: Performance metrics for MFI.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	18.25
Minimum parasitic energy [kJ/kg CO_2]	1567.63
Purity [%] at minimum parasitic energy	65.24
Cost [$/ton of CO_2 captured and compressed]	33.51
Purity [%] at optimum cost	93.20
Recovery [%] at optimum cost	92.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	214.06

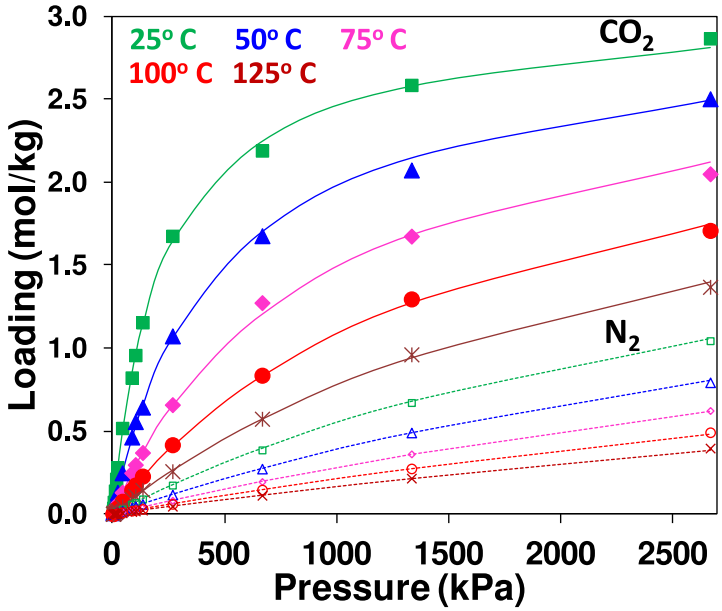

Figure S70: Adsorption isotherms of MFI. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S143: Dual-site Langmuir isotherm parameters for MFI.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.44	2.65
b^o [m^3 mol^{-1}]	7.60×10^{-5}	9.00×10^{-6}
ΔU [kJ mol^{-1}]	0	10.75
Site 2		
q^{sat} [mol kg^{-1}]	3.44	0
b^o [m^3 mol^{-1}]	9.40×10^{-7}	9.00×10^{-6}
ΔU [kJ mol^{-1}]	22.98	13.40

MON

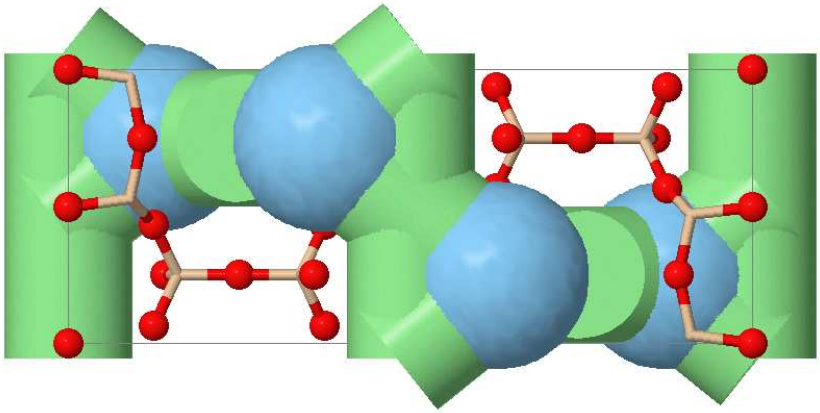

Figure S71: Main pore system of MON from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S144: Physical properties for MON.

Property	Value
Pore limiting diamater, PLD [Å]	3.5
Largest cavity diameter, LCD [Å]	4.9
Solid density [kg m^{-3}]	1761

Table S145: Adsorption and geometric properties for MON.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.08434	0.00067
Heat of adsorption at 298 K [kJ mol^{-1}]	38.0	17.3
Accessible volume [cm^3 g^{-1}]	0.267	0.318
Accessible surface area [m^2 g^{-1}]	1633	1633

Table S146: Performance metrics for MON.

Property	Value
Shape selectivity	–
Size selectivity	0.16
Adsorption selectivity	126.5
Minimum parasitic energy [kJ/kg CO_2]	891.00
Purity [%] at minimum parasitic energy	88.92
Cost [$/ton of CO_2 captured and compressed]	34.34
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	202.76

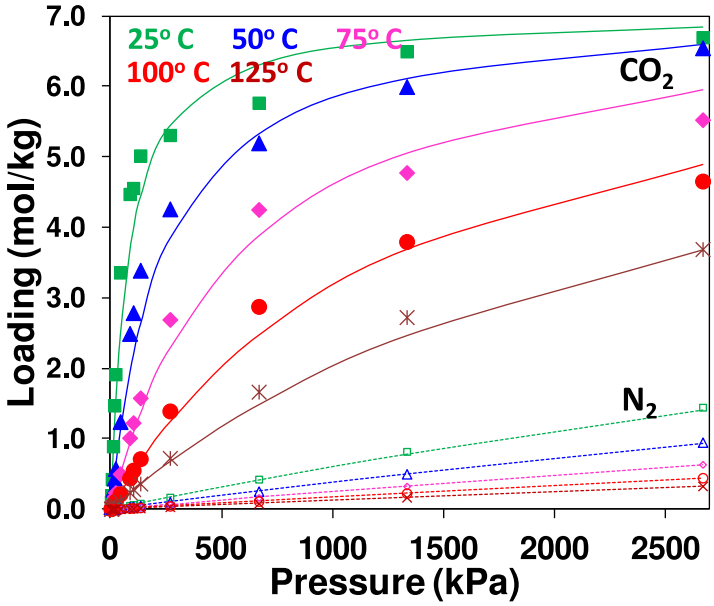

Figure S72: Adsorption isotherms of MON. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S147: Dual-site Langmuir isotherm parameters for MON.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	6.06	7.34
b^o [m^3 mol^{-1}]	0	1.00×10^{-6}
ΔU [kJ mol^{-1}]	3.26	13.30
Site 2		
q^{sat} [mol kg^{-1}]	7.34	0
b^o [m^3 mol^{-1}]	1.00×10^{-7}	0
ΔU [kJ mol^{-1}]	31.36	50.00

MOR

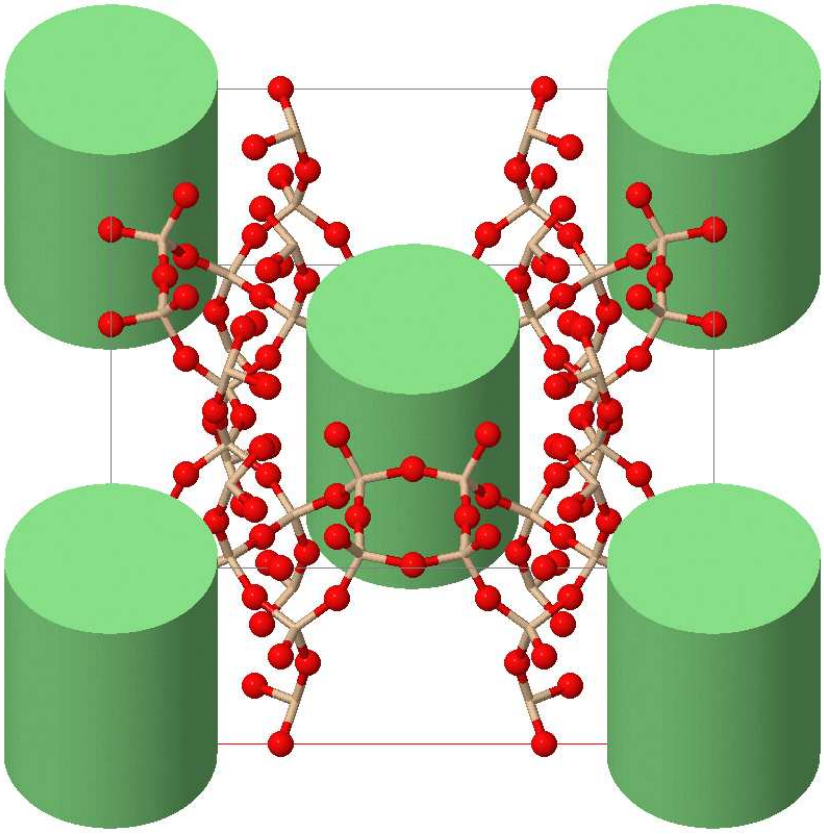

Figure S73: Main pore system of MOR from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S148: Physical properties for MOR.

Property	Value
Pore limiting diamater, PLD [Å]	6.5
Largest cavity diameter, LCD [Å]	6.5
Solid density [kg m^{-3}]	1694

Table S149: Adsorption and geometric properties for MOR.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.04816	0.00111
Heat of adsorption at 298 K [kJ mol^{-1}]	27.7	14.7
Accessible volume [cm^3 g^{-1}]	0.256	0.256
Accessible surface area [m^2 g^{-1}]	2079	2079

Table S150: Performance metrics for MOR.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	43.27
Minimum parasitic energy [kJ/kg CO_2]	947.06
Purity [%] at minimum parasitic energy	83.81
Cost [$/ton of CO_2 captured and compressed]	35.85
Purity [%] at optimum cost	98.77
Recovery [%] at optimum cost	90.18
Energy penalty [kWh/ton CO_2 captured] at optimum cost	276.71

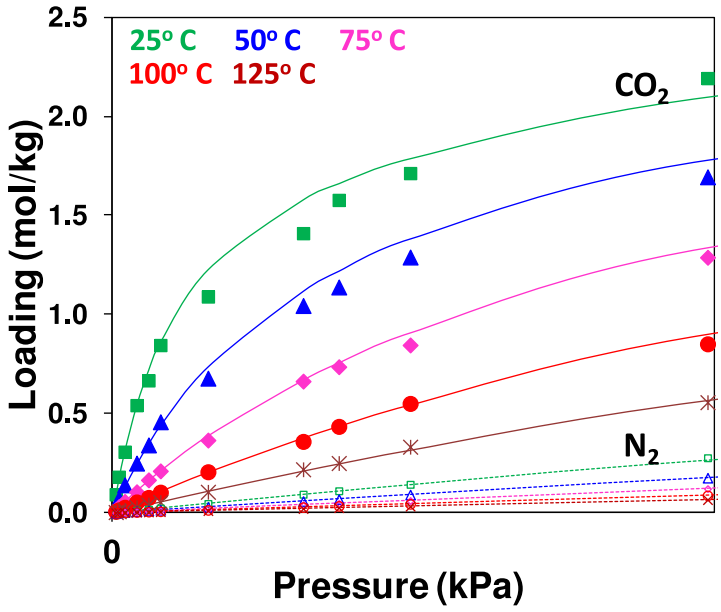

Figure S74: Adsorption isotherms of MOR. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S151: Dual-site Langmuir isotherm parameters for MOR.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.72	4.72
b^o [m^3 mol^{-1}]	3.60×10^{-7}	4.00×10^{-6}
ΔU [kJ mol^{-1}]	18.89	12.13
Site 2		
q^{sat} [mol kg^{-1}]	2.82	0
b^o [m^3 mol^{-1}]	4.00×10^{-7}	0
ΔU [kJ mol^{-1}]	29.49	38.08

MOZ

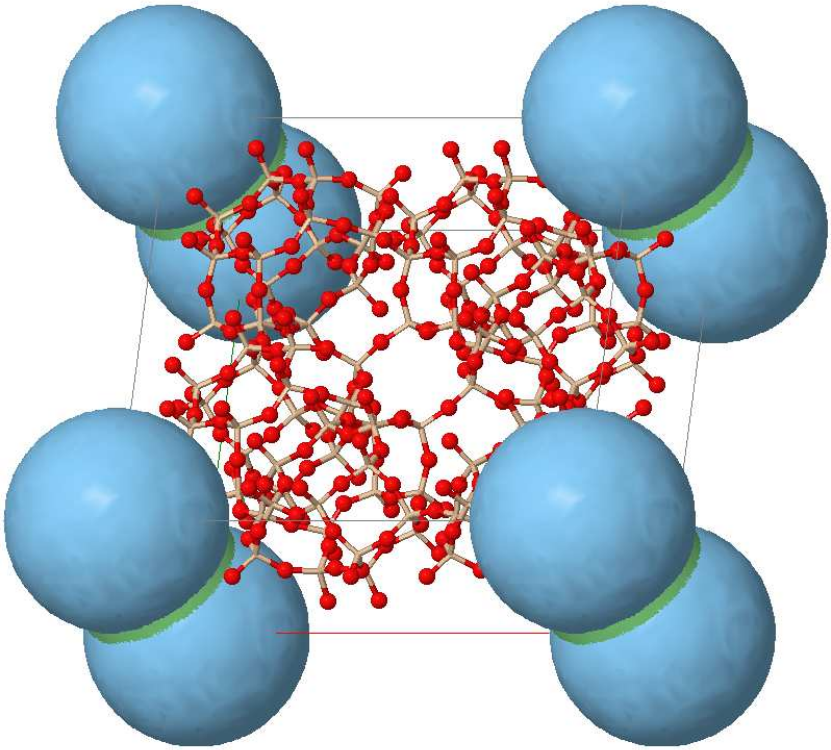

Figure S75: Main pore system of MOZ from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S152: Physical properties for MOZ.

Property	Value
Pore limiting diamater, PLD [Å]	8.2
Largest cavity diameter, LCD [Å]	10.7
Solid density [kg m^{-3}]	1693

Table S153: Adsorption and geometric properties for MOZ.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01476	0.00060
Heat of adsorption at 298 K [kJ mol^{-1}]	27.0	14.7
Accessible volume [cm^3 g^{-1}]	0.114	0.222
Accessible surface area [m^2 g^{-1}]	551	1178

Table S154: Performance metrics for MOZ.

Property	Value
Shape selectivity	–
Size selectivity	0.49
Adsorption selectivity	24.65
Minimum parasitic energy [kJ/kg CO_2]	1430.19
Purity [%] at minimum parasitic energy	70.16
Cost [$/ton of CO_2 captured and compressed]	31.83
Purity [%] at optimum cost	90.10
Recovery [%] at optimum cost	92.58
Energy penalty [kWh/ton CO_2 captured] at optimum cost	181.21

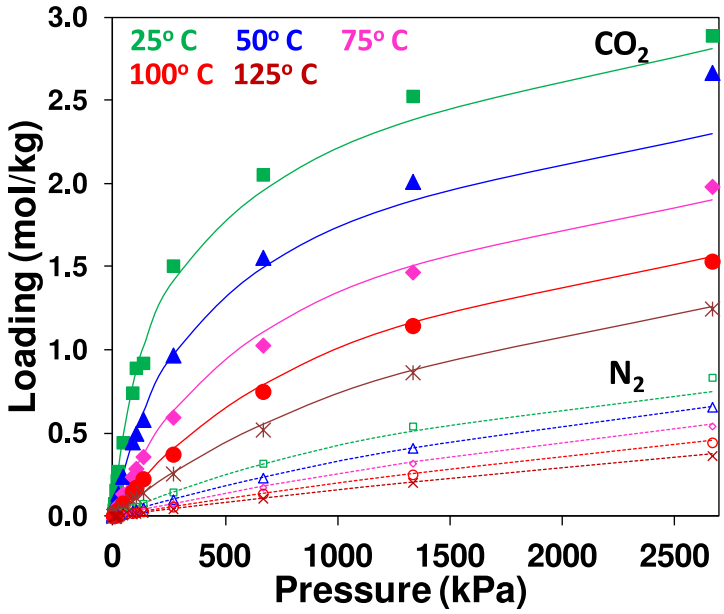

Figure S76: Adsorption isotherms of MOZ. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S155: Dual-site Langmuir isotherm parameters for MOZ.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	1.79	1.45
b^o [m^3 mol^{-1}]	2.00×10^{-6}	1.40×10^{-5}
ΔU [kJ mol^{-1}]	22.47	0
Site 2		
q^{sat} [mol kg^{-1}]	3.47	3.47
b^o [m^3 mol^{-1}]	1.20×10^{-7}	8.00×10^{-6}
ΔU [kJ mol^{-1}]	21.32	9.97

MSO

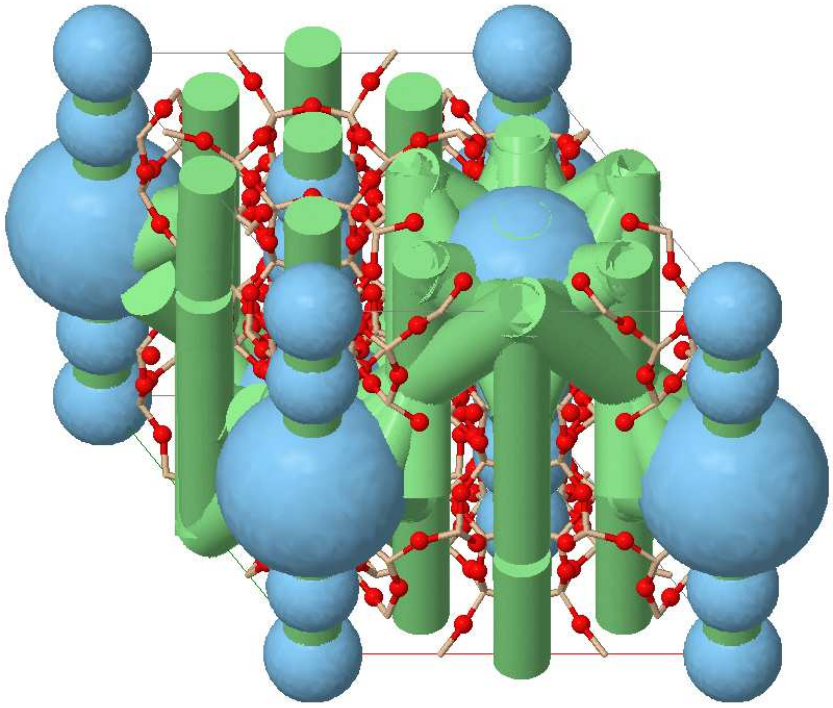

Figure S77: Main pore system of MSO from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S156: Physical properties for MSO.

Property	Value
Pore limiting diamater, PLD [Å]	2.6
Largest cavity diameter, LCD [Å]	7.9
Solid density [kg m^{-3}]	1779

Table S157: Adsorption and geometric properties for MSO.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00526	0.00063
Heat of adsorption at 298 K [kJ mol^{-1}]	22.7	10.9
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S158: Performance metrics for MSO.

Property	Value
Shape selectivity	0.28
Size selectivity	–
Adsorption selectivity	8.35
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	32.23
Purity [%] at optimum cost	87.99
Recovery [%] at optimum cost	81.33
Energy penalty [kWh/ton CO_2 captured] at optimum cost	207.91

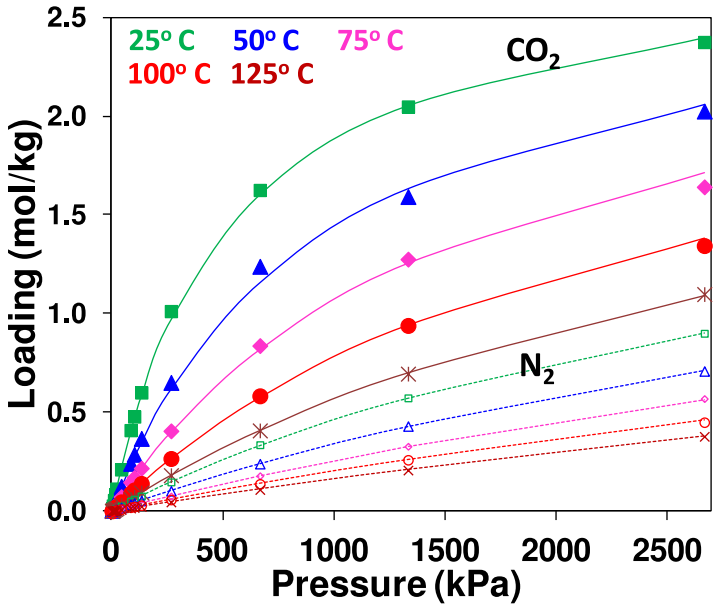

Figure S78: Adsorption isotherms of MSO. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S159: Dual-site Langmuir isotherm parameters for MSO.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.85	2.30
b^o [m^3 mol^{-1}]	0	8.00×10^{-6}
ΔU [kJ mol^{-1}]	21.86	10.72
Site 2		
q^{sat} [mol kg^{-1}]	2.85	0.92
b^o [m^3 mol^{-1}]	5.00×10^{-6}	1.38×10^{-4}
ΔU [kJ mol^{-1}]	17.04	0

MTN

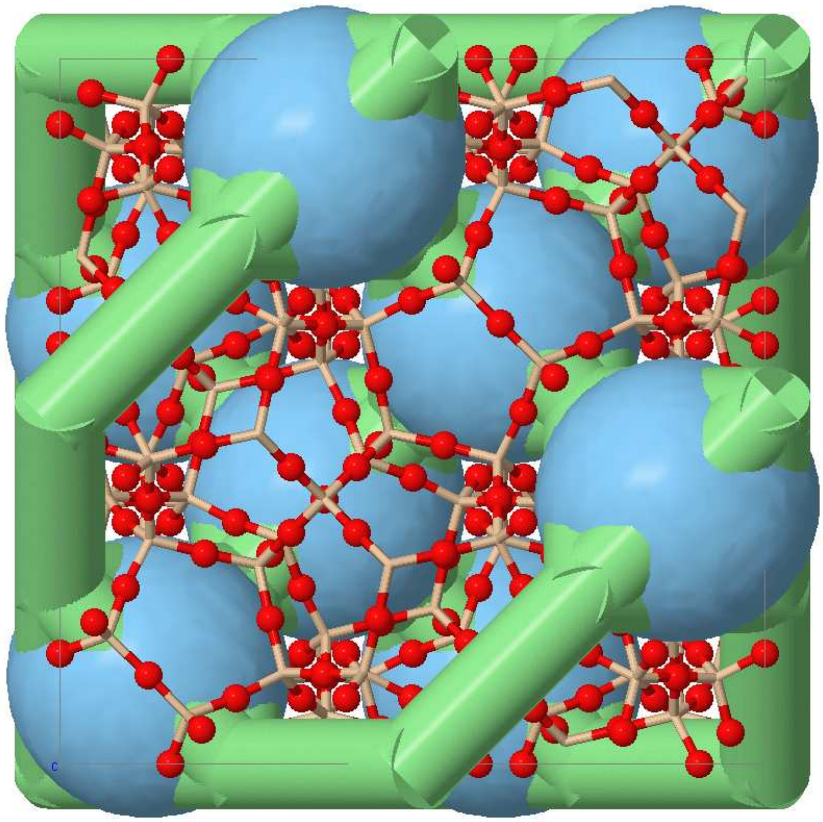

Figure S79: Main pore system of MTN from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S160: Physical properties for MTN.

Property	Value
Pore limiting diamater, PLD [Å]	2.5
Largest cavity diameter, LCD [Å]	8.0
Solid density [kg m^{-3}]	1713

Table S161: Adsorption and geometric properties for MTN.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00287	0.00054
Heat of adsorption at 298 K [kJ mol^{-1}]	2.5	13.6
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S162: Performance metrics for MTN.

Property	Value
Shape selectivity	0.13
Size selectivity	–
Adsorption selectivity	5.31
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	36.73
Purity [%] at optimum cost	85.70
Recovery [%] at optimum cost	73.70
Energy penalty [kWh/ton CO_2 captured] at optimum cost	226.27

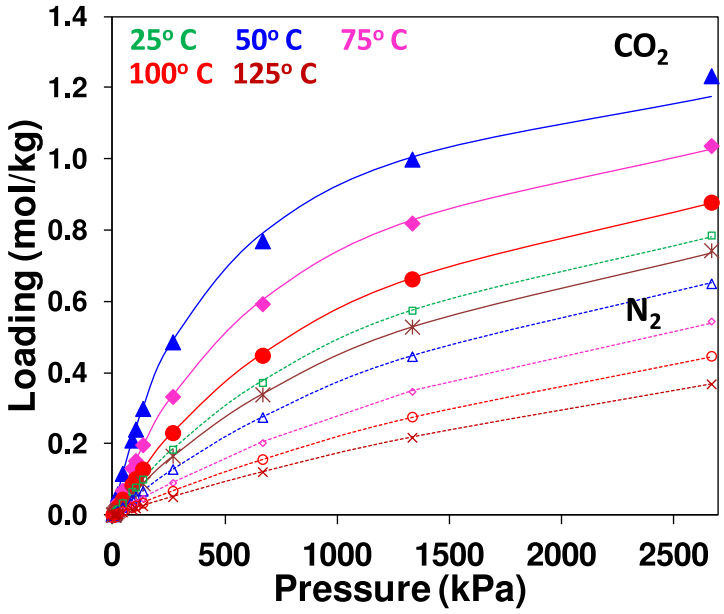

Figure S80: Adsorption isotherms of MTN. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S163: Dual-site Langmuir isotherm parameters for MTN.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	1.48	1.48
b^o [m^3 mol^{-1}]	6.00×10^{-6}	1.30×10^{-5}
ΔU [kJ mol^{-1}]	9.81	11.44
Site 2		
q^{sat} [mol kg^{-1}]	1.32	0.10
b^o [m^3 mol^{-1}]	9.00×10^{-6}	2.48×10^{-4}
ΔU [kJ mol^{-1}]	17.48	2.58

MVY

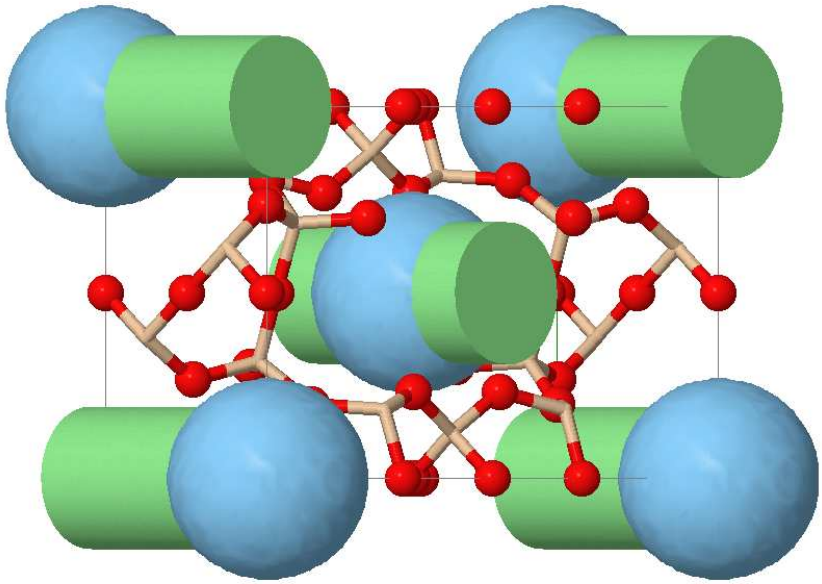

Figure S81: Main pore system of MVY from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S164: Physical properties for MVY.

Property	Value
Pore limiting diamater, PLD [Å]	3.1
Largest cavity diameter, LCD [Å]	4.4
Solid density [kg m^{-3}]	2093

Table S165: Adsorption and geometric properties for MVY.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.04530	0.00002
Heat of adsorption at 298 K [kJ mol^{-1}]	41.2	2.5
Accessible volume [cm^3 g^{-1}]	–	0.193
Accessible surface area [m^2 g^{-1}]	–	380

Table S166: Performance metrics for MVY.

Property	Value
Shape selectivity	0.34
Size selectivity	1.00
Adsorption selectivity	2709
Minimum parasitic energy [kJ/kg CO_2]	926.30
Purity [%] at minimum parasitic energy	96.57
Cost [$/ton of CO_2 captured and compressed]	26.74
Purity [%] at optimum cost	95.29
Recovery [%] at optimum cost	96.57
Energy penalty [kWh/ton CO_2 captured] at optimum cost	156.07

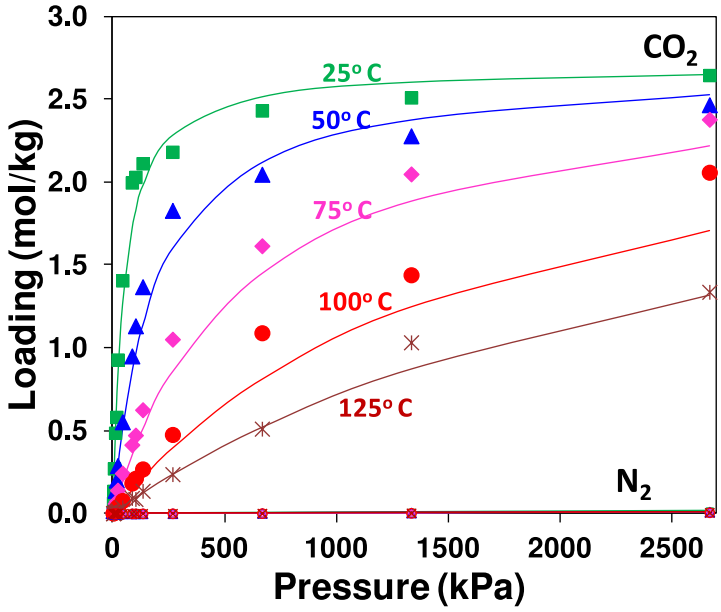

Figure S82: Adsorption isotherms of MVY. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S167: Dual-site Langmuir isotherm parameters for MVY.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.04	3.18
b^o [m^3 mol^{-1}]	0	1.90×10^{-7}
ΔU [kJ mol^{-1}]	49.97	7.67
Site 2		
q^{sat} [mol kg^{-1}]	2.90	3.18
b^o [m^3 mol^{-1}]	1.00×10^{-8}	0
ΔU [kJ mol^{-1}]	37.78	14.90

NAB

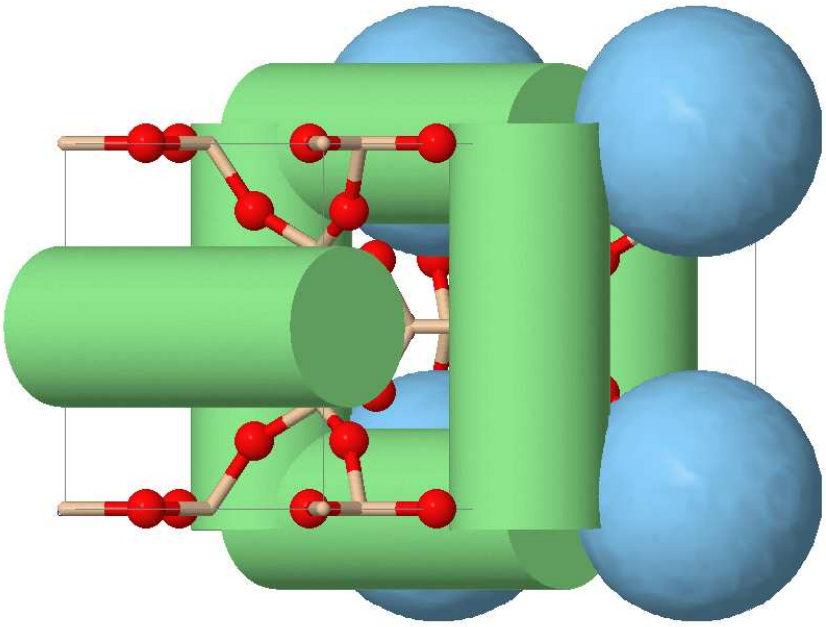

Figure S83: Main pore system of NAB from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S168: Physical properties for NAB.

Property	Value
Pore limiting diamater, PLD [Å]	3.2
Largest cavity diameter, LCD [Å]	5.0
Solid density [kg m^{-3}]	1605

Table S169: Adsorption and geometric properties for NAB.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01799	0.00042
Heat of adsorption at 298 K [kJ mol^{-1}]	32.0	12.3
Accessible volume [cm^3 g^{-1}]	–	0.408
Accessible surface area [m^2 g^{-1}]	–	615

Table S170: Performance metrics for NAB.

Property	Value
Shape selectivity	–
Size selectivity	1.00
Adsorption selectivity	42.74
Minimum parasitic energy [kJ/kg CO_2]	1249.07
Purity [%] at minimum parasitic energy	80.94
Cost [$/ton of CO_2 captured and compressed]	26.01
Purity [%] at optimum cost	93.99
Recovery [%] at optimum cost	91.20
Energy penalty [kWh/ton CO_2 captured] at optimum cost	161.42

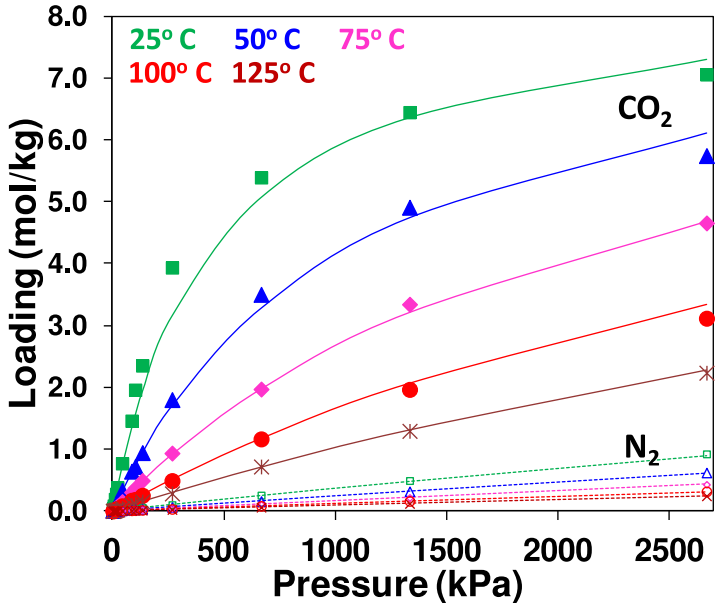

Figure S84: Adsorption isotherms of NAB. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S171: Dual-site Langmuir isotherm parameters for NAB.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	8.47	8.47
b^o [m^3 mol^{-1}]	7.00×10^{-6}	1.00×10^{-6}
ΔU [kJ mol^{-1}]	0	10.86
Site 2		
q^{sat} [mol kg^{-1}]	8.47	8.47
b^o [m^3 mol^{-1}]	2.50×10^{-7}	0
ΔU [kJ mol^{-1}]	24.82	50.00

NON

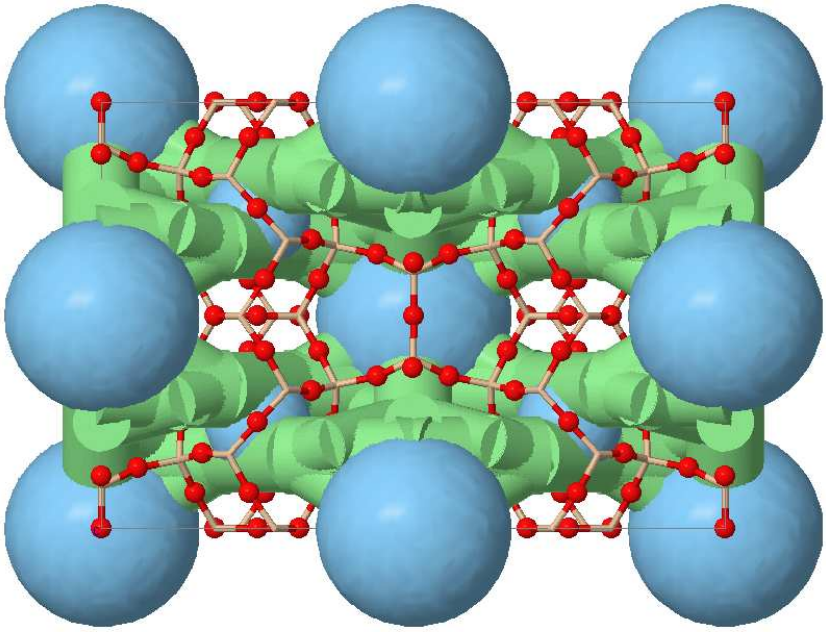

Figure S85: Main pore system of NON from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S172: Physical properties for NON.

Property	Value
Pore limiting diamater, PLD [Å]	2.9
Largest cavity diameter, LCD [Å]	7.1
Solid density [kg m^{-3}]	1760

Table S173: Adsorption and geometric properties for NON.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00636	0.00067
Heat of adsorption at 298 K [kJ mol^{-1}]	23.2	14.1
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S174: Performance metrics for NON.

Property	Value
Shape selectivity	0.41
Size selectivity	–
Adsorption selectivity	9.53
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	32.68
Purity [%] at optimum cost	89.92
Recovery [%] at optimum cost	79.50
Energy penalty [kWh/ton CO_2 captured] at optimum cost	224.58

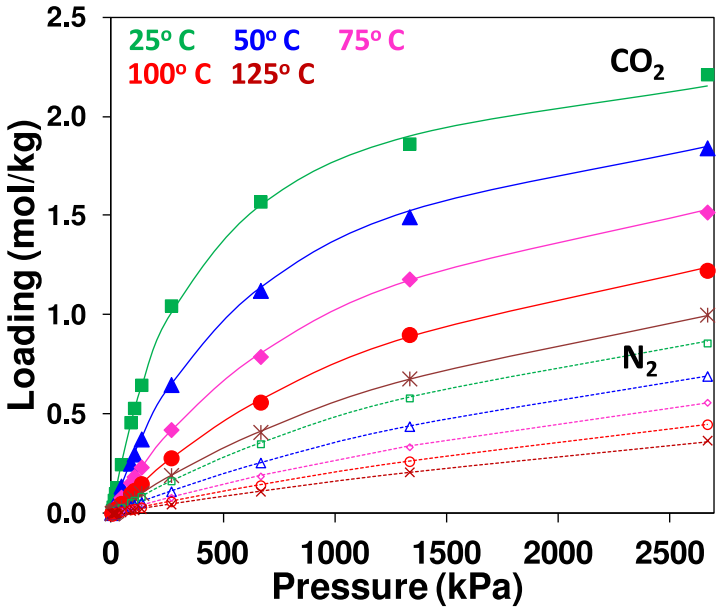

Figure S86: Adsorption isotherms of NON. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S175: Dual-site Langmuir isotherm parameters for NON.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.66	1.82
b^o [m^3 mol^{-1}]	8.40×10^{-5}	1.50×10^{-5}
ΔU [kJ mol^{-1}]	0	10.18
Site 2		
q^{sat} [mol kg^{-1}]	2.66	0.01
b^o [m^3 mol^{-1}]	3.00×10^{-6}	2.80×10^{-4}
ΔU [kJ mol^{-1}]	18.63	2.90

OFF

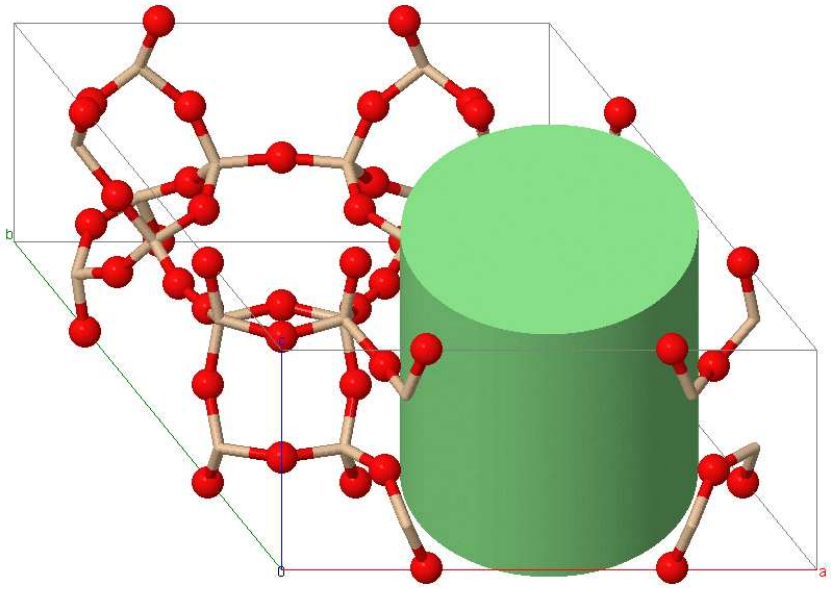

Figure S87: Main pore system of OFF from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S176: Physical properties for OFF.

Property	Value
Pore limiting diamater, PLD [Å]	7.3
Largest cavity diameter, LCD [Å]	7.3
Solid density [kg m^{-3}]	1606

Table S177: Adsorption and geometric properties for OFF.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01976	0.00106
Heat of adsorption at 298 K [kJ mol^{-1}]	25.7	12.2
Accessible volume [cm^3 g^{-1}]	0.181	0.330
Accessible surface area [m^2 g^{-1}]	960	2579

Table S178: Performance metrics for OFF.

Property	Value
Shape selectivity	–
Size selectivity	0.45
Adsorption selectivity	18.59
Minimum parasitic energy [kJ/kg CO_2]	1391.65
Purity [%] at minimum parasitic energy	67.60
Cost [$/ton of CO_2 captured and compressed]	29.30
Purity [%] at optimum cost	90.15
Recovery [%] at optimum cost	90.28
Energy penalty [kWh/ton CO_2 captured] at optimum cost	173.27

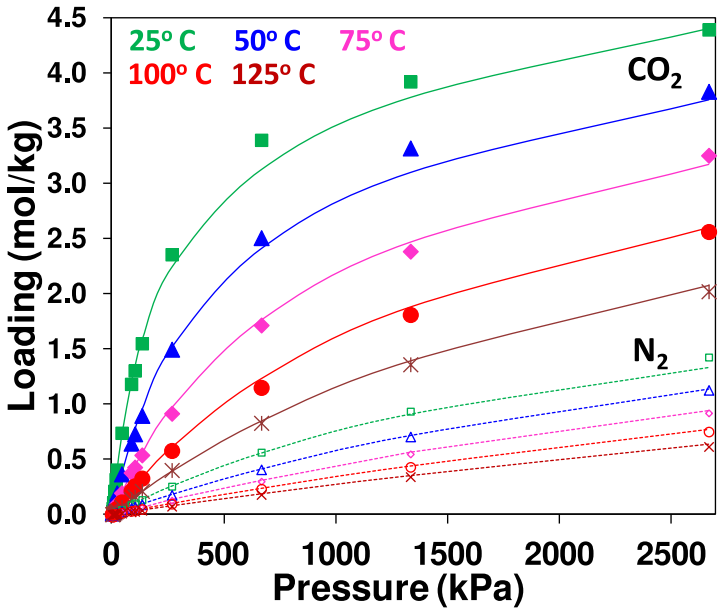

Figure S88: Adsorption isotherms of OFF. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S179: Dual-site Langmuir isotherm parameters for OFF.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	5.27	5.27
b^o [m^3 mol^{-1}]	6.20×10^{-7}	9.00×10^{-6}
ΔU [kJ mol^{-1}]	16.87	9.94
Site 2		
q^{sat} [mol kg^{-1}]	3.08	0
b^o [m^3 mol^{-1}]	2.00×10^{-6}	0
ΔU [kJ mol^{-1}]	22.88	50.00

RRO

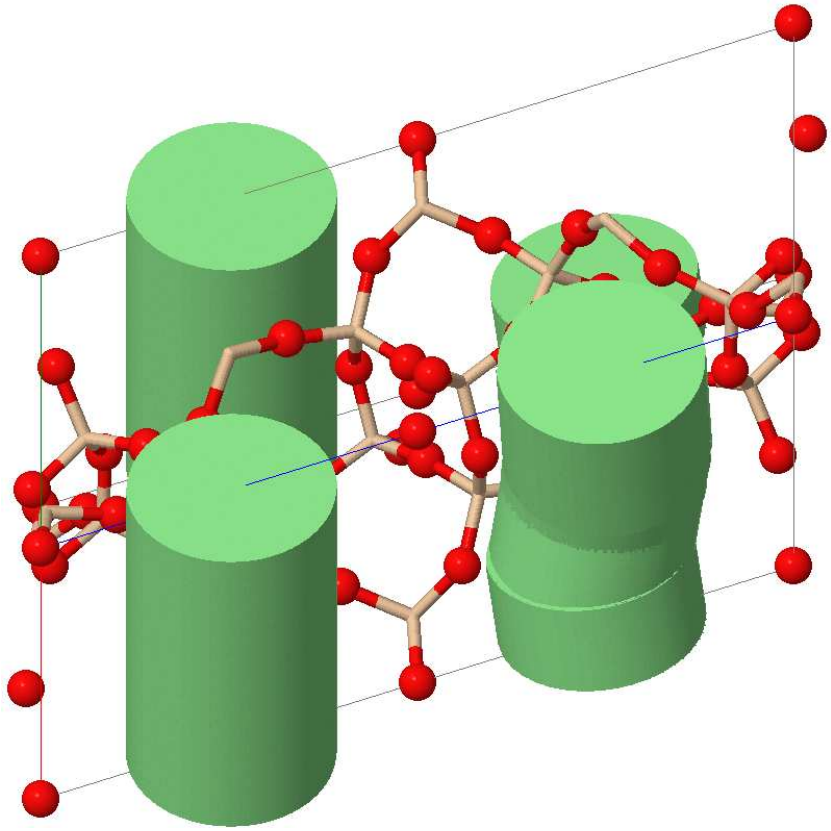

Figure S89: Main pore system of RRO from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S180: Physical properties for RRO.

Property	Value
Pore limiting diamater, PLD [Å]	4.4
Largest cavity diameter, LCD [Å]	4.4
Solid density [kg m^{-3}]	1782

Table S181: Adsorption and geometric properties for RRO.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.03302	0.00045
Heat of adsorption at 298 K [kJ mol^{-1}]	32.6	17.0
Accessible volume [cm^3 g^{-1}]	0.151	0.151
Accessible surface area [m^2 g^{-1}]	1094	1094

Table S182: Performance metrics for RRO.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	73.53
Minimum parasitic energy [kJ/kg CO_2]	880.80
Purity [%] at minimum parasitic energy	89.34
Cost [$/ton of CO_2 captured and compressed]	29.68
Purity [%] at optimum cost	90.18
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	154.06

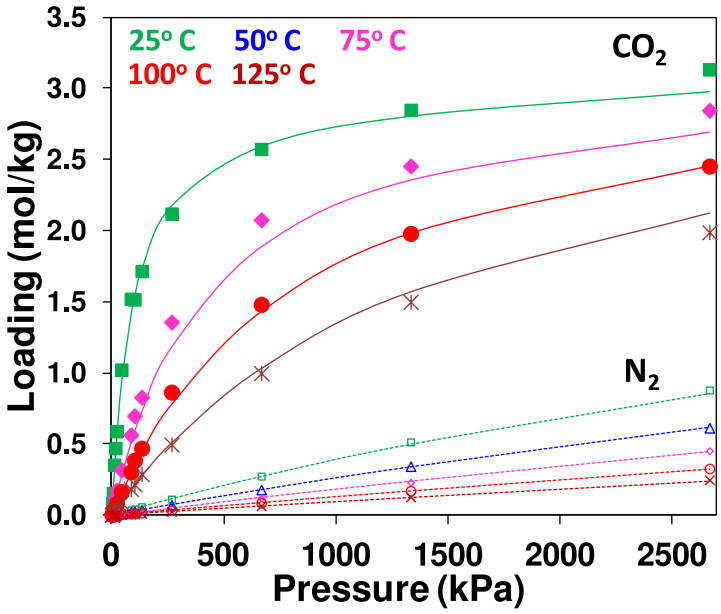

Figure S90: Adsorption isotherms of RRO. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S183: Dual-site Langmuir isotherm parameters for RRO.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.76	3.76
b^o [m^3 mol^{-1}]	0	2.00×10^{-6}
ΔU [kJ mol^{-1}]	50.00	12.17
Site 2		
q^{sat} [mol kg^{-1}]	3.76	0
b^o [m^3 mol^{-1}]	2.00×10^{-6}	3.00×10^{-8}
ΔU [kJ mol^{-1}]	23.36	30.89

RWR

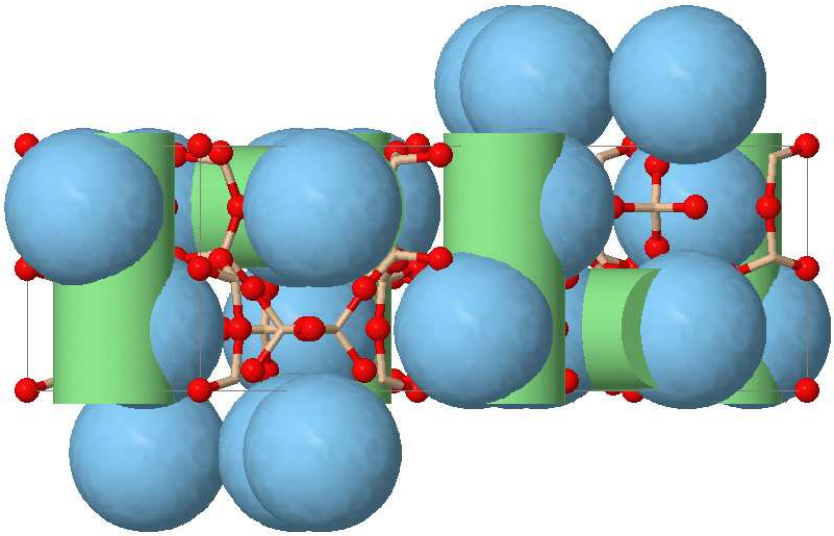

Figure S91: Main pore system of RWR from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S184: Physical properties for RWR.

Property	Value
Pore limiting diamater, PLD [Å]	3.8
Largest cavity diameter, LCD [Å]	5.1
Solid density [kg m^{-3}]	1791

Table S185: Adsorption and geometric properties for RWR.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.06993	0.00071
Heat of adsorption at 298 K [kJ mol^{-1}]	35.2	18.1
Accessible volume [cm^3 g^{-1}]	0.251	0.251
Accessible surface area [m^2 g^{-1}]	1320	1320

Table S186: Performance metrics for RWR.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	97.81
Minimum parasitic energy [kJ/kg CO_2]	903.26
Purity [%] at minimum parasitic energy	88.46
Cost [$/ton of CO_2 captured and compressed]	29.14
Purity [%] at optimum cost	90.06
Recovery [%] at optimum cost	90.44
Energy penalty [kWh/ton CO_2 captured] at optimum cost	168.41

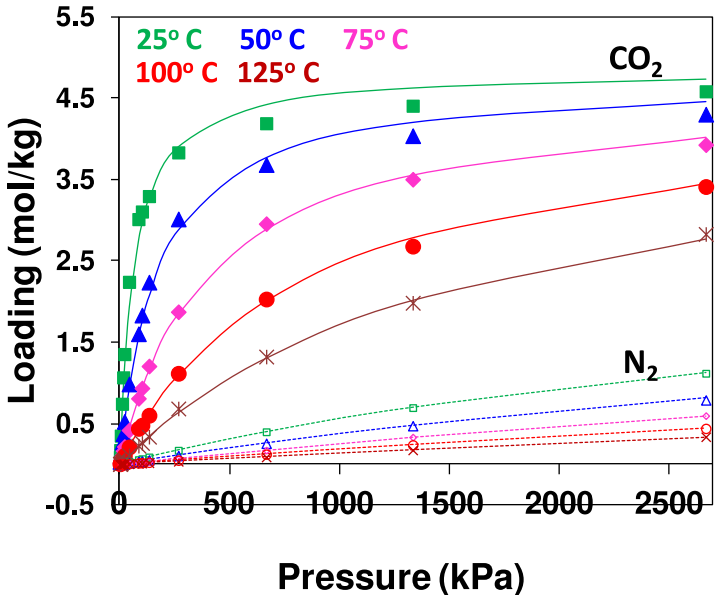

Figure S92: Adsorption isotherms of RWR. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S187: Dual-site Langmuir isotherm parameters for RWR.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.49	2.91
b^o [m^3 mol^{-1}]	0	3.00×10^{-6}
ΔU [kJ mol^{-1}]	4.02	12.93
Site 2		
q^{sat} [mol kg^{-1}]	5.50	0
b^o [m^3 mol^{-1}]	2.10×10^{-7}	2.90×10^{-7}
ΔU [kJ mol^{-1}]	29.69	23.90

RWY

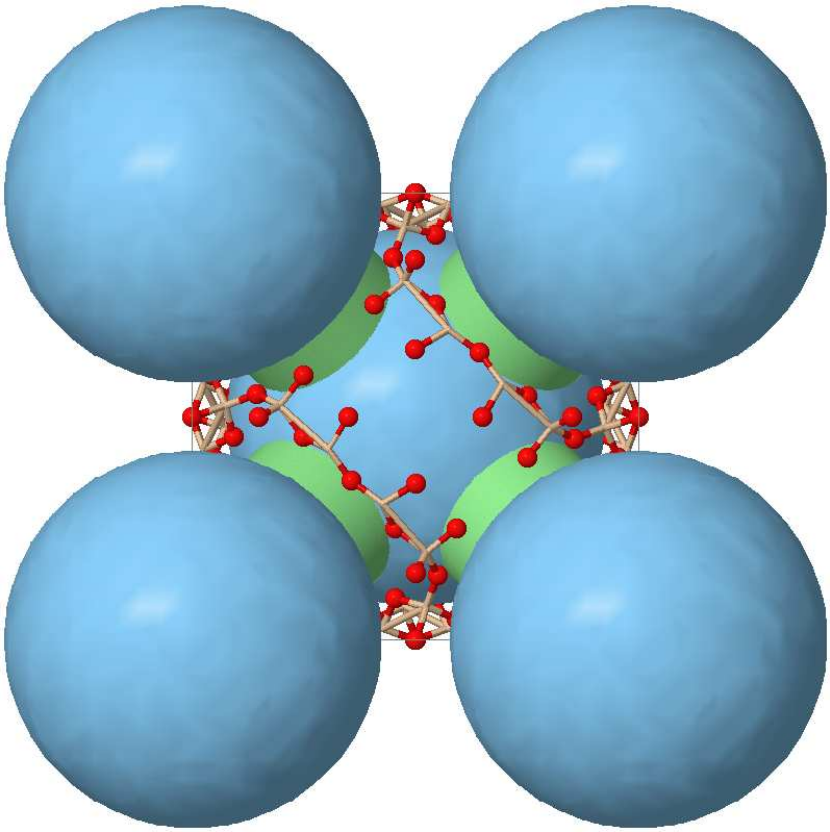

Figure S93: Main pore system of RWY from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S188: Physical properties for RWY.

Property	Value
Pore limiting diamater, PLD [Å]	6.9
Largest cavity diameter, LCD [Å]	15.0
Solid density [kg m^{-3}]	855

Table S189: Adsorption and geometric properties for RWY.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00428	0.00107
Heat of adsorption at 298 K [kJ mol^{-1}]	17.2	8.1
Accessible volume [cm^3 g^{-1}]	0.903	0.922
Accessible surface area [m^2 g^{-1}]	1492	1688

Table S190: Performance metrics for RWY.

Property	Value
Shape selectivity	–
Size selectivity	0.02
Adsorption selectivity	4.00
Minimum parasitic energy [kJ/kg CO_2]	3953.60
Purity [%] at minimum parasitic energy	30.43
Cost [$/ton of CO_2 captured and compressed]	55.90
Purity [%] at optimum cost	86.40
Recovery [%] at optimum cost	82.20
Energy penalty [kWh/ton CO_2 captured] at optimum cost	248.21

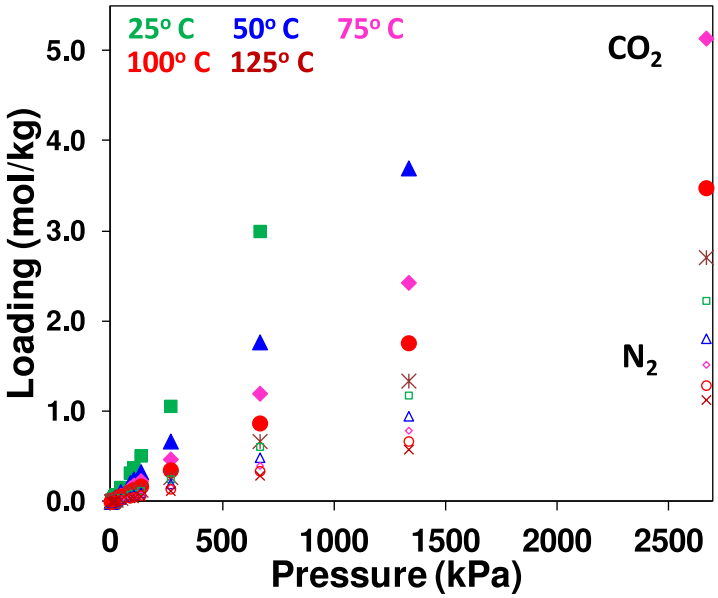

Figure S94: Adsorption isotherms of RWY. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S191: Dual-site Langmuir isotherm parameters for RWY.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	12.03	12.22
b^o [m^3 mol^{-1}]	5.02×10^{-1}	6.92×10^{-1}
ΔU [kJ mol^{-1}]	33.15	23.66
Site 2		
q^{sat} [mol kg^{-1}]	7.37	21.35
b^o [m^3 mol^{-1}]	7.65×10^{-1}	7.73×10^{-1}
ΔU [kJ mol^{-1}]	2.18	14.82

SAO

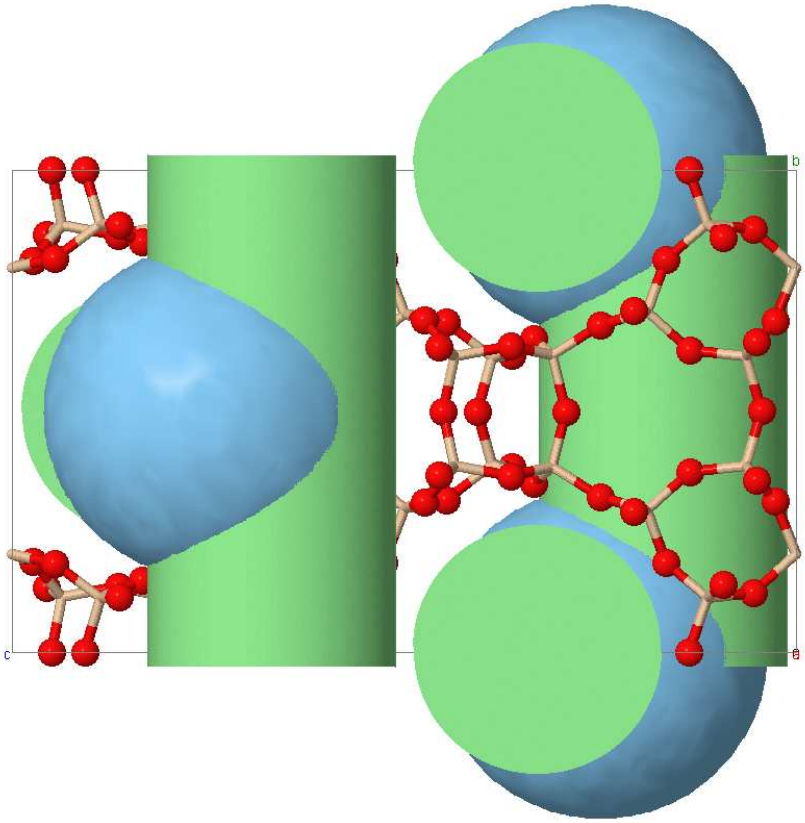

Figure S95: Main pore system of SAO from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S192: Physical properties for SAO.

Property	Value
Pore limiting diamater, PLD [Å]	6.9
Largest cavity diameter, LCD [Å]	9.3
Solid density [kg m^{-3}]	1415

Table S193: Adsorption and geometric properties for SAO.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00321	0.00107
Heat of adsorption at 298 K [kJ mol^{-1}]	20.6	9.5
Accessible volume [cm^3 g^{-1}]	0.398	0.398
Accessible surface area [m^2 g^{-1}]	2018	2018

Table S194: Performance metrics for SAO.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	3.00
Minimum parasitic energy [kJ/kg CO_2]	3237.27
Purity [%] at minimum parasitic energy	39.68
Cost [$/ton of CO_2 captured and compressed]	35.18
Purity [%] at optimum cost	69.90
Recovery [%] at optimum cost	70.40
Energy penalty [kWh/ton CO_2 captured] at optimum cost	192.04

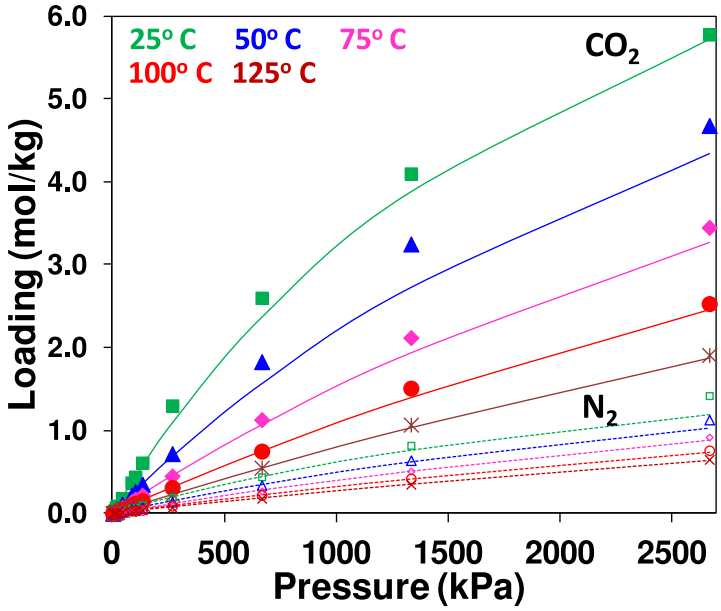

Figure S96: Adsorption isotherms of SAO. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S195: Dual-site Langmuir isotherm parameters for SAO.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	6.94	3.76
b^o [m^3 mol^{-1}]	4.00×10^{-6}	0
ΔU [kJ mol^{-1}]	14.12	36.52
Site 2		
q^{sat} [mol kg^{-1}]	6.94	6.94
b^o [m^3 mol^{-1}]	3.00×10^{-6}	1.60×10^{-5}
ΔU [kJ mol^{-1}]	12.38	7.13

SGT

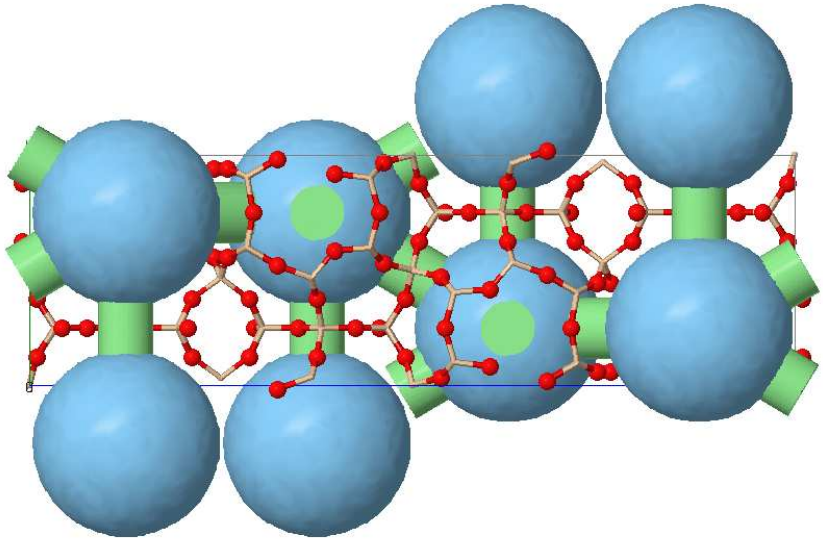

Figure S97: Main pore system of SGT from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S196: Physical properties for SGT.

Property	Value
Pore limiting diamater, PLD [Å]	2.7
Largest cavity diameter, LCD [Å]	8.4
Solid density [kg m^{-3}]	1742

Table S197: Adsorption and geometric properties for SGT.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00583	0.00103
Heat of adsorption at 298 K [kJ mol^{-1}]	22.5	14.2
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S198: Performance metrics for SGT.

Property	Value
Shape selectivity	0.27
Size selectivity	–
Adsorption selectivity	5.65
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	46.05
Purity [%] at optimum cost	89.91
Recovery [%] at optimum cost	48.67
Energy penalty [kWh/ton CO_2 captured] at optimum cost	353.21

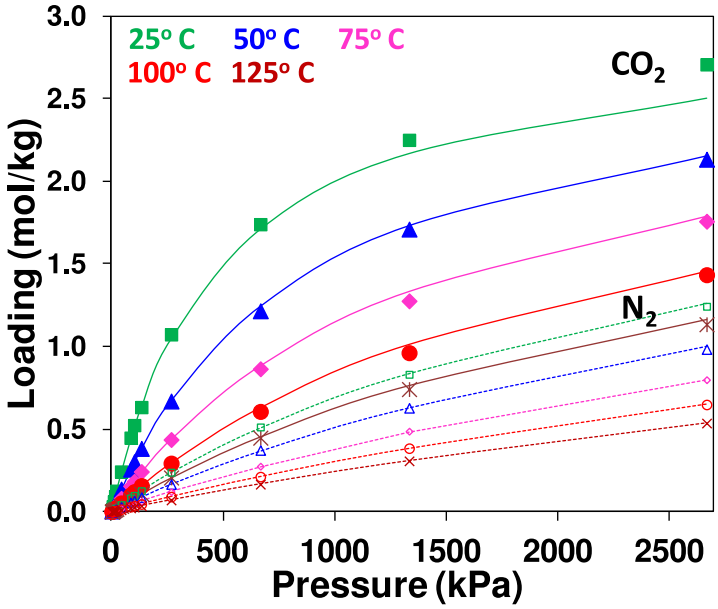

Figure S98: Adsorption isotherms of SGT. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S199: Dual-site Langmuir isotherm parameters for SGT.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.25	1.35
b^o [m^3 mol^{-1}]	5.00×10^{-6}	7.10×10^{-5}
ΔU [kJ mol^{-1}]	16.77	4.57
Site 2		
q^{sat} [mol kg^{-1}]	0.20	2.58
b^o [m^3 mol^{-1}]	0	5.00×10^{-6}
ΔU [kJ mol^{-1}]	0	12.60

SIV

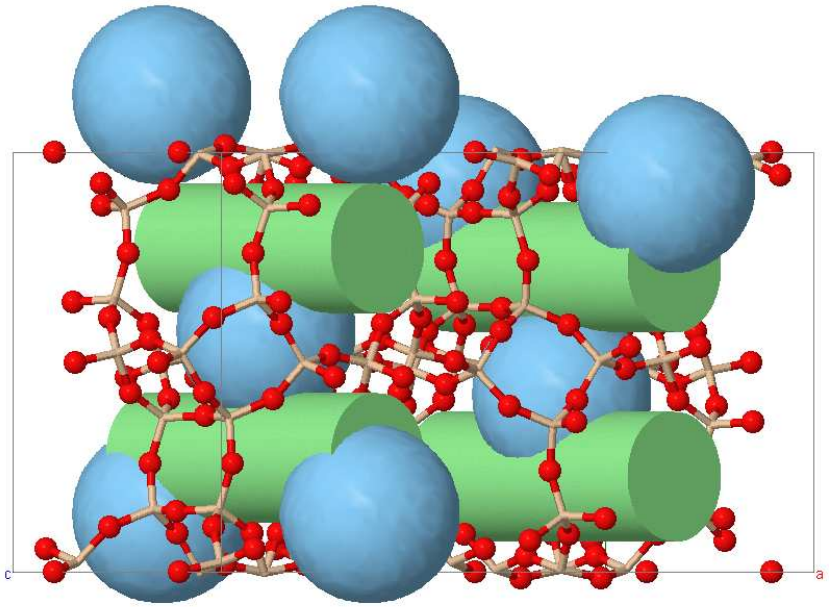

Figure S99: Main pore system of SIV from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S200: Physical properties for SIV.

Property	Value
Pore limiting diamater, PLD [Å]	4.4
Largest cavity diameter, LCD [Å]	6.0
Solid density [kg m^{-3}]	1633

Table S201: Adsorption and geometric properties for SIV.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.10188	0.00114
Heat of adsorption at 298 K [kJ mol^{-1}]	33.7	15.7
Accessible volume [cm^3 g^{-1}]	0.361	0.361
Accessible surface area [m^2 g^{-1}]	1252	1252

Table S202: Performance metrics for SIV.

Property	Value
Shape selectivity	–
Size selectivity	–
Adsorption selectivity	89.08
Minimum parasitic energy [kJ/kg CO_2]	839.32
Purity [%] at minimum parasitic energy	86.97
Cost [$/ton of CO_2 captured and compressed]	32.54
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	191.30

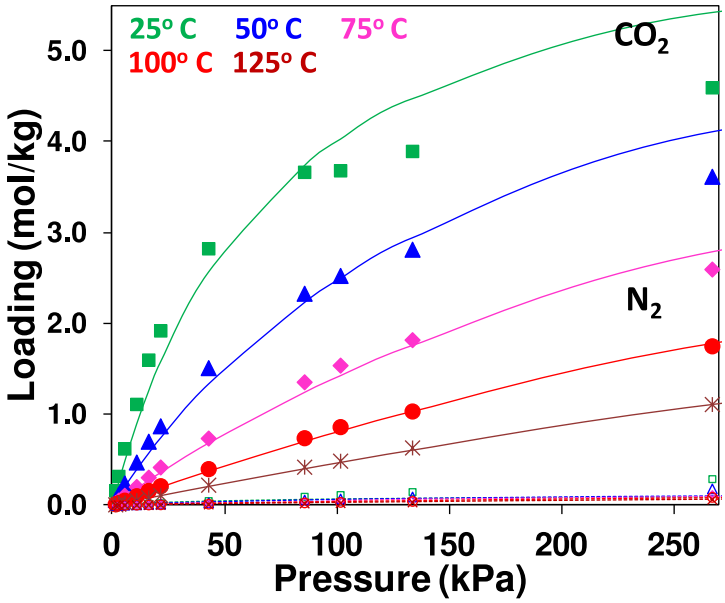

Figure S100: Adsorption isotherms of SIV. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S203: Dual-site Langmuir isotherm parameters for SIV.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	7.02	5.26
b^o [m^3 mol^{-1}]	8.40×10^{-7}	2.00×10^{-6}
ΔU [kJ mol^{-1}]	26.27	14.00
Site 2		
q^{sat} [mol kg^{-1}]	6.17	0
b^o [m^3 mol^{-1}]	0	0
ΔU [kJ mol^{-1}]	28.58	20.64

SOD

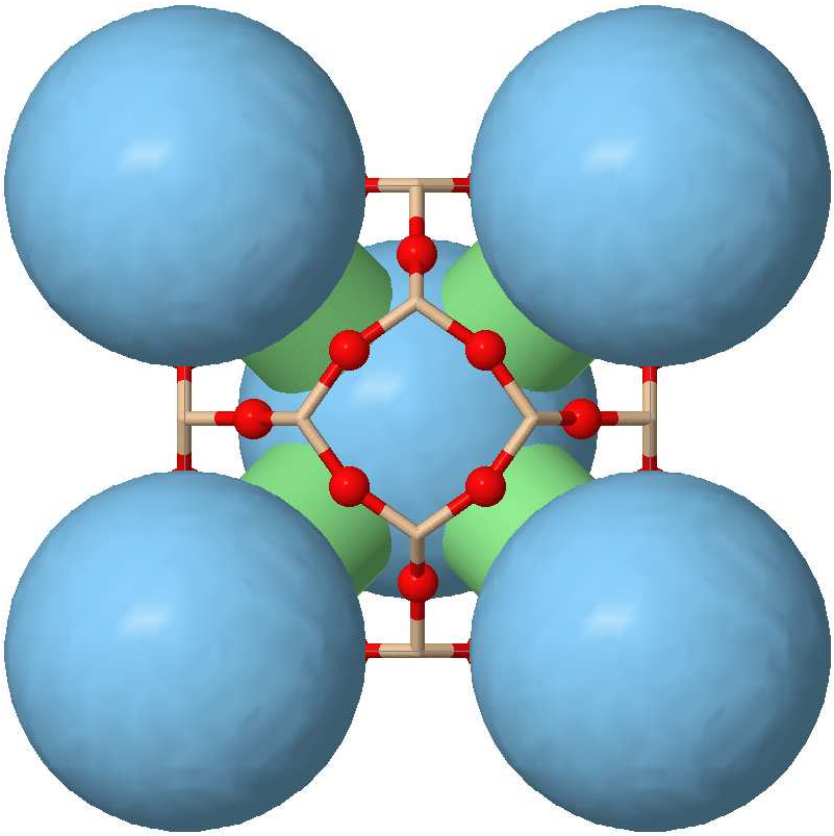

Figure S101: Main pore system of SOD from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S204: Physical properties for SOD.

Property	Value
Pore limiting diamater, PLD [Å]	3.2
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1662

Table S205: Adsorption and geometric properties for SOD.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01152	0.00200
Heat of adsorption at 298 K [kJ mol^{-1}]	25.1	16.4
Accessible volume [cm^3 g^{-1}]	–	0.406
Accessible surface area [m^2 g^{-1}]	–	2021

Table S206: Performance metrics for SOD.

Property	Value
Shape selectivity	0.24
Size selectivity	1.00
Adsorption selectivity	5.75
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	42.42
Purity [%] at optimum cost	71.29
Recovery [%] at optimum cost	63.78
Energy penalty [kWh/ton CO_2 captured] at optimum cost	298.30

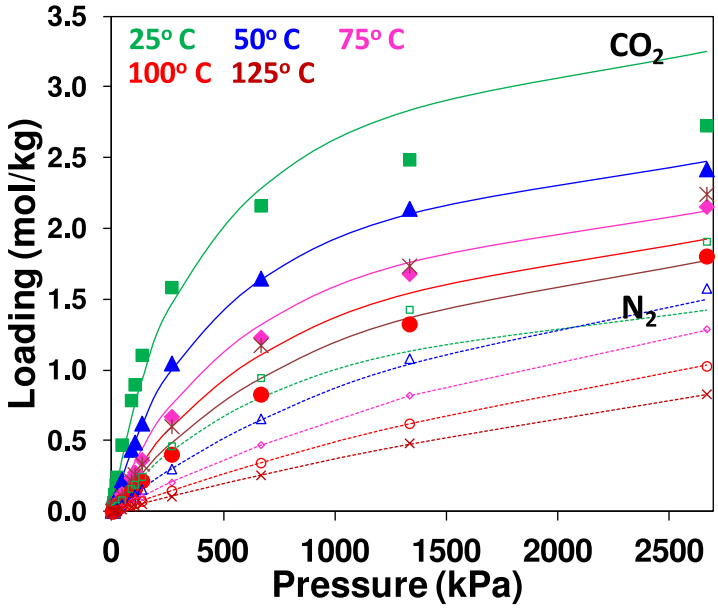

Figure S102: Adsorption isotherms of SOD. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S207: Dual-site Langmuir isotherm parameters for SOD.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.28	3.28
b^o [m^3 mol^{-1}]	0	8.00×10^{-6}
ΔU [kJ mol^{-1}]	50.00	13.02
Site 2		
q^{sat} [mol kg^{-1}]	2.49	0.69
b^o [m^3 mol^{-1}]	1.54×10^{-4}	0
ΔU [kJ mol^{-1}]	9.81	8.69

TOL

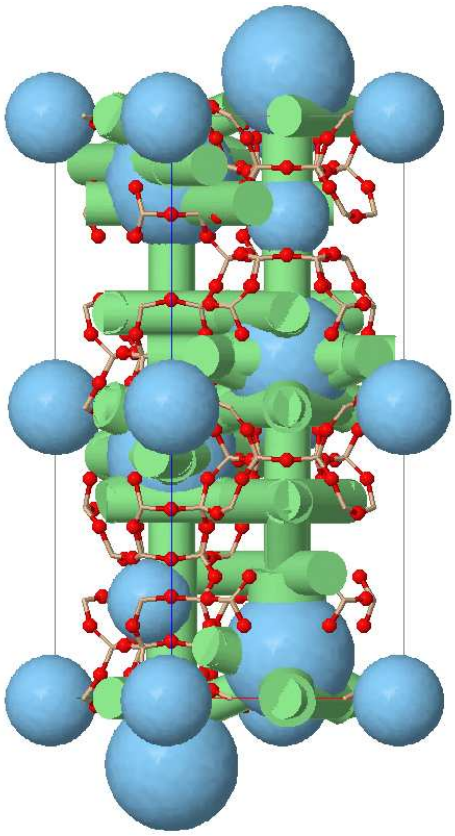

Figure S103: Main pore system of TOL from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S208: Physical properties for TOL.

Property	Value
Pore limiting diamater, PLD [Å]	2.6
Largest cavity diameter, LCD [Å]	7.0
Solid density [kg m^{-3}]	1782

Table S209: Adsorption and geometric properties for TOL.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00234	0.00059
Heat of adsorption at 298 K [kJ mol^{-1}]	2.5	14.1
Accessible volume [cm^3 g^{-1}]	–	–
Accessible surface area [m^2 g^{-1}]	–	–

Table S210: Performance metrics for TOL.

Property	Value
Shape selectivity	0.41
Size selectivity	–
Adsorption selectivity	3.97
Minimum parasitic energy [kJ/kg CO_2]	–
Purity [%] at minimum parasitic energy	–
Cost [$/ton of CO_2 captured and compressed]	38.24
Purity [%] at optimum cost	57.32
Recovery [%] at optimum cost	74.56
Energy penalty [kWh/ton CO_2 captured] at optimum cost	182.09

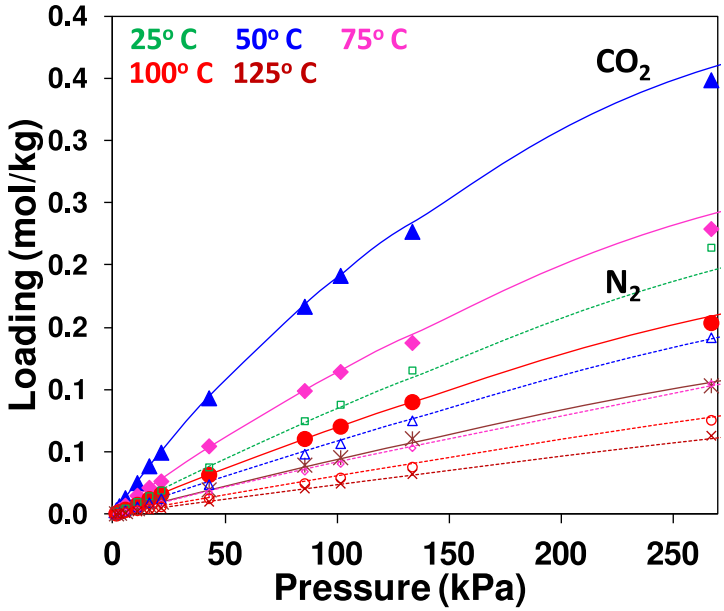

Figure S104: Adsorption isotherms of TOL. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S211: Dual-site Langmuir isotherm parameters for TOL.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	0.90	0.90
b^o [m^3 mol^{-1}]	0	3.80×10^{-5}
ΔU [kJ mol^{-1}]	12.61	10.42
Site 2		
q^{sat} [mol kg^{-1}]	0.90	0
b^o [m^3 mol^{-1}]	3.00×10^{-6}	2.40×10^{-5}
ΔU [kJ mol^{-1}]	20.88	10.78

TON

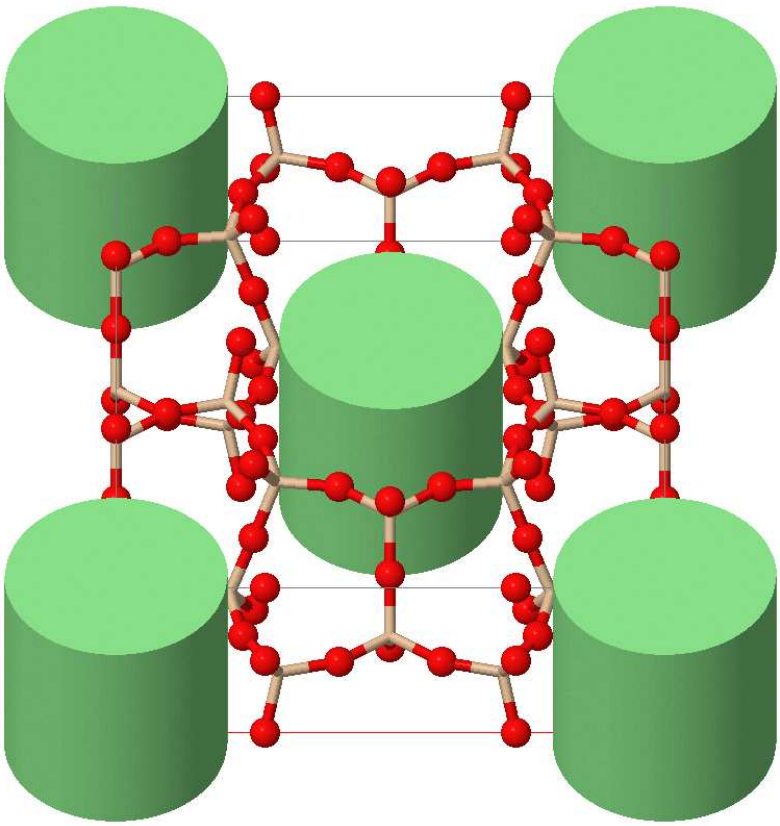

Figure S105: Main pore system of TON from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S212: Physical properties for TON.

Property	Value
Pore limiting diamater, PLD [Å]	5.7
Largest cavity diameter, LCD [Å]	5.7
Solid density [kg m^{-3}]	1810

Table S213: Adsorption and geometric properties for TON.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00887	0.00046
Heat of adsorption at 298 K [kJ mol^{-1}]	26.5	10.7
Accessible volume [cm^3 g^{-1}]	0.126	0.179
Accessible surface area [m^2 g^{-1}]	653	1468

Table S214: Performance metrics for TON.

Property	Value
Shape selectivity	–
Size selectivity	0.30
Adsorption selectivity	19.21
Minimum parasitic energy [kJ/kg CO_2]	1606.28
Purity [%] at minimum parasitic energy	66.50
Cost [$/ton of CO_2 captured and compressed]	28.93
Purity [%] at optimum cost	90.81
Recovery [%] at optimum cost	90.43
Energy penalty [kWh/ton CO_2 captured] at optimum cost	159.32

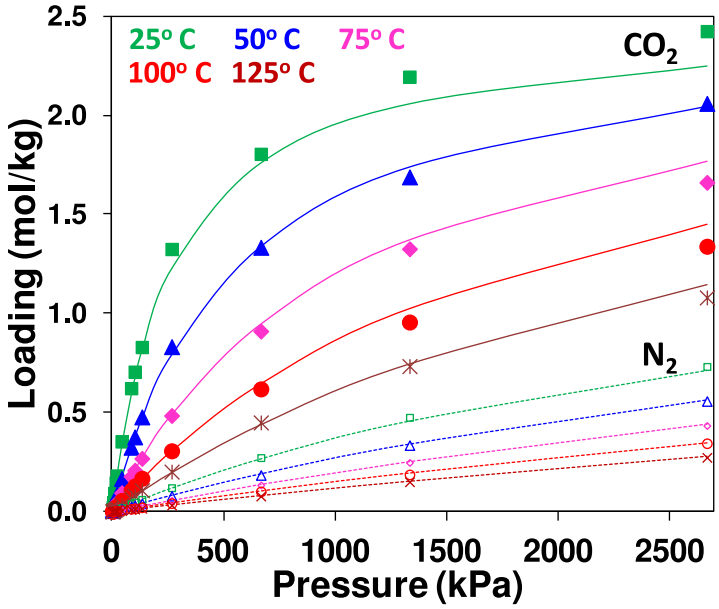

Figure S106: Adsorption isotherms of TON. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S215: Dual-site Langmuir isotherm parameters for TON.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	2.71	1.63
b^o [m^3 mol^{-1}]	0	1.20×10^{-5}
ΔU [kJ mol^{-1}]	3.09	10.27
Site 2		
q^{sat} [mol kg^{-1}]	2.48	0.02
b^o [m^3 mol^{-1}]	2.00×10^{-6}	0
ΔU [kJ mol^{-1}]	21.11	50.00

VNI

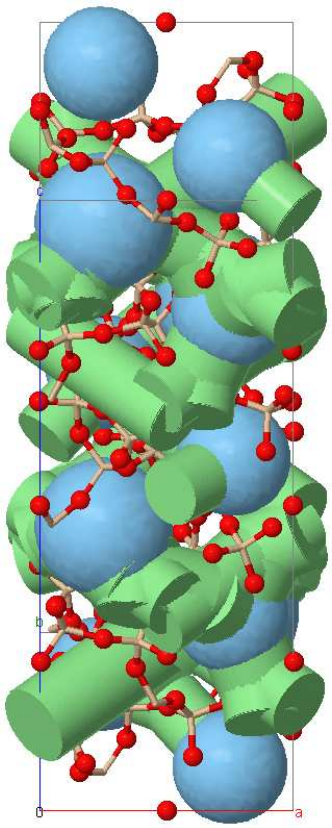

Figure S107: Main pore system of VNI from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S216: Physical properties for VNI.

Property	Value
Pore limiting diamater, PLD [Å]	3.2
Largest cavity diameter, LCD [Å]	5.4
Solid density [kg m^{-3}]	1753

Table S217: Adsorption and geometric properties for VNI.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.00708	0.00045
Heat of adsorption at 298 K [kJ mol^{-1}]	30.5	17.4
Accessible volume [cm^3 g^{-1}]	–	0.078
Accessible surface area [m^2 g^{-1}]	–	376

Table S218: Performance metrics for VNI.

Property	Value
Shape selectivity	–
Size selectivity	1.00
Adsorption selectivity	15.86
Minimum parasitic energy [kJ/kg CO_2]	2297.32
Purity [%] at minimum parasitic energy	58.57
Cost [$/ton of CO_2 captured and compressed]	28.11
Purity [%] at optimum cost	90.12
Recovery [%] at optimum cost	90.63
Energy penalty [kWh/ton CO_2 captured] at optimum cost	167.60

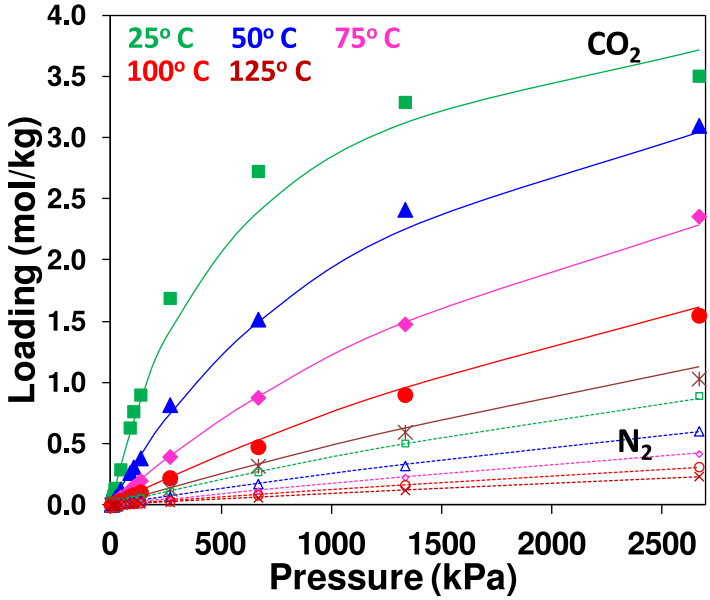

Figure S108: Adsorption isotherms of VNI. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S219: Dual-site Langmuir isotherm parameters for VNI.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.21	4.21
b^o [m^3 mol^{-1}]	6.30×10^{-5}	2.00×10^{-6}
ΔU [kJ mol^{-1}]	0	12.24
Site 2		
q^{sat} [mol kg^{-1}]	4.21	0.01
b^o [m^3 mol^{-1}]	1.70×10^{-7}	0
ΔU [kJ mol^{-1}]	25.28	35.14

WEI

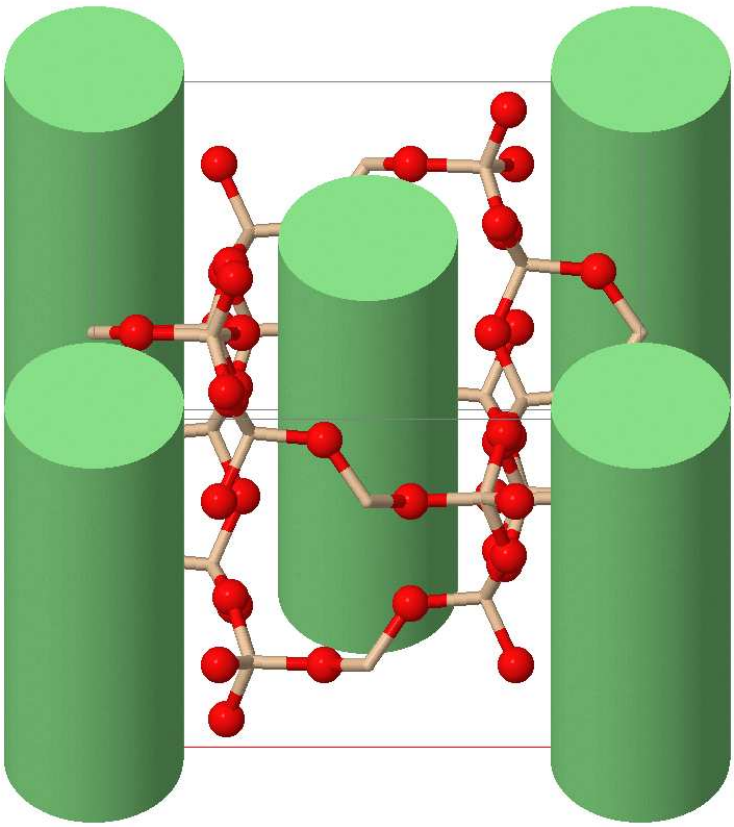

Figure S109: Main pore system of WEI from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S220: Physical properties for WEI.

Property	Value
Pore limiting diamater, PLD [Å]	3.9
Largest cavity diameter, LCD [Å]	3.9
Solid density [kg m^{-3}]	1647

Table S221: Adsorption and geometric properties for WEI.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01629	0.00009
Heat of adsorption at 298 K [kJ mol^{-1}]	30.6	24.0
Accessible volume [cm^3 g^{-1}]	0.239	0.308
Accessible surface area [m^2 g^{-1}]	1211	1988

Table S222: Performance metrics for WEI.

Property	Value
Shape selectivity	–
Size selectivity	0.22
Adsorption selectivity	188.5
Minimum parasitic energy [kJ/kg CO_2]	732.44
Purity [%] at minimum parasitic energy	95.71
Cost [$/ton of CO_2 captured and compressed]	27.29
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	146.95

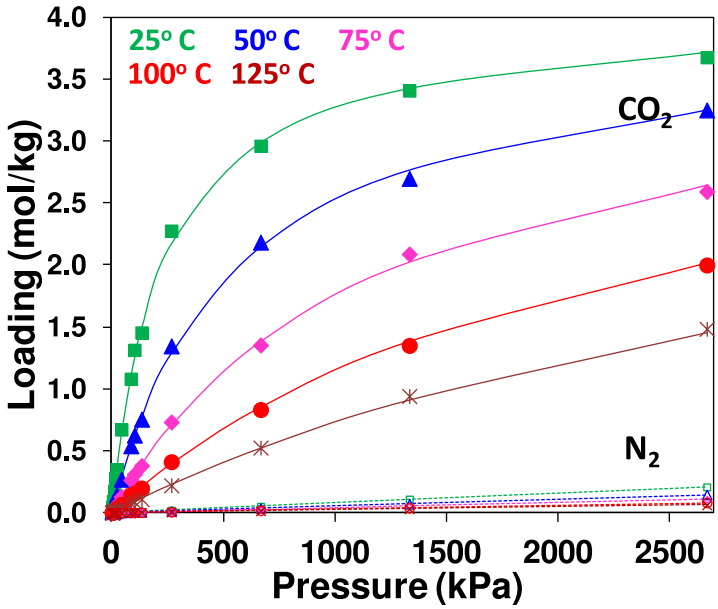

Figure S110: Adsorption isotherms of WEI. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S223: Dual-site Langmuir isotherm parameters for WEI.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	4.41	4.41
b^o [m^3 mol^{-1}]	1.60×10^{-5}	1.00×10^{-6}
ΔU [kJ mol^{-1}]	0	9.29
Site 2		
q^{sat} [mol kg^{-1}]	4.41	0
b^o [m^3 mol^{-1}]	2.10×10^{-7}	1.00×10^{-6}
ΔU [kJ mol^{-1}]	26.73	17.47

ZON

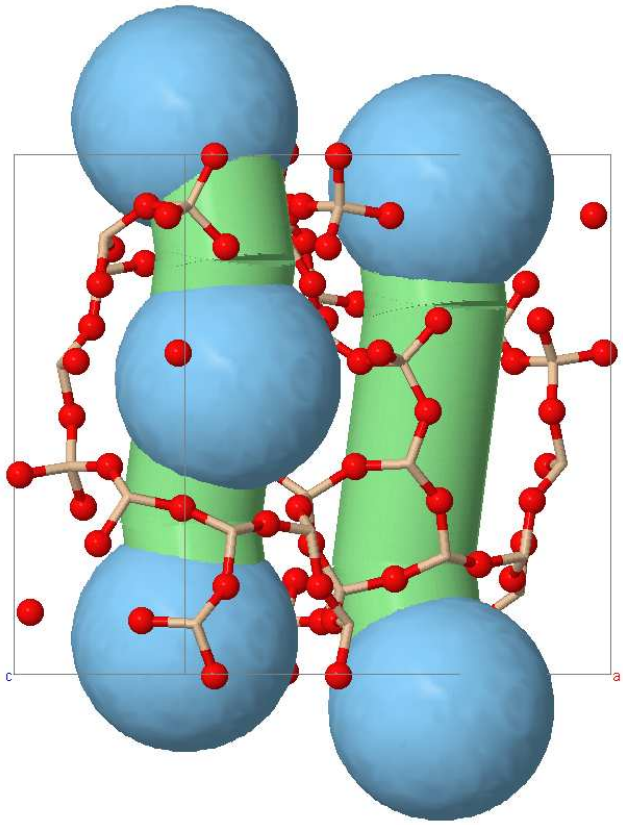

Figure S111: Main pore system of ZON from ZEOMICS. A unit cell is displayed where channels are green, cages are blue, and oxygen atoms of the zeolite structure are red.

Table S224: Physical properties for ZON.

Property	Value
Pore limiting diamater, PLD [Å]	4.0
Largest cavity diameter, LCD [Å]	6.5
Solid density [kg m^{-3}]	1801

Table S225: Adsorption and geometric properties for ZON.

Property	CO_2	N_2
Henry constant [mol kg^{-1} kPa^{-1}]	0.01537	0.00112
Heat of adsorption at 298 K [kJ mol^{-1}]	27.6	15.1
Accessible volume [cm^3 g^{-1}]	0.238	0.288
Accessible surface area [m^2 g^{-1}]	1248	1662

Table S226: Performance metrics for ZON.

Property	Value
Shape selectivity	–
Size selectivity	0.17
Adsorption selectivity	13.77
Minimum parasitic energy [kJ/kg CO_2]	1650.66
Purity [%] at minimum parasitic energy	60.32
Cost [$/ton of CO_2 captured and compressed]	33.09
Purity [%] at optimum cost	90.00
Recovery [%] at optimum cost	90.00
Energy penalty [kWh/ton CO_2 captured] at optimum cost	211.08

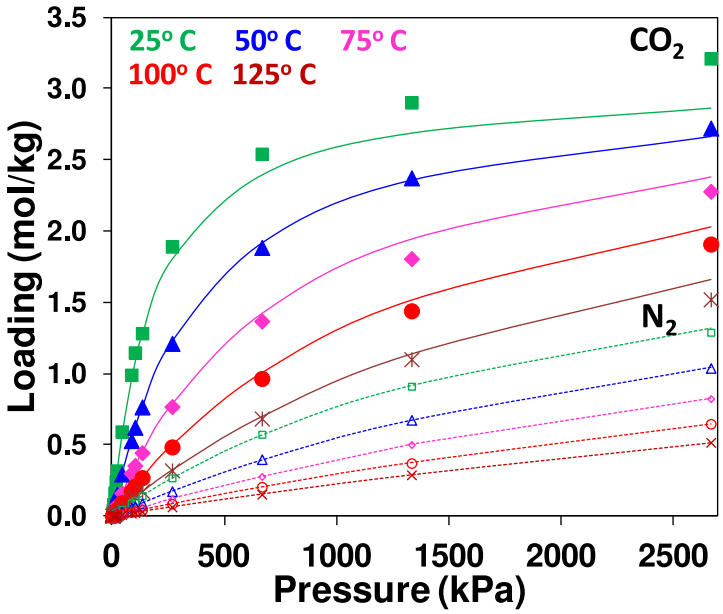

Figure S112: Adsorption isotherms of ZON. Symbols represent GCMC data, and lines represent predictions using the fitted dual-site Langmuir model (solid lines are for CO_2 and dashed lines are for N_2).

Table S227: Dual-site Langmuir isotherm parameters for ZON.

Parameter	CO_2	N_2
Site 1		
q^{sat} [mol kg^{-1}]	3.85	2.35
b^o [m^3 mol^{-1}]	0	9.00×10^{-6}
ΔU [kJ mol^{-1}]	2.67	12.08
Site 2		
q^{sat} [mol kg^{-1}]	3.06	0
b^o [m^3 mol^{-1}]	2.00×10^{-6}	0
ΔU [kJ mol^{-1}]	21.78	31.83