Supplementary Information (SI) for Sustainable Energy & Fuels.

A Sustainable Multi-Zeolite Synthetic Framework from a Single Natural Clay: CO_2/H_2O Adsorption Performance and Life Cycle Assessment Benefits

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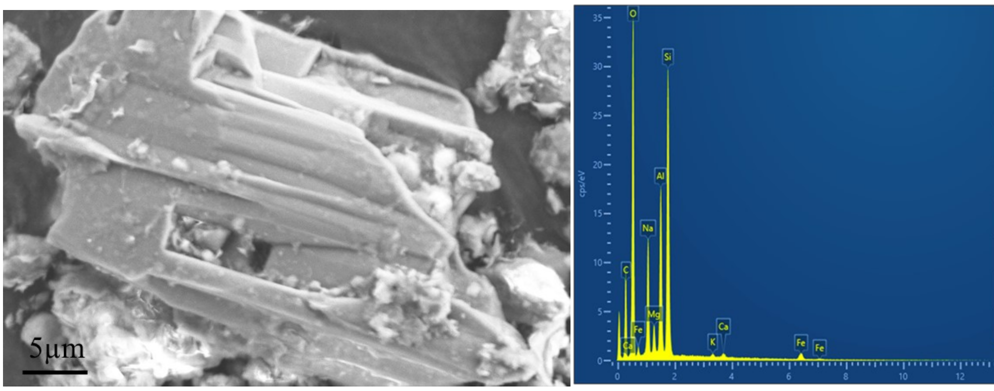
Supplementary information

Figure S1. SEM image of the natural bentonite clay precursor showing its characteristic layered, plate-like morphology, together with the corresponding EDX spectrum and elemental composition.



Element	Composition (Wt.%)
Si	48.8
Al	22.5
Na	13.5
Fe	9.3
Mg	3.8
Ca	1.2
K	0.9

Figure S2. Powder X-ray diffraction (PXRD) data of bentonite clay and high-angle region of Zeolites. (a) PXRD of the starting bentonite clay, normalized to the most intense peak. (b-d) High-angle zoom (50-100° 2θ) of normalized PXRD patterns for the synthesized zeolites and their commercial references (b) Zeolite 4A (LTA), (c) Zeolite 13X (FAU-X), (d) Zeolite Y (FAU-Y).

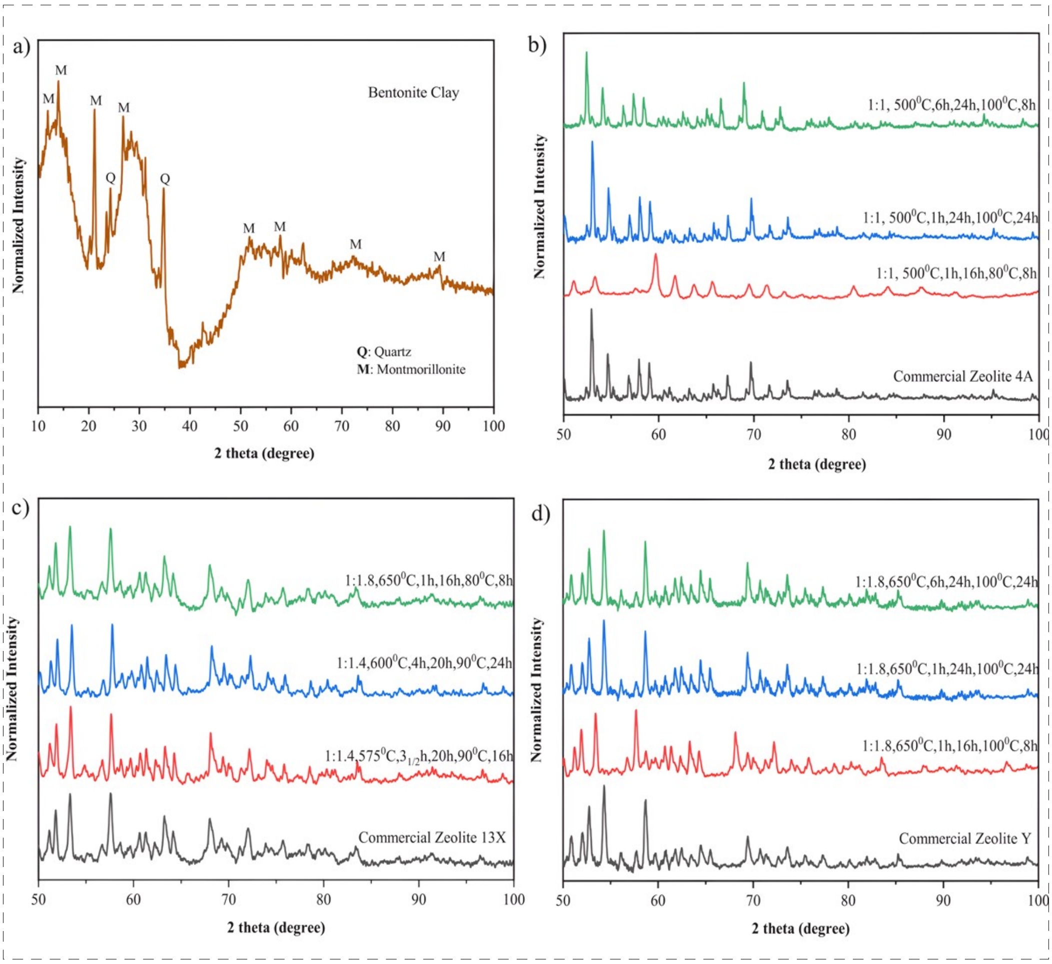


Table S1: Integrated peak areas and calculated relative crystallinity of all samples within each zeolite category

No	Zeolite type	Sample code	∑Synthesized zeolite	∑Commercial	Relative crystallinity (%)
1.	Zeolite 4A	1:1,500^{0}C,1h,16h,80^{0}C,8h	34028.53	39057.68	87.12
		1:1,500^{0}C,1h,24h,100^{0}C,24h	14619.87		37.43
		1:1, 500^{0}C,6h,24h,100^{0}C,8h	45835.33		117.35
2.	Zeolite 13X	1:1.4,575^{0}C,31/2h,20h,90^{0}C,16h	23742.16	26038.94	91.18
		1:1.4,600^{0}C,4h,20h,90^{0}C,24h	25051.65		96.21
		1:1.8,650^{0}C,1h,16h,80^{0}C,8h	25812.63		99.13
3.	Zeolite Y	1:1.8,650^{0}C,1h,16h,100^{0}C,8h	28127.11	56985.11	49.36
		1:1.8,650^{0}C,1h,24h,100^{0}C,24h	49604.34		87.05
		1:1.8,650^{0}C,6h,24h,100^{0}C,24h	51763.74		90.83731

Table S2: Literature ranges of -Q_{st} for commercial Zeolites

Zeolite (commercial)	−Qst (kJ mol⁻¹)	Typical T set (K)	Used method	References
Na-4A (Zeolite 4A)	40-50	273-333	Clausius-Clapeyron	[1,2]
Na-13X (Zeolite 13X)	35-45	288-333	Clausius-Clapeyron	[3,4]
Na-Y (Zeolite Y)	30-40	303-473	Clausius-Clapeyron	[5]

Figure S3: Schematic of the water-vapour adsorption setup.

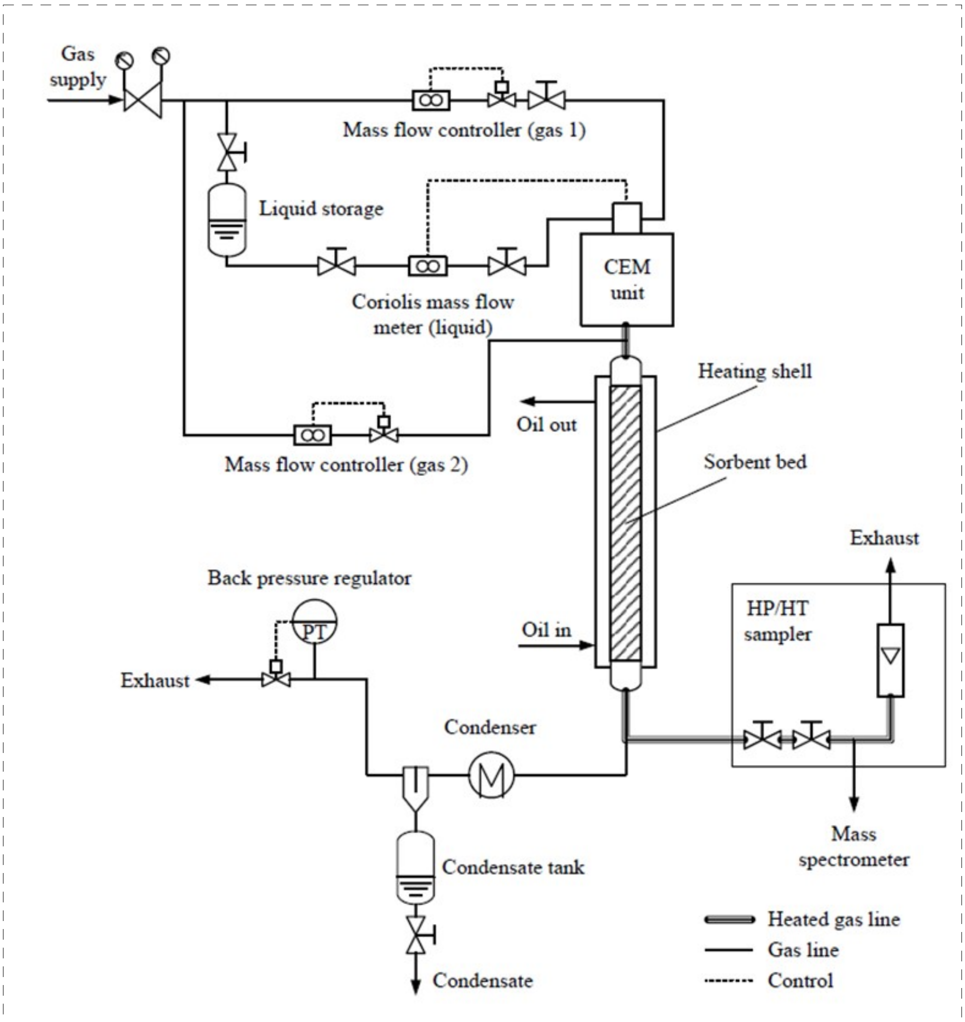


Table S3: Water sorption isotherms experiment summary for Zeolite 13x

Experiment	$T(^0C)$	P (bar)	P_{H2O} (bar)	Water breakthrough	Capacity_ g_{ads}/g_{sorb}	Asymmetry	R^2
Cycle-1	200	10	1	454.0797	0.245	12.3666	0.99755
Cycle-2	200	10	1	440.7093	0.23223	14.2052	0.99918
Cycle-3	200	10	1	433.763	0.23069	12.0599	0.9986
Cycle-4	200	10	1	431.5597	0.23889	11.6919	0.9975
Cycle-5	200	10	1	431.7157	0.23226	12.3833	0.9982
Cycle-1	300	10	0.2	158.1974	0.090942	41.7925	0.99914
Cycle-2	300	10	1	171.6267	0.10229	10.993	0.99687
Cycle-3	300	10	2	140.8708	0.14589	0.13133	0.98777
Cycle-4	300	10	4	67.5509	0.209	7.8738	0.98974
Cycle-5	200	10	1	153.4941	0.097125	15.6047	0.99729
Cycle-1	250	10	1	89.433	0.060627	6.6705	0.99605
Cycle-2	250	10	2	91.3596	0.11961	11.5258	0.98526
Cycle-3	250	10	4	58.4256	0.22475	6.6953	0.97692
Cycle-4	200	10	1	137.2601	0.083252	11.0361	0.99755
Cycle-1	200	10	2	77.77935	0.11145	3.3251	0.9752
Cycle-2	200	10	4	52.44405	0.16185	8.1972	0.9734
Cycle-3	200	10	1	122.0814	0.074027	9.0471	0.99714
Cycle-1	350	10	1	40.2686	0.028051	27.9609	0.9886
Cycle-2	350	10	2	44.882	0.056479	2274206	0.98531
Cycle-3	350	10	4	25.4186	0.14413	19.473	0.9982

Table 3 : Water sorption isotherms experiment summary for Zeolite Y

Experiment	T (^{0}C)	P (bar)	P_{H2O} (bar)	Water breakthrough	Capacity g_{ads}/g_{sorb}	Asymmetry	R^2
cycle_1	200	10	1	55.1944	0.044952	6.648	0.99233
cycle_2	200	10	1	52.237	0.042793	6.1018	0.99277
cycle_3	200	10	1	62.5122	0.044937	9.8074	0.99034
cycle_4	200	10	1	61.181	0.044515	11.2117	0.99121
cycle_1	300	10	1	35.4	0.01615	3.1619	0.99981
cycle_2	300	10	2	44.8306	0.041515	2913914	0.94738
cycle_3	300	10	4	46.4234	0.14262	10.6098	0.98058
cycle_4	200	10	1	65.4551	0.040156	71.0653	0.99184
cycle_1	250	10	1	41.6704	0.021732	34.8541	0.99374
cycle_2	250	10	2	62.7583	0.04916	727115.4	0.8199
cycle_3	250	10	4	80.7054	0.16694	68.4583	0.97101
cycle_4	200	10	1	60.965	0.041882	12.1009	0.99253
cycle_1	200	10	1	61.0004	0.035197	34.6106	0.98256
cycle_2	200	10	2	56.7048	0.082596	6.46	0.97332
cycle_3	350	10	1	24.34	0.0111	41.8146	0.99999
cycle_4	350	10	2	37.3566	0.035542	3983026	0.88235
cycle_5	350	10	4	16.4687	0.11368	3.8097	0.9911
cycle_6	200	10	1	56.6759	0.03255	36.4957	0.98924
cycle_1	300	10	1	31.1059	0.022459	435486.7	0.95641
cycle_2	200	10	4	74.8009	0.16284	0.40687	0.95959

Table 4: Input and output inventories to produce 1kg of Zeolite 13X from Bentonite clay.

	Category	Unit	Value	Database for provider source
Input	Bentonite Clay	kg	0.417	Ecoinvent 3.1
	Sodium hydroxide	kg	0.583	OZLCI2019
	Demineralized water	m3	0.0096	OZLCI2019
	Electricity	MJ	108.00	Electricity Mix-CH

Output	Bentonite clay-Zeolite 13x	Kg	1.00	This Work
Emission	Wastewater	m3	0.0094	This work, Ecoinvent 3.1

Table 5: Input and output inventories to produce 1kg of Zeolite 13X from chemical precursors. Reference work: International Intellectual Property : WO 2023/119309[6]

	Category	**Unit**	**Value**	**Database source for Provider**
Input	Sodium Silicate	Kg	1.517	Ecoinvent 3.1 USEEI , OZLCI2019
	Sodium Aluminate	Kg	0.540	Ecoinvent 3.1 OZLCI2019
	Sodium hydroxide	Kg	0.443	OZLCI2019
	Demineralized water	m3	0.00878	OZLCI2019
	Electricity	MJ	122.760	Electricity Mix-EU-27
Output	Chemical-Zeolite 13X	Kg	1.00	Patent (WO 2023/119309 AI)[6]
Emission	Wastewater	m3	0.00852	Patent (WO 2023/119309 AI)[6]

Table 6: Input and output inventories for 1kg sodium silicate production

	Category	**Unit**	**Value**	**Database source for Provider**
Input	Ground Quartzite	Kg	0.772	Ecoinvent 3.1, OZLCI2019, Reference[7]
	Fine Sand	Kg	0.65	Ecoinvent 3.1 , OZLCI2019, Reference [7]
	Crashed limestone	Kg	0.022	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Sodium hydroxide	Kg	0.209	OZLCI2019, Reference[7]
	Sodium chloride	kg	0.123	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Demineralized water	m3	0.8288	OZLCI2019, Reference [7]
	Electricity	MJ	3.118	Electricity grid mix, AC, < 1kV
	Diesel	Kg	0.144	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Light fuel oil	MJ	0.456	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Natural gas	MJ	1.27	Ecoinvent 3.1 , OZLCI2019, Reference[7]
Output	Sodium Silicate	Kg	1.00	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Inorganic salts and acids	g	1.034	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Metals	g	0.0173	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Chlorides	g	6.316	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Suspended solids	g	0.892	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Dust	g	0.667	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Non-methane volatile organic component (NMVOC)	g	2.451	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Mineral waste (ash)	g	0.0202	Ecoinvent 3.1 , OZLCI2019, Reference[7]
Emission	Carbon dioxide, fossil	kg	0.288	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Nitrogen oxides , NO	g	1.748	Ecoinvent 3.1 , OZLCI2019, Reference[7]
	Sulfur oxides	g	2.186	Ecoinvent 3.1 , OZLCI2019, Reference[7]

	Carbon monoxide	g	0.218	Ecoinvent 3.1 , OZLCI2019, Reference[7]

Table 7: Input and output inventories for 1kg sodium aluminate production

	Category	**Unit**	**Value**	**Database source for Provider**
Input	Bauxite	Kg	1.9	Ecoinvent 3.1, OZLCI2019, Reference[8]
	Steam	Kg	4.48	Ecoinvent 3.1 , OZLCI2019
	Sodium hydroxide	Kg	1.6	OZLCI2019
	Demineralized water	m3	0.4	OZLCI2019
	Electricity	MJ	7.44	Electricity grid mix, AC, < 1kV
Output	Sodium Aluminate	Kg	1.00	Reference [9]
	Red mud (dry)	kg	1.8	OZLCI2019, Reference [9]
Emission	Carbon dioxide, fossil	kg	0.8	Reference [9]

Table S8: Isotherms at 3 different temperatures(25 °C - 60 °C) and the dual site Langmuir fitting values

https://docs.google.com/spreadsheets/d/1GybRSNRkiNCSuc45NeOd8owEQzvJ5CVM/edit?usp=drive_link&ouid=100721013064026322254&rtpof=true&sd=true

Table S9: Unit prices and material cost contributions for the chemical based synthesis of 1 kg Zeolite 13X.

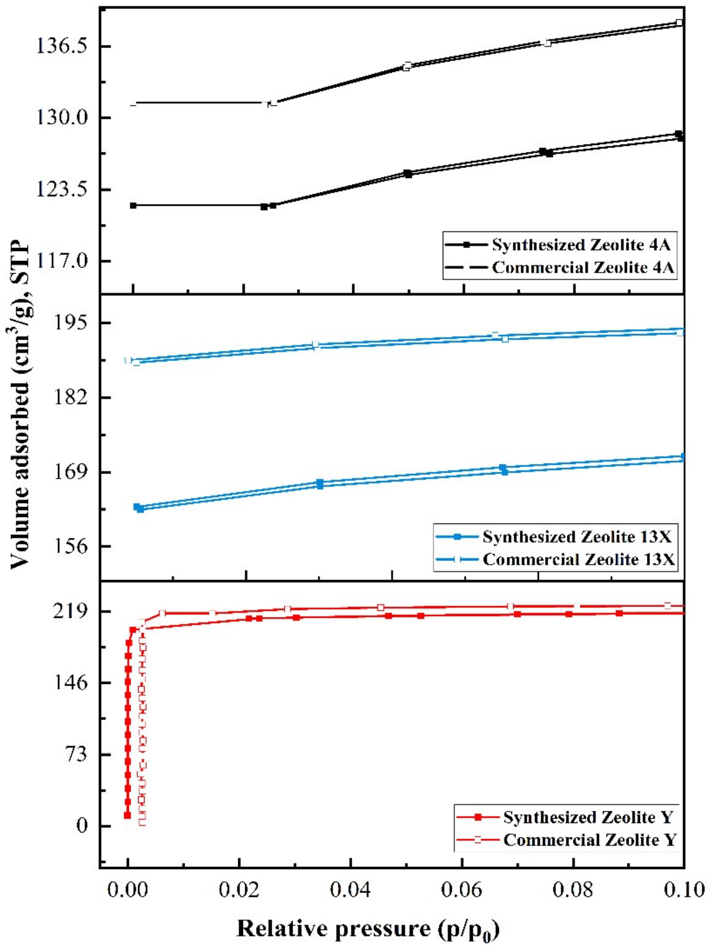
Item	**Amount**	**Unit price**	**Cost (EUR)**
Sodium silicate	1.517 kg	0.60 €/kg	0.91

Sodium aluminate	0.540 kg	1.20 €/kg	0.65
NaOH	0.443 kg	0.50 €/kg	0.22
Demineralized water	0.00878 m³	1.0 €/m³	0.009
Electricity	122.8 MJ = 34.1 kWh	0.12 €/kWh	4.09

Table S10: Unit prices and material cost contributions for the clay based synthesis of 1 kg Zeolite 13X

Input	Amount	Unit price	Cost (€)
Bentonite clay	0.417 kg	0.10 €/kg	0.042
NaOH	0.583 kg	0.50 €/kg	0.292
Demineralized water	0.0096 m³	1.0 €/m³	0.01
Electricity	108 MJ = 30.0 kWh	0.12 €/kWh	3.6

Figure S4: Expanded view of the low relative pressure region ($p/p_0 \leq 0.10$) of the nitrogen adsorption-desorption isotherms shown in Figure 5a.



Reference

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