

# Supplementary Materials

## Impact of Na<sup>+</sup> and Ca<sup>2+</sup> cations on the adsorption of H<sub>2</sub>S on binderfree LTA zeolites

Annika Starke,<sup>1</sup> Christoph Pasel,<sup>1</sup> Christian Bläker,<sup>1</sup> Tobias Eckardt,<sup>2</sup> Jens Zimmermann,<sup>3</sup> and Dieter Bathen,<sup>1,4</sup>

<sup>1</sup> University of Duisburg-Essen, Thermal Process Engineering, D-47057 Duisburg, Germany.

<sup>2</sup> BASF Catalysts Germany GmbH, D-31582 Nienburg, Germany.

<sup>3</sup> Chemiewerk Bad Köstritz GmbH, D-07586 Bad Köstritz, Germany.

<sup>4</sup> Institute of Energy and Environmental Technology IUTA e. V., D-47229 Duisburg, Germany.

Correspondence should be addressed to Annika Starke; annika.starke@uni-due.de

Table S1: Chemical properties of LTA zeolite materials (Determined by XRF (X-ray fluorescence spectroscopy))

Zeolite	Al <sub>2</sub> O <sub>3</sub> [wt%]	SiO <sub>2</sub> [wt%]	Na <sub>2</sub> O [wt%]	CaO [wt%]	Sodium Exchange [%]
NaA BF	31.0	35.2	19.6	0.165	0
CaNaA(19 %) BF	31.4	35.4	16.0	3.22	18.6
CaNaA(35 %) BF	31.1	35.0	12.5	6.05	35.4
CaNaA(50 %) BF	30.7	34.8	9.72	8.43	50.1
CaNaA(70 %) BF	30.1	34.0	5.66	11.6	70.3
CaNaA(82 %) BF	29.9	33.9	3.21	13.6	82.4

Table S2: Parameters of isothermal fit of H<sub>2</sub>S on the LTA zeolites at 25 °C

Zeolite	X <sub>mon1</sub> [mol/kg]	b <sub>1</sub> [-]	X <sub>mon2</sub> [mol/kg]	b <sub>2</sub> [-]	R <sup>2</sup>
NaA	0.292	0.066	2.248	2.31E-4	0.998
CaNaA 19%	0.558	0.036	2.928	1.83E-4	0.998
CaNaA 35%	0.712	0.006	5.237	1.00E-4	0.999
CaNaA 50%	0.469	0.011	2.526	5.92E-4	0.999
CaNaA 70%	0.476	0.020	2.606	7.78E-4	0.999
CaNaA 82%	0.930	0.009	2.327	9.67E-4	0.999
CaNaA 89%	1.626	0.007	1.977	5.55E-4	0.999
CaNaA 92%	0.890	0.010	2.485	1.36E-3	0.999

18

Table S3: Parameters of isothermal fit of H<sub>2</sub>S on the LTA zeolites at 85 °C

Zeolite	X <sub>mon1</sub> [mol/kg]	b <sub>1</sub> [-]	X <sub>mon2</sub> [mol/kg]	b <sub>2</sub> [-]	R <sup>2</sup>
NaA	0.210	0.174	0.388	2.62E-4	0.997
CaNaA 19%	0.076	0.068	0.371	6.14E-4	0.998
CaNaA 35%	0.066	0.008	1.111	1.40E-4	0.999
CaNaA 50%	0.044	0.005	2.985	4.37E-5	0.999
CaNaA 70%	0.085	0.003	2.038	8.21E-5	0.999
CaNaA 82%	0.026	0.072	1.788	1.79E-4	0.999
CaNaA 89%	0.030	0.026	2.362	1.37E-4	0.999
CaNaA 92%	0.017	0.055	2.922	1.10E-4	0.999

19

Table S4: Measured equilibrium loading of H<sub>2</sub>S on the LTA zeolites at 25 °C

Zeolite	Concentration [ppm <sub>mol</sub> ]	Loading [mol/kg]
NaA	43	0.24
	187	0.35
	412	0.49
	620	0.57
	826	0.66
	1065	0.73
	1285	0.79
	1407	0.82
	1610	0.90
	1794	0.95
	1981	1.00
CaNaA 19 %	48	0.38
	191	0.57
	411	0.73
	615	0.84
	825	0.93
	1063	1.04
	1269	1.09
	1400	1.13
	1605	1.19

20

	1795	1.27
	1977	1.35
CaNaA 35 %	44	0.18
	196	0.46
	411	0.71
	618	0.87
	824	0.99
	1068	1.13
	1271	1.20
	1403	1.28
	1609	1.36
	1790	1.42
	1982	1.55
CaNaA 50 %	48	0.23
	199	0.57
	411	0.88
	618	1.09
	823	1.24
	1064	1.41
	1277	1.52
	1401	1.58
	1602	1.66
	1788	1.74
	1979	1.82
CaNaA 70 %	42	0.30
	200	0.72
	411	1.06
	619	1.29
	828	1.48
	1068	1.64
	1285	1.75
	1406	1.81
	1613	1.90

	1798	1.99
	1984	2.06
CaNaA 82 %	36	0.27
	199	0.96
	411	1.39
	620	1.67
	830	1.85
	1067	2.00
	1285	2.13
	1408	2.19
	1612	2.27
	1798	2.38
	1982	2.44
CaNaA 89 %	46	0.43
	199	1.12
	402	1.54
	618	1.81
	828	2.00
	1068	2.16
	1283	2.27
	1405	2.34
	1613	2.42
	1797	2.49
	1980	2.54
CaNaA 92 %	45	0.38
	201	1.10
	412	1.58
	619	1.85
	832	2.08
	1064	2.32
	1273	2.40
	1401	2.46
	1605	2.52

1788 2.57  
1974 2.66

21  
22

Table S5: Measured equilibrium loading of H<sub>2</sub>S on the LTA zeolites at 85 °C

Zeolite	Concentration [ppm <sub>mol</sub> ]	Loading [mol/kg]
NaA	45	0.19
	196	0.22
	411	0.25
	617	0.27
	825	0.28
	1066	0.29
	1283	0.31
	1404	0.31
	1610	0.32
	1796	0.33
	1983	0.35
CaNaA(19 %) BF	48	0.07
	199	0.11
	411	0.15
	617	0.17
	827	0.20
	1068	0.22
	1283	0.24
	1403	0.25
	1609	0.26
	1793	0.27
	1979	0.28
CaNaA(35 %) BF	48	0.03
	200	0.07
	412	0.11
	618	0.14
	828	0.17
	1068	0.21
	1284	0.23

	1404	0.24
	1611	0.26
	1796	0.29
	1981	0.30
CaNaA(50 %) BF	45	0.01
	201	0.05
	411	0.08
	619	0.11
	826	0.14
	1065	0.17
	1281	0.20
	1402	0.21
	1611	0.24
	1793	0.26
	1980	0.28
CaNaA(70 %) BF	47	0.02
	200	0.06
	410	0.11
	617	0.15
	824	0.19
	1063	0.23
	1280	0.26
	1400	0.28
	1604	0.31
	1788	0.33
	1973	0.36
CaNaA(82 %) BF	49	0.04
	200	0.07
	411	0.15
	618	0.20
	823	0.25
	1064	0.31
	1281	0.36

	1402	0.39
	1607	0.42
	1790	0.46
	1975	0.49
CaNaA(89 %) BF	49	0.03
	199	0.09
	411	0.15
	619	0.22
	826	0.27
	1064	0.33
	1279	0.38
	1398	0.41
	1604	0.45
	1786	0.49
	1972	0.53
CaNaA(92 %) BF	50	0.03
	201	0.08
	412	0.15
	620	0.21
	829	0.27
	1067	0.33
	1282	0.38
	1404	0.41
	1615	0.46
	1798	0.50
	1983	0.54

23

24 Table S6: Massbalance after H<sub>2</sub>S desorption at 25 °C for some of the materials. Desorption was measured  
25 immediately after adsorption until no concentration was detectable by μ-GC.

Zeolite	Concentration [ppm <sub>mol</sub> ]	Loading after adsorption [mol/kg]	Loading which desorpted [mol/kg]	Difference [mol/kg]
NaA	1727.73	0.95	0.78	0.17

CaNaA(19 %)	1500.20	1.02	0.93	0.09
CaNaA(35 %)	1498.46	1.23	1.21	0.02

---