Supporting Information:

In silico screening of zeolites for high-pressure hydrogen drying

Máté Erdős,[†] Daan F. Geerdink,[†] Ana Martin-Calvo,[‡] Evgeny A. Pidko,[¶] Leo J. P. van den Broeke,[†] Sofia Calero,[§] Thijs J. H. Vlugt,[†] and Othonas A. Moultos[*,†]

[†]*Engineering Thermodynamics, Process & Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Leeghwaterstraat 39, 2628CB Delft, The Netherlands*

[‡]*Department of Physical, Chemical, and Natural Systems, Universidad Pablo de Olavide, Ctra. Utrera km, 1. ES-41013 Seville, Spain*

[¶]*Inorganic Systems Engineering, Chemical Engineering Department, Faculty of Applied Sciences, Delft University of Technology, Van der Maasweg 9, 2629HZ Delft, The Netherlands*

[§]*Materials Simulation & Modelling, Department of Applied Physics, Eindhoven University of Technology, 5600MB Eindhoven, The Netherlands*

E-mail: o.moultos@tudelft.nl

In Figure S1, the amount of adsorbed H_2 on the LTA4A zeolite is shown as a function of the pressure at $T = 77$ K.

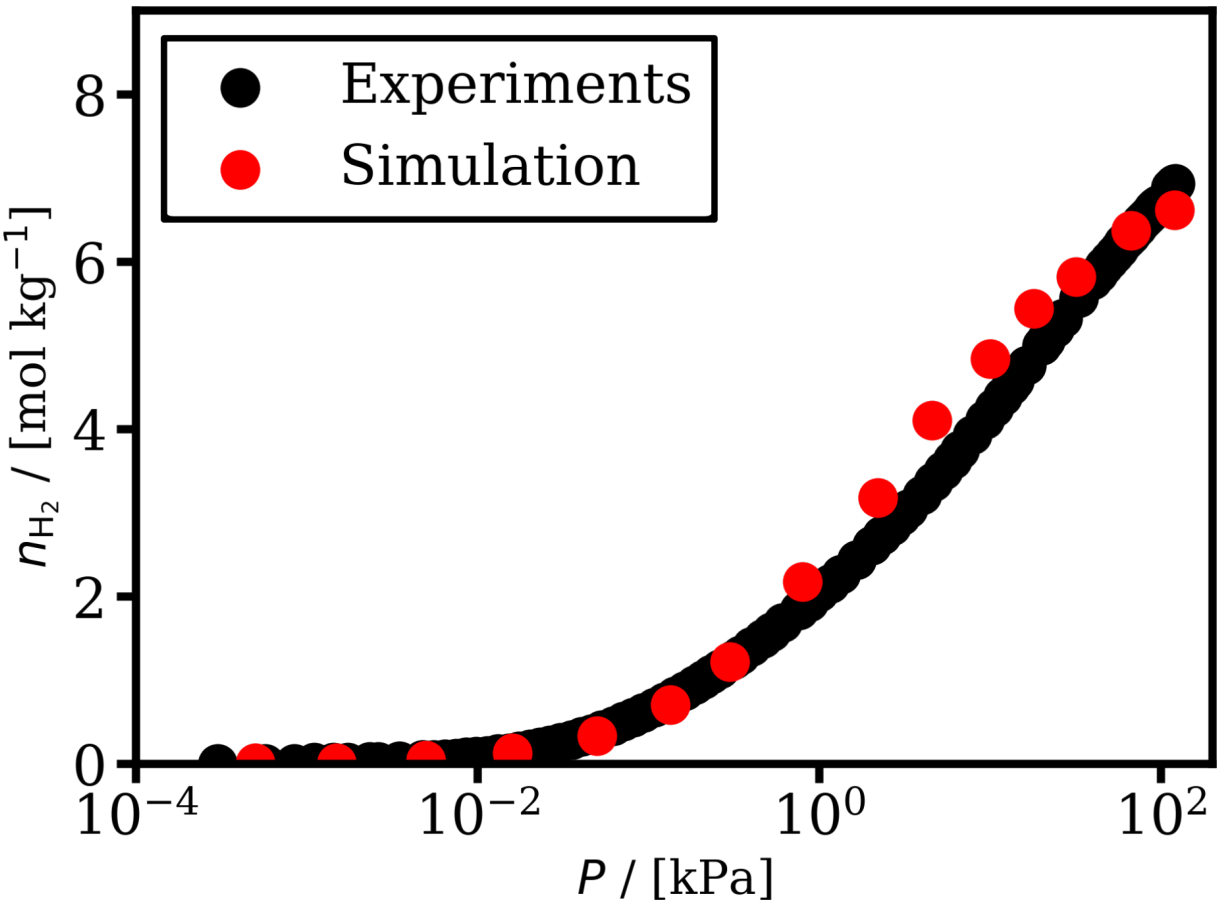

Figure S1: Amount of adsorbed hydrogen on the LTA4A as a function of pressure at T = 77 K. The red and black symbols represent computational and experimentally measured[S1] results, respectively.

Diffusion of hydrogen on the LTA4A zeolite

The calculated mean square displacement of H_2 as a function of time in LTA4A is shown in Figure S2. It can be observed that hydrogen molecules have limited displacement inside the zeolite with the fitted force field parameters, as indicated by the almost flat MSD curve. Based on the computed MSD, the computed diffusivity of H_2 inside the LTA4A is lower than ca. 8×10^{-13} m^2 s^{-1}. To the best of our knowledge, no experimental diffusion data of H_2 on LTA4A is available, thus it is unclear whether or not our force field can accurately describe the mass transport of hydrogen in zeolite frameworks with non-framework Na^+ cations. Ideally, we would like to develop a transferable force field that is applicable to all zeolite structures. However, fitting a transferable force field that can describe both dynamics and adsorption thermodynamics requires a large number of experimental data, which are largely lacking. For this reason, and because the focus of our work is on high-pressure hydrogen drying, we feel that the development of a transferable force field is beyond the scope of our study.

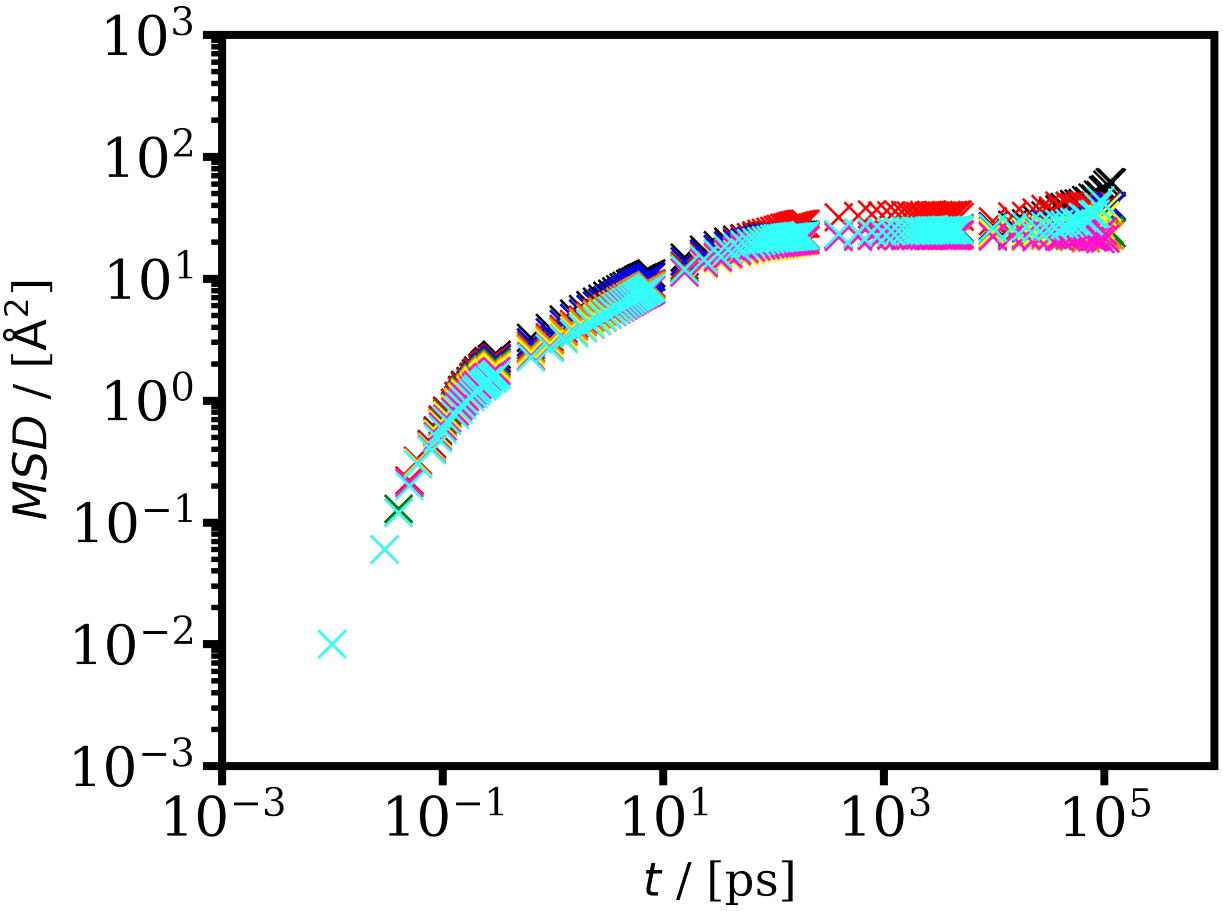

Figure S2: Mean squared displacement of H_2 in LTA4A as a function of time at $T = 77$ K. The colors represent simulations with different number of H_2 molecules in the alpha cages of the LTA4A. The black, red, blue, green, orange, yellow, magenta and cyan colors represent the simulations with 1, 2, 3, 4, 5, 6, 7, and 8 H_2 molecules per alpha cage, respectively.

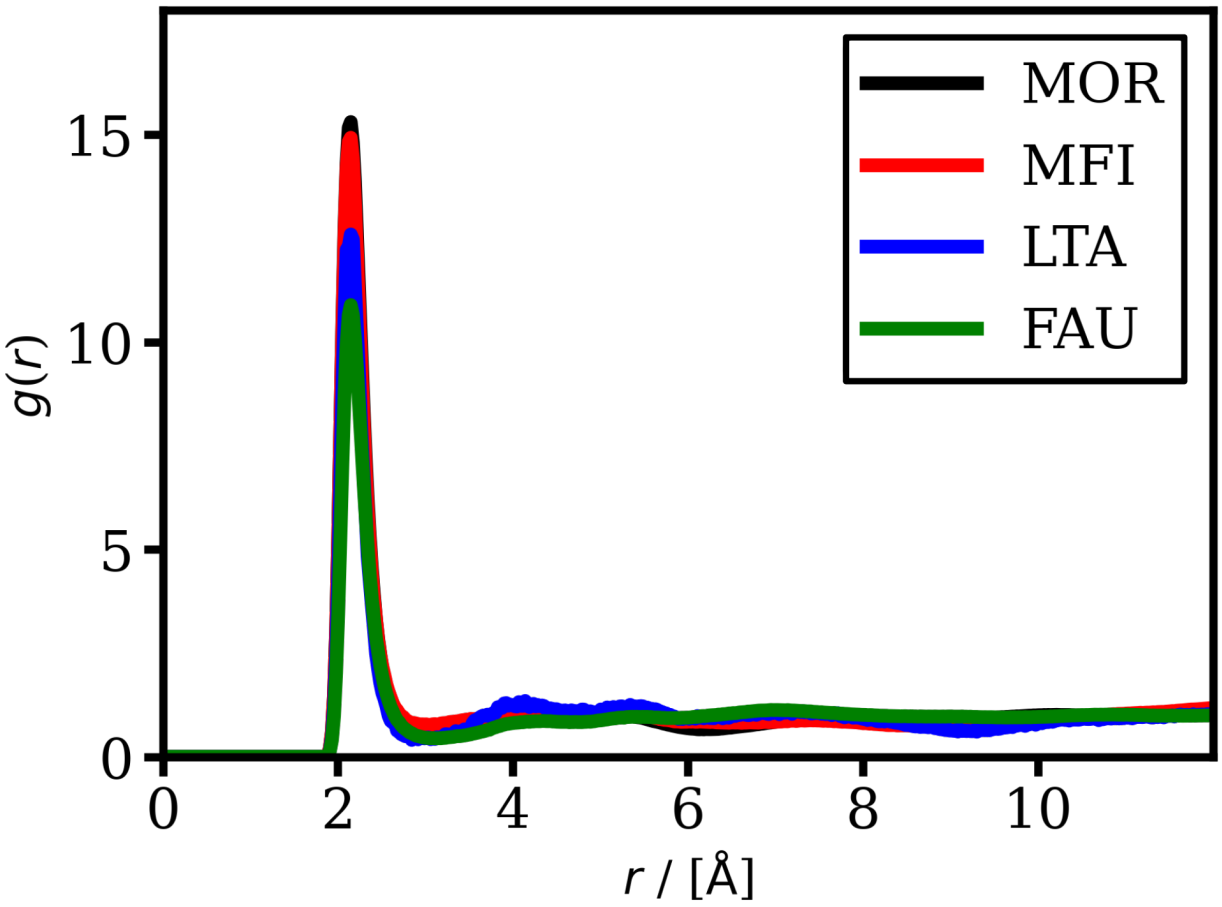

Figure S3: The radial distribution functions for the oxygen atoms of the water molecules and the Na^+ cations on MOR- (black), MFI- (red), LTA- (blue), and FAU-type (green) zeolites with the lowest Si/Al ratio at $P = 875$ bar, $T = 310$ K, and $y_{H_2O} = 12.3$ ppm (molar). The computed loading of each component and the Si/Al ratio of each zeolite type are listed in Tables S6 and S7, respectively.

Table S1: Lennard-Jones parameters and atomic charges used in the simulations. $Oa_{Zeolite}$ represents the oxygen atoms of the zeolite connected to an Al atom, $O_{Zeolite}$ represents the oxygen atoms of the zeolite connected to only Si atoms, O_{water} is the oxygen atom of the water molecule, L_{water} is dummy atom of the TIP5P/Ew water model,[S2] H_{water} is the hydrogen atom of the water molecule.[S3]

Atom type	ϵ / [K]	σ / [Å]	Atomic charge
$Si_{Zeolite}$[S4]	0	0	0.786
$Al_{Zeolite}$[S4]	0	0	0.486
$O_{Zeolite}$[S4]	0	0	-0.393
$Oa_{Zeolite}$[S4]	0	0	-0.414
O_{water}[S2]	89.52	3.10	0
L_{water}[S2]	0	0	-0.241
H_{water}[S2]	0	0	0.241
$Na_{Zeolite}$[S4]	251.78	3.14	0.383
H_{H_2}[S3]	36.73	2.96	0

Table S2: Lennard-Jones parameters for the interaction between specific interaction sites. $Oa_{Zeolite}$ represents the oxygen atoms of the zeolite connected to an Al atom, $O_{Zeolite}$ represents the oxygen atoms of the zeolite connected to only Si atoms, O_{water} is the oxygen atom of the water molecule, L_{water} is dummy atom of the TIP5P/Ew water model,[S2] H_{H_2} is the interaction site of the one-site hydrogen model[S3]

Site 1	Site 2	ϵ / [K]	σ / [Å]
H_{H_2}	$Si_{Zeolite}$	28.26[S3]	1.85[S3]
H_{H_2}	$Al_{Zeolite}$	26.51	1.99
H_{H_2}	$O_{Zeolite}$	66.06[S3]	2.89[S3]
H_{H_2}	$Oa_{Zeolite}$	66.06	2.89
H_{H_2}	$Na_{Zeolite}$	220	3
$O_{Zeolite}$	$Na_{Zeolite}$	33[S4]	3.2[S4]
$O_{Zeolite}$	O_{water}	13.71[S4]	3.38[S4]
$Oa_{Zeolite}$	$Na_{Zeolite}$	23[S4]	3.4[S4]
$Oa_{Zeolite}$	O_{water}	13.71[S4]	3.38[S4]
$Na_{Zeolite}$	O_{water}	75[S4]	2.39[S4]

Table S3: Fugacity coefficients of water and H_2 in the infinitely diluted water/H_2 mixture at 400 and 875 bar calculated by performing CFCMC simulations in the NPT ensemble.[S5,S6] Fugacity coefficients of bulk H_2 reported in the NIST reference fluid thermodynamic and transport properties (REFPROP) database[S7] at $P = 400$ and 875 bar, and $T = 310$ K.

Component	Fugacity coefficient		Source
	$P = 400$ bar	$P = 875$ bar	
Water	1.10	1.46	This work
Hydrogen	1.26	1.68	This work
Hydrogen	1.27	1.70	REFPROP[S7]

Table S4: The adsorption selectivity (S_{H_2O,H_2}), the number of adsorbed H_2 and H_2O molecules per unit cell, and the amount of H_2 gas that can be dried by 1 dm^3 of zeolite for each investigated zeolite structure at $P = 400$ bar, $T = 310$ K, and $y_{H_2O} = 12.3$ ppm (molar). The values of $\sigma_{N_{H_2O}}$ and $\sigma_{N_{H_2}}$ represent the standard deviation of the mean of the water and hydrogen loadings calculated from the five independent simulations, respectively. The Si/Al ratio of each zeolite type is listed in Table S7.

Name	$\boldsymbol{S_{H_2O,H_2}}$ / [%]	$\boldsymbol{N_{H_2}}$ / [molecules (unit cell)$^{-1}$]	$\boldsymbol{\sigma_{N_{H_2}}}$	$\boldsymbol{N_{H_2O}}$ / [molecules (unit cell)$^{-1}$]	$\boldsymbol{\sigma_{N_{H_2O}}}$	$\boldsymbol{V_{H_2}}$ / [dm^3]
ABW	100.00	0.00	0.00	2.22	0.01	5246
ACO	94.43	0.36	0.01	6.11	0.02	6765
AEI	92.22	2.19	0.11	25.89	1.29	8731
AEL	100.00	0.00	0.00	11.95	0.02	6164
AEN	100.00	0.00	0.00	13.88	0.04	6259
AET	89.76	2.64	0.13	23.13	1.16	6291
AFG	98.98	0.21	0.00	20.33	0.06	7711
AFI	90.26	0.93	0.01	8.65	0.05	6545
AFN	99.40	0.07	0.00	11.85	0.59	6927
AFO	99.99	0.00	0.00	10.45	0.15	5394
AFR	67.26	5.10	0.05	10.47	0.08	5337
AFS	80.84	6.52	0.33	27.50	1.38	7727
AFT	87.90	4.97	0.14	36.09	0.12	8120
AFV	86.85	1.96	0.02	12.93	0.06	7292
AFX	84.65	4.18	0.03	23.03	0.03	7765
AFY	88.91	1.35	0.00	10.83	0.04	10279
AHT	100.00	0.00	0.00	5.28	0.26	4551
ANA	100.00	0.00	0.00	3.62	0.03	1561
APC	99.70	0.02	0.00	8.10	0.00	4813

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
APD	99.99	0.00	0.00	8.09	0.01	4892
AST	99.30	0.16	0.01	23.27	0.04	9896
ASV	100.00	0.00	0.00	7.95	0.01	8166
ATN	82.45	1.10	0.02	5.17	0.00	6186
ATO	99.80	0.02	0.00	9.67	0.01	5425
ATS	91.13	1.04	0.05	10.72	0.54	7718
ATT	72.38	1.48	0.01	3.87	0.01	5920
ATV	100.00	0.00	0.00	4.17	0.01	3537
AVL	82.52	3.48	0.02	16.43	0.04	6660
AWO	99.31	0.07	0.00	10.51	0.53	4291
AWW	82.04	1.48	0.00	6.76	0.01	5128
BCT	0.80	0.01	0.00	0.00	0.00	0
BEA	87.24	4.95	0.01	33.82	0.02	8703
BEC	83.46	3.21	0.14	16.19	0.34	8226
BIK	98.92	0.03	0.00	2.41	0.12	4025
BOF	98.87	0.09	0.01	7.86	0.08	6437
BOG	90.59	5.01	0.10	48.20	0.12	8669
BOZ	52.43	25.50	1.28	28.11	1.41	4250
BPH	84.36	2.80	0.14	15.09	0.75	8477
BRE	94.27	0.27	0.01	4.45	0.22	5480
BSV	100.00	0.00	0.00	39.62	0.01	8298
CAN	97.44	0.12	0.01	4.73	0.24	7161

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
CAS	99.31	0.04	0.00	5.57	0.01	4682
CDO	96.44	0.43	0.00	11.76	0.01	6342
CFI	95.61	0.57	0.00	12.51	0.06	7049
CGF	99.01	0.09	0.00	8.93	0.02	5070
CGS	98.82	0.16	0.01	13.58	0.02	7708
CHA	91.98	1.65	0.03	18.91	0.07	8502
CSV	96.23	0.43	0.02	11.04	0.55	9643
CZP	100.00	0.00	0.00	6.32	0.32	6031
DAC	94.77	0.42	0.00	7.52	0.01	5884
DDR	91.11	3.10	0.01	31.77	0.06	5088
DFO	85.04	13.47	0.03	76.55	0.11	9286
DFT	61.38	0.82	0.01	1.30	0.01	3085
DOH	92.75	0.81	0.05	10.33	0.07	5538
DON	97.17	0.81	0.03	27.92	0.15	8031
EAB	97.84	0.41	0.02	18.52	0.07	8825
EDI	40.85	0.95	0.05	0.65	0.03	2288
EEI	89.94	5.70	0.28	50.93	2.55	4910
EMT	72.69	20.33	1.02	54.11	2.71	8073
EON	88.74	2.55	0.04	20.14	0.17	6079
EPI	97.41	0.20	0.01	7.48	0.37	5925
ERI	95.05	0.92	0.03	17.74	0.06	8517
ESV	99.43	0.09	0.00	15.45	0.04	6144

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ETL	88.83	2.33	0.05	18.57	0.04	5005
ETR	82.22	4.39	0.02	20.31	0.01	7031
EUO	90.28	4.06	0.02	37.68	0.11	6195
EZT	97.34	0.56	0.03	20.40	0.11	7859
FAR	99.78	0.08	0.01	36.77	0.07	8046
FAU	77.06	35.99	1.80	120.86	6.04	9008
FER	98.36	0.20	0.00	12.23	0.02	6414
FRA	98.12	0.54	0.01	28.43	0.01	7972
GIS	96.26	0.26	0.00	6.56	0.02	7227
GIU	99.40	0.24	0.01	40.57	0.05	7786
GME	84.42	2.16	0.04	11.71	0.06	7900
GON	99.18	0.07	0.01	8.52	0.04	5413
GOO	99.70	0.03	0.00	8.90	0.00	5670
HEU	88.62	1.53	0.03	11.95	0.01	6254
IFO	96.02	0.73	0.04	17.62	0.88	10233
IFR	96.86	0.52	0.02	16.10	0.05	9281
IFW	88.14	4.02	0.02	29.89	0.06	7934
IFY	96.23	0.76	0.04	19.41	0.97	7673
IHW	98.05	0.75	0.07	37.89	0.31	6718
IMF	96.26	3.76	0.00	96.69	0.02	6313
IRN	86.93	6.51	0.10	43.30	0.22	7753
IRR	55.18	18.79	0.02	23.13	0.04	5625

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Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ISV	83.17	6.63	0.01	32.77	0.02	8282
ITE	93.21	2.29	0.07	31.39	0.09	8293
ITG	94.49	1.59	0.08	27.31	0.12	8698
ITH	97.70	0.52	0.03	22.11	1.11	7397
ITR	96.00	1.72	0.06	41.17	0.19	6859
ITT	58.81	13.78	0.10	19.67	0.24	5899
ITW	98.86	0.09	0.00	8.14	0.03	6465
IWR	94.19	2.08	0.13	33.71	0.19	10125
IWS	79.08	18.23	0.23	68.92	0.56	8061
IWV	79.65	17.98	0.29	70.38	0.79	7480
IWW	89.19	5.55	0.09	45.76	0.07	7305
JBW	99.46	0.01	0.00	1.27	0.01	4274
JNT	100.00	0.00	0.00	6.12	0.31	4225
JOZ	72.26	1.67	0.01	4.35	0.04	3825
JRY	100.00	0.00	0.00	7.60	0.14	6288
JSN	99.23	0.04	0.00	4.67	0.01	5610
JSR	56.35	29.39	0.04	37.94	0.08	5220
JST	55.98	9.75	0.05	12.40	0.13	3975
JSW	100.00	0.00	0.00	16.19	0.03	6682
KFI	82.63	10.65	0.00	50.65	0.01	8495
LAU	97.50	0.22	0.01	8.52	0.43	6871
LEV	93.86	1.67	0.00	25.50	0.04	8090

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
LIO	99.66	0.04	0.00	13.07	0.02	6886
LOS	99.47	0.05	0.00	10.07	0.02	7607
LOV	74.30	1.49	0.02	4.30	0.00	4319
LTA	85.75	24.42	1.22	146.95	7.35	10674
LTF	78.23	7.64	0.15	27.44	0.47	4614
LTJ	99.76	0.01	0.00	4.10	0.20	5108
LTL	67.41	3.68	0.01	7.61	0.04	3803
LTN	96.75	11.27	0.39	335.43	0.57	7980
MAR	99.95	0.01	0.00	27.92	0.01	7411
MAZ	84.34	2.14	0.11	11.52	0.58	5731
MEI	88.68	2.64	0.08	20.70	0.18	9603
MEL	97.59	0.92	0.06	37.17	0.23	7229
MEP	97.28	0.33	0.00	11.86	0.05	4954
MER	97.24	0.36	0.02	12.80	0.64	7041
MFI	99.44	0.19	0.06	33.42	0.15	6896
MFS	96.59	0.45	0.02	12.65	0.63	6590
MON	42.17	2.39	0.12	1.74	0.09	2063
MOR	90.38	1.68	0.01	15.84	0.03	6023
MOZ	76.07	8.42	0.07	26.78	0.00	4524
MRE	99.98	0.00	0.00	11.67	0.01	5137
MSE	86.12	7.14	0.00	44.29	0.05	6960
MSO	99.96	0.02	0.00	37.96	0.06	8087

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
MTF	99.99	0.00	0.00	11.78	0.04	5974
MTN	92.52	3.00	0.01	37.16	0.08	5045
MTT	96.02	0.30	0.02	7.22	0.05	5894
MTW	93.44	0.50	0.02	7.09	0.02	4967
MVY	100.00	0.00	0.00	1.85	0.02	3471
MWF	71.03	177.00	8.85	434.00	21.70	5210
MWW	87.25	4.58	0.04	31.35	0.08	7462
NAB	41.51	1.91	0.00	1.36	0.01	2347
NAT	88.30	0.93	0.03	7.04	0.05	6147
NES	87.60	7.37	0.02	52.04	0.14	6766
NON	86.62	3.12	0.04	20.19	0.13	4352
NPO	94.01	0.09	0.00	1.34	0.00	4483
NPT	58.62	8.53	0.43	12.08	0.60	4855
NSI	99.88	0.00	0.00	2.30	0.02	3869
OBW	53.27	20.94	0.01	23.87	0.09	4298
OFF	77.68	1.66	0.08	5.76	0.29	5546
OKO	96.18	1.16	0.04	29.18	0.05	8079
OSI	98.27	0.17	0.01	9.95	0.50	5932
OSO	67.43	1.82	0.01	3.78	0.03	6014
OWE	89.51	0.64	0.02	5.50	0.01	6336
PAU	95.24	16.25	0.32	325.13	0.36	8269
PCR	99.88	0.02	0.00	18.30	0.06	6149

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
PHI	95.21	0.68	0.02	13.49	0.05	7427
PON	99.99	0.00	0.00	9.37	0.12	7629
POS	85.31	5.39	0.11	31.31	0.21	8176
PSI	100.00	0.00	0.00	23.56	0.09	3619
PUN	86.02	2.79	0.00	17.15	0.04	7667
RHO	91.13	3.06	0.03	31.43	0.07	10180
RRO	87.02	0.77	0.04	5.15	0.26	5499
RSN	68.57	3.56	0.05	7.76	0.04	3895
RTE	83.72	1.38	0.01	7.08	0.06	5442
RTH	94.14	0.99	0.00	15.85	0.01	8570
RUT	90.97	1.16	0.02	11.72	0.01	6349
RWR	99.99	0.00	0.00	8.04	0.00	5189
RWY	26.68	33.07	0.02	12.03	0.04	2309
SAF	99.67	0.06	0.01	19.07	0.12	6088
SAO	83.50	7.25	0.07	36.68	0.12	9992
SAS	93.53	1.26	0.06	18.25	0.91	9167
SAT	97.09	1.01	0.04	33.78	0.11	8282
SAV	88.04	3.41	0.01	25.09	0.01	8215
SBE	80.09	19.57	0.06	78.68	0.15	9078
SBN	65.82	1.10	0.01	2.13	0.02	3690
SBS	85.36	12.01	0.07	70.05	0.12	10766
SBT	84.50	19.13	0.28	104.32	0.37	10683

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
SEW	92.32	2.18	0.05	26.21	0.09	7268
SFE	95.55	0.28	0.02	5.99	0.06	7784
SFF	98.84	0.18	0.01	15.03	0.03	9012
SFG	96.36	0.98	0.05	25.96	1.30	6656
SFH	82.31	5.13	0.26	23.86	1.19	6613
SFN	87.19	1.92	0.08	13.04	0.20	7254
SFO	73.94	4.30	0.08	12.20	0.18	6218
SFS	95.73	1.23	0.08	27.45	0.21	8766
SFV	87.83	32.50	2.41	234.50	12.44	5657
SFW	86.00	8.55	0.17	52.54	0.10	7894
SGT	89.40	2.21	0.03	18.62	0.02	5461
SIV	95.92	1.14	0.03	26.79	0.20	7366
SOD	99.85	0.01	0.00	5.63	0.00	8398
SOF	91.89	1.49	0.05	16.88	0.07	7453
SOS	81.85	1.62	0.02	7.29	0.07	5540
SSF	98.84	0.33	0.02	28.32	0.21	9281
SSY	85.41	1.75	0.06	10.26	0.12	6652
STF	97.87	0.34	0.03	15.65	0.08	8874
STI	96.25	1.33	0.04	34.21	0.15	8530
STO	99.45	0.20	0.02	36.06	0.16	6475
STT	93.85	1.76	0.04	26.90	0.13	7666
STW	94.33	1.55	0.09	25.81	0.13	7584

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
SVV	94.87	1.14	0.06	21.07	1.05	7295
SZR	80.00	2.16	0.01	8.63	0.08	4546
TER	96.85	1.12	0.02	34.52	0.11	7909
THO	58.40	1.42	0.01	1.99	0.02	3368
TOL	99.95	0.01	0.00	26.42	1.32	7050
TON	97.63	0.16	0.02	6.65	0.07	5404
TSC	74.84	74.83	0.53	222.60	1.24	8240
TUN	92.21	5.86	0.20	69.35	0.41	6839
UEI	97.34	0.42	0.05	15.41	0.18	6030
UFI	83.27	6.21	0.11	30.91	0.12	7895
UOS	94.93	0.39	0.02	7.36	0.02	5812
UOV	83.85	13.57	0.12	70.47	0.27	6991
UOZ	100.00	0.00	0.00	14.43	0.06	7578
USI	97.59	0.62	0.03	25.21	1.26	10783
UTL	86.78	6.26	0.13	41.06	0.31	9063
UWY	86.00	3.87	0.19	23.80	0.29	6956
VET	99.99	0.00	0.00	4.73	0.07	6043
VFI	78.82	5.19	0.01	19.30	0.07	8346
VNI	74.55	3.61	0.12	10.59	0.10	3333
VSV	55.84	4.64	0.02	5.86	0.07	2943
WEI	81.65	1.31	0.01	5.82	0.02	5161
YUG	92.43	0.29	0.01	3.57	0.02	4307

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Table S4 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ZON	92.81	0.85	0.04	10.99	0.04	6664

Table S5: The adsorption selectivity (S_{H_2O,H_2}), the number of adsorbed H_2 and H_2O molecules per unit cell, and the amount of H_2 gas that can be dried by 1 dm^3 of zeolite for each investigated zeolite structure at $P = 400$ bar, $T = 310$ K, and $y_{H_2O} = 478$ ppm (molar). The value of $\sigma_{N_{H_2O}}$ and $\sigma_{N_{H_2}}$ represent the standard deviation of the mean of the water and hydrogen loadings calculated from the five independent simulations, respectively. The Si/Al ratio of each zeolite type is listed in Table S7.

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ABW	100.00	0.00	0.00	2.74	0.01	167
ACO	99.00	0.09	0.01	9.37	0.05	267
AEI	98.21	0.64	0.02	34.92	0.08	303
AEL	100.00	0.00	0.00	13.36	0.67	177
AEN	100.00	0.00	0.00	16.50	0.83	191
AET	100.00	0.00	0.00	36.34	1.82	254
AFG	99.73	0.06	0.00	23.73	0.04	232
AFI	99.99	0.00	0.00	13.82	0.03	269
AFN	99.75	0.04	0.00	15.13	0.06	228
AFO	100.00	0.00	0.00	13.37	0.03	178
AFR	99.15	0.22	0.03	25.34	0.09	332
AFS	99.52	0.26	0.04	52.68	0.30	381
AFT	97.78	1.19	0.04	52.29	0.24	303
AFV	97.31	0.52	0.01	18.77	0.04	272
AFX	97.67	0.83	0.05	34.70	0.14	301
AFY	97.96	0.31	0.02	14.99	0.01	366
AHT	100.00	0.00	0.00	7.83	0.01	174
ANA	100.00	0.00	0.00	7.97	0.04	88
APC	99.42	0.05	0.01	8.84	0.07	135

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
APD	99.99	0.00	0.00	9.69	0.10	151
AST	99.85	0.04	0.00	27.18	0.04	297
ASV	100.00	0.00	0.00	8.52	0.01	225
ATN	85.07	1.03	0.05	5.89	0.29	181
ATO	99.94	0.01	0.00	11.61	0.02	168
ATS	99.47	0.08	0.01	15.12	0.04	280
ATT	81.33	1.09	0.02	4.76	0.03	187
ATV	100.00	0.00	0.00	6.54	0.08	143
AVL	96.28	0.94	0.01	24.37	0.05	254
AWO	99.87	0.02	0.00	17.86	0.14	188
AWW	96.69	0.38	0.01	11.01	0.05	215
BCT	27.97	0.02	0.00	0.01	0.00	0
BEA	99.25	0.38	0.03	50.47	0.38	334
BEC	98.90	0.29	0.01	25.59	0.03	335
BIK	99.52	0.01	0.00	2.92	0.01	126
BOF	99.91	0.01	0.00	10.15	0.05	214
BOG	99.69	0.21	0.00	68.76	0.18	318
BOZ	85.40	11.23	0.17	65.70	0.49	256
BPH	99.35	0.17	0.01	26.33	0.10	380
BRE	96.70	0.20	0.00	5.92	0.01	187
BSV	100.00	0.00	0.00	45.87	0.02	247
CAN	99.23	0.05	0.00	5.88	0.01	229

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
CAS	99.66	0.03	0.00	7.58	0.01	164
CDO	99.02	0.15	0.00	15.52	0.03	215
CFI	99.68	0.05	0.00	16.48	0.01	239
CGF	99.47	0.06	0.00	11.91	0.01	174
CGS	99.92	0.02	0.00	18.64	0.01	272
CHA	97.91	0.55	0.02	25.83	0.04	299
CSV	99.79	0.03	0.00	14.57	0.03	327
CZP	100.00	0.00	0.00	7.61	0.02	187
DAC	98.94	0.11	0.01	10.52	0.02	212
DDR	98.06	0.94	0.04	47.56	0.09	196
DFO	99.68	0.38	0.01	118.50	3.56	370
DFT	83.46	0.47	0.02	2.37	0.12	145
DOH	99.26	0.11	0.00	14.96	0.03	206
DON	99.89	0.04	0.00	36.29	0.03	269
EAB	99.67	0.08	0.01	23.39	0.06	287
EDI	63.99	0.69	0.02	1.22	0.01	110
EEI	97.64	1.80	0.01	74.64	0.31	185
EMT	99.48	0.57	0.03	109.69	0.09	421
EON	96.66	1.02	0.05	29.58	0.03	230
EPI	99.03	0.10	0.00	10.00	0.50	204
ERI	99.28	0.16	0.01	22.59	0.10	279
ESV	99.90	0.02	0.00	19.40	0.04	199

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ETL	93.54	1.84	0.01	26.57	0.09	184
ETR	99.84	0.06	0.01	38.01	0.27	339
EUO	98.63	0.73	0.05	52.23	0.25	221
EZT	99.73	0.07	0.00	25.41	0.07	252
FAR	99.97	0.01	0.00	42.02	0.02	237
FAU	99.43	1.27	0.06	222.65	11.13	427
FER	99.48	0.08	0.00	15.23	0.01	206
FRA	99.28	0.25	0.01	34.14	1.71	246
GIS	98.87	0.10	0.00	9.09	0.02	258
GIU	99.90	0.05	0.00	47.88	0.10	236
GME	97.90	0.38	0.00	17.51	0.03	304
GON	99.97	0.00	0.00	10.46	0.04	171
GOO	99.80	0.03	0.00	13.79	0.17	226
HEU	93.75	1.02	0.01	15.37	0.01	207
IFO	99.99	0.00	0.00	22.52	0.14	336
IFR	99.71	0.06	0.00	19.94	0.03	296
IFW	99.37	0.28	0.01	44.04	0.07	301
IFY	99.72	0.07	0.00	24.58	0.06	250
IHW	99.87	0.06	0.01	46.17	0.10	211
IMF	98.82	1.50	0.05	126.00	3.78	212
IRN	98.82	0.78	0.00	65.29	0.01	301
IRR	98.88	0.86	0.02	76.29	0.03	477

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ISV	98.85	0.60	0.01	51.55	0.08	335
ITE	99.01	0.41	0.02	41.47	0.01	282
ITG	99.65	0.13	0.01	36.27	1.81	297
ITH	99.80	0.06	0.00	27.67	0.08	238
ITR	99.72	0.15	0.03	52.44	0.24	225
ITT	99.43	0.34	0.01	58.65	0.07	453
ITW	99.54	0.05	0.00	10.46	0.05	214
IWR	99.68	0.14	0.02	43.62	0.07	337
IWS	98.64	1.62	0.09	117.53	0.36	354
IWV	98.93	1.33	0.10	122.97	0.26	336
IWW	99.16	0.57	0.02	67.81	0.43	279
JBW	99.61	0.01	0.00	1.53	0.01	132
JNT	100.00	0.00	0.00	7.67	0.03	136
JOZ	83.99	1.37	0.02	7.21	0.04	163
JRY	100.00	0.00	0.00	9.82	0.08	209
JSN	99.77	0.02	0.00	6.51	0.33	201
JSR	90.47	9.34	0.04	88.74	0.10	314
JST	82.93	5.35	0.09	26.00	0.23	214
JSW	100.00	0.00	0.00	17.72	0.03	188
KFI	95.26	3.39	0.08	68.27	0.25	295
LAU	99.75	0.02	0.00	10.03	0.04	208
LEV	98.98	0.35	0.01	33.82	0.01	276

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
LIO	99.94	0.01	0.00	15.81	0.04	214
LOS	99.81	0.02	0.00	12.23	0.05	238
LOV	87.84	0.93	0.05	6.74	0.34	174
LTA	93.70	13.37	0.05	198.97	0.31	372
LTF	93.66	3.16	0.03	46.74	0.03	202
LTJ	99.94	0.00	0.00	6.12	0.03	196
LTL	98.95	0.19	0.01	17.79	0.02	229
LTN	99.70	1.27	0.26	417.06	1.88	255
MAR	99.97	0.01	0.00	33.95	0.15	232
MAZ	95.31	0.91	0.00	18.42	0.04	236
MEI	99.01	0.30	0.01	30.04	0.07	359
MEL	99.81	0.09	0.00	47.94	0.07	240
MEP	99.36	0.10	0.02	15.86	0.02	171
MER	98.97	0.19	0.01	18.72	0.09	265
MFI	99.96	0.02	0.00	41.15	2.06	219
MFS	99.11	0.15	0.02	17.02	0.06	228
MON	73.72	1.64	0.02	4.60	0.02	140
MOR	98.67	0.32	0.01	23.69	0.03	232
MOZ	96.55	1.69	0.07	47.36	0.29	206
MRE	99.99	0.00	0.00	12.72	0.05	144
MSE	98.42	1.04	0.01	64.85	0.17	262
MSO	99.99	0.00	0.00	44.20	0.06	242

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
MTF	100.00	0.00	0.00	13.75	0.05	179
MTN	98.10	1.00	0.00	51.80	0.06	181
MTT	99.57	0.04	0.01	8.89	0.05	187
MTW	99.72	0.03	0.00	11.65	0.01	210
MVY	100.00	0.00	0.00	2.10	0.10	101
MWF	86.15	109.00	3.27	678.00	20.34	209
MWW	99.16	0.41	0.03	48.21	0.02	295
NAB	71.98	1.39	0.07	3.58	0.18	159
NAT	94.28	0.50	0.01	8.17	0.02	184
NES	98.19	1.40	0.02	75.65	0.23	253
NON	94.32	1.63	0.05	27.13	0.16	151
NPO	94.69	0.08	0.00	1.44	0.07	124
NPT	84.95	4.14	0.06	23.40	0.01	242
NSI	99.91	0.00	0.00	2.91	0.15	126
OBW	84.45	9.91	0.03	53.80	0.07	249
OFF	94.12	0.58	0.01	9.20	0.03	228
OKO	99.73	0.10	0.02	37.37	0.14	266
OSI	99.62	0.05	0.00	12.73	0.64	195
OSO	84.83	1.08	0.05	6.03	0.30	247
OWE	96.06	0.32	0.03	7.77	0.01	230
PAU	99.02	4.38	0.00	440.83	0.02	289
PCR	99.97	0.01	0.00	22.18	0.04	192

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
PHI	99.13	0.17	0.02	18.99	0.06	269
PON	100.00	0.00	0.00	11.16	0.05	234
POS	99.10	0.44	0.01	48.06	0.01	323
PSI	100.00	0.00	0.00	25.72	0.02	102
PUN	96.70	0.85	0.02	25.02	0.06	288
RHO	99.45	0.24	0.04	43.21	0.12	360
RRO	93.86	0.46	0.00	7.08	0.01	194
RSN	83.77	2.52	0.03	13.01	0.11	168
RTE	97.23	0.31	0.01	10.83	0.01	214
RTH	98.94	0.22	0.01	20.32	1.02	283
RUT	93.17	0.93	0.05	12.63	0.63	176
RWR	100.00	0.00	0.00	9.44	0.02	157
RWY	76.50	17.86	0.00	58.14	0.01	287
SAF	99.99	0.00	0.00	23.74	1.19	195
SAO	99.36	0.36	0.02	55.95	0.06	392
SAS	98.08	0.46	0.01	23.45	0.13	303
SAT	99.58	0.17	0.01	41.01	0.03	259
SAV	97.60	0.89	0.02	35.97	0.11	303
SBE	99.39	0.89	0.04	144.96	7.25	430
SBN	80.14	0.83	0.01	3.37	0.02	150
SBS	99.76	0.26	0.02	108.69	0.12	430
SBT	99.76	0.39	0.00	161.95	0.30	427

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
SEW	99.52	0.17	0.01	36.18	0.15	258
SFE	99.79	0.02	0.00	8.11	0.04	271
SFF	99.96	0.01	0.00	18.07	0.08	279
SFG	99.31	0.23	0.02	33.14	0.12	219
SFH	98.49	0.57	0.00	37.25	0.15	266
SFN	99.55	0.09	0.01	19.43	0.08	278
SFO	98.87	0.29	0.04	25.22	0.06	331
SFS	99.87	0.05	0.00	36.82	0.04	303
SFV	97.66	7.75	0.23	323.00	9.69	201
SFW	97.69	1.84	0.07	77.61	0.24	300
SGT	97.12	0.74	0.01	24.89	0.07	188
SIV	98.68	0.50	0.02	37.16	1.86	263
SOD	99.91	0.01	0.00	6.31	0.32	242
SOF	99.35	0.16	0.01	23.68	1.18	269
SOS	97.71	0.29	0.01	12.24	0.61	239
SSF	99.94	0.02	0.00	34.15	0.11	288
SSY	99.57	0.07	0.01	15.43	0.04	257
STF	99.89	0.02	0.00	19.52	0.04	285
STI	98.99	0.44	0.03	42.86	0.14	275
STO	99.97	0.01	0.00	42.30	0.15	195
STT	99.29	0.25	0.01	34.99	0.17	257
STW	99.41	0.20	0.00	34.65	0.02	262

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
SVV	97.92	0.53	0.01	25.06	0.01	223
SZR	91.10	1.38	0.05	14.14	0.15	192
TER	99.89	0.05	0.00	46.38	0.12	273
THO	80.59	0.89	0.02	3.68	0.03	160
TOL	99.98	0.00	0.00	31.10	0.03	214
TON	99.73	0.02	0.00	9.04	0.45	189
TSC	98.90	4.79	0.04	433.03	0.22	412
TUN	99.55	0.43	0.04	94.29	0.20	239
UEI	99.94	0.01	0.00	22.86	1.14	230
UFI	97.35	1.23	0.06	45.22	2.26	297
UOS	98.90	0.11	0.01	10.17	0.51	207
UOV	98.64	1.53	0.12	110.77	0.24	283
UOZ	100.00	0.00	0.00	15.70	0.78	212
USI	99.98	0.01	0.00	31.78	0.07	350
UTL	99.53	0.30	0.01	61.97	3.10	352
UWY	99.57	0.16	0.00	36.85	0.16	277
VET	100.00	0.00	0.00	5.70	0.28	187
VFI	99.94	0.02	0.00	36.58	1.83	407
VNI	88.78	2.22	0.11	17.60	0.88	143
VSV	79.55	3.19	0.16	12.43	0.62	161
WEI	93.01	0.72	0.01	9.57	0.03	218
YUG	97.96	0.14	0.01	6.49	0.32	201

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Table S5 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ZON	95.16	0.66	0.01	12.94	0.01	202

Table S6: The adsorption selectivity (S_{H_2O,H_2}), the number of adsorbed H_2 and H_2O molecules per unit cell, and the amount of H_2 gas that can be dried by 1 dm^3 of zeolite for each investigated zeolite structure at $P = 875$ bar, $T = 310$ K, and $y_{H_2O} = 12.3$ ppm (molar). The value of $\sigma_{N_{H_2O}}$ and $\sigma_{N_{H_2}}$ represent the standard deviation of the mean of the water and hydrogen loadings calculated from the five independent simulations, respectively. The Si/Al ratio of each zeolite type is listed in Table S7.

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ABW	99.99	0.00	0.00	2.39	0.12	3188
ACO	92.21	0.59	0.03	6.93	0.35	4330
AEI	87.92	3.73	0.06	27.16	0.10	5170
AEL	100.00	0.00	0.00	12.37	0.01	3602
AEN	100.00	0.00	0.00	14.94	0.07	3803
AET	92.51	2.11	0.11	26.06	0.25	4001
AFG	98.08	0.42	0.02	21.27	1.06	4555
AFI	94.43	0.61	0.01	10.39	0.06	4440
AFN	98.66	0.17	0.01	12.68	0.63	4185
AFO	99.99	0.00	0.00	11.56	0.58	3371
AFR	71.08	5.51	0.11	13.54	0.20	3895
AFS	81.91	7.21	0.23	32.65	0.58	5179
AFT	85.68	6.62	0.00	39.62	0.01	5031
AFV	83.41	2.76	0.14	13.88	0.69	4421
AFX	81.51	5.61	0.03	24.73	0.02	4708
AFY	86.13	1.87	0.09	11.62	0.58	6227
AHT	100.00	0.00	0.00	6.55	0.33	3183
ANA	100.00	0.00	0.00	5.42	0.03	1317
APC	99.22	0.06	0.01	8.20	0.01	2750

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
APD	99.96	0.00	0.00	8.33	0.02	2842
AST	98.66	0.33	0.02	24.12	0.05	5789
ASV	100.00	0.00	0.00	8.11	0.03	4702
ATN	78.61	1.50	0.03	5.50	0.02	3715
ATO	99.56	0.05	0.00	10.19	0.01	3227
ATS	91.50	1.12	0.03	12.06	0.06	4901
ATT	65.69	2.08	0.10	3.99	0.20	3446
ATV	100.00	0.00	0.00	4.43	0.04	2121
AVL	77.93	5.02	0.25	17.75	0.89	4060
AWO	98.06	0.24	0.00	12.24	0.01	2822
AWW	78.01	2.04	0.02	7.23	0.05	3095
BCT	0.90	0.04	0.00	0.00	0.00	1
BEA	85.40	6.30	0.16	36.88	0.31	5358
BEC	79.04	4.52	0.16	17.04	0.30	4887
BIK	98.32	0.04	0.00	2.59	0.01	2443
BOF	98.55	0.13	0.00	8.50	0.02	3928
BOG	90.17	5.74	0.08	52.69	0.06	5350
BOZ	47.50	36.09	0.25	32.64	0.35	2786
BPH	85.26	3.05	0.15	17.64	0.88	5592
BRE	89.00	0.61	0.01	4.92	0.05	3416
BSV	100.00	0.00	0.00	41.60	2.08	4917
CAN	95.44	0.24	0.01	4.97	0.25	4249

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
CAS	98.43	0.10	0.00	6.14	0.08	2913
CDO	94.25	0.78	0.03	12.80	0.04	3898
CFI	95.13	0.68	0.02	13.35	0.05	4247
CGF	97.71	0.23	0.00	9.82	0.06	3146
CGS	98.54	0.22	0.03	14.95	0.12	4791
CHA	87.97	2.75	0.04	20.11	0.01	5104
CSV	95.96	0.50	0.03	11.94	0.60	5885
CZP	100.00	0.00	0.00	6.80	0.02	3663
DAC	91.21	0.78	0.02	8.08	0.03	3565
DDR	87.10	5.17	0.00	34.88	0.04	3152
DFO	81.43	18.02	0.01	78.99	0.01	5409
DFT	51.78	1.34	0.02	1.44	0.02	1930
DOH	92.81	0.91	0.03	11.70	0.05	3542
DON	97.40	0.80	0.04	30.10	1.51	4889
EAB	96.98	0.62	0.01	19.79	0.05	5324
EDI	35.61	1.46	0.00	0.81	0.01	1595
EEI	85.61	9.03	0.05	53.71	0.28	2923
EMT	75.12	21.42	0.98	64.68	1.77	5447
EON	85.12	3.87	0.03	22.13	0.26	3771
EPI	94.45	0.47	0.00	8.02	0.03	3587
ERI	92.50	1.51	0.01	18.58	0.03	5036
ESV	98.89	0.18	0.02	16.36	0.03	3673

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ETL	86.14	3.33	0.02	20.69	0.06	3148
ETR	82.97	4.85	0.14	23.60	0.27	4611
EUO	88.95	5.07	0.01	40.79	0.01	3785
EZT	96.02	0.89	0.04	21.52	0.07	4682
FAR	99.67	0.13	0.01	39.18	1.96	4839
FAU	79.32	37.06	1.42	142.13	2.56	5980
FER	96.90	0.41	0.02	12.93	0.05	3826
FRA	96.27	1.15	0.01	29.59	0.01	4685
GIS	94.23	0.45	0.01	7.35	0.04	4571
GIU	98.91	0.48	0.01	43.44	0.10	4706
GME	80.91	2.97	0.15	12.59	0.63	4793
GON	99.07	0.08	0.01	8.96	0.05	3215
GOO	99.29	0.07	0.01	10.37	0.10	3731
HEU	82.91	2.63	0.02	12.75	0.06	3765
IFO	96.91	0.60	0.00	18.92	0.01	6200
IFR	95.61	0.78	0.03	16.93	0.11	5509
IFW	86.10	5.12	0.26	31.74	1.59	4754
IFY	95.22	1.04	0.06	20.65	0.09	4609
IHW	97.36	1.09	0.06	40.24	0.17	4028
IMF	94.20	6.30	0.26	102.30	0.51	3770
IRN	84.31	8.67	0.01	46.59	0.02	4710
IRR	49.70	25.98	0.10	25.67	0.19	3523

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ISV	79.61	8.90	0.16	34.74	0.25	4957
ITE	90.82	3.35	0.00	33.17	0.01	4946
ITG	93.45	2.05	0.04	29.27	0.10	5260
ITH	97.29	0.66	0.01	23.68	0.04	4472
ITR	94.89	2.36	0.08	43.72	0.06	4112
ITT	56.01	17.87	0.05	22.76	0.08	3852
ITW	98.18	0.16	0.01	8.78	0.04	3934
IWR	92.92	2.71	0.11	35.58	0.12	6033
IWS	78.96	20.83	0.69	78.17	1.20	5161
IWV	81.45	19.07	0.67	83.74	1.27	5023
IWW	86.75	7.56	0.07	49.49	0.18	4459
JBW	96.99	0.04	0.01	1.31	0.02	2491
JNT	100.00	0.00	0.00	6.74	0.03	2623
JOZ	60.48	3.25	0.03	4.97	0.02	2469
JRY	100.00	0.00	0.00	8.15	0.04	3808
JSN	98.19	0.10	0.00	5.19	0.03	3516
JSR	52.08	39.74	0.02	43.19	0.04	3355
JST	52.73	13.08	0.08	14.59	0.18	2639
JSW	100.00	0.00	0.00	16.32	0.06	3801
KFI	79.52	13.41	0.14	52.08	0.18	4930
LAU	96.30	0.34	0.02	8.92	0.01	4062
LEV	90.94	2.69	0.13	26.98	1.35	4831

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
LIO	99.40	0.08	0.01	13.62	0.02	4050
LOS	99.04	0.10	0.01	10.56	0.53	4505
LOV	70.98	2.00	0.01	4.88	0.02	2766
LTA	83.11	31.42	1.57	154.55	7.73	6337
LTF	74.85	10.59	0.15	31.52	0.24	2992
LTJ	99.57	0.02	0.00	4.54	0.06	3193
LTL	65.39	4.57	0.04	8.63	0.10	2433
LTN	96.43	13.20	0.40	356.63	0.77	4789
MAR	99.88	0.04	0.00	30.13	1.51	4514
MAZ	81.48	3.06	0.05	13.47	0.07	3781
MEI	87.97	3.17	0.05	23.17	0.09	6067
MEL	97.27	1.13	0.01	40.37	0.10	4431
MEP	96.35	0.52	0.02	13.83	0.05	3262
MER	95.29	0.73	0.04	14.72	0.04	4573
MFI	99.20	0.29	0.05	35.46	0.12	4131
MFS	94.85	0.75	0.03	13.82	0.05	4065
MON	42.01	3.08	0.01	2.23	0.06	1493
MOR	87.82	2.37	0.03	17.06	0.01	3664
MOZ	71.35	11.72	0.11	29.19	0.22	2783
MRE	99.98	0.00	0.00	11.97	0.03	2974
MSE	83.49	9.46	0.09	47.81	0.06	4241
MSO	99.95	0.02	0.00	39.97	0.19	4807

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
MTF	99.97	0.00	0.00	12.18	0.04	3486
MTN	89.52	4.87	0.01	41.60	0.05	3189
MTT	94.17	0.47	0.06	7.56	0.07	3482
MTW	91.89	0.70	0.02	7.91	0.07	3126
MVY	100.00	0.00	0.00	1.95	0.10	2068
MWF	63.33	271.00	13.55	468.00	23.40	3171
MWW	86.34	5.46	0.22	34.50	0.46	4635
NAB	41.09	2.60	0.01	1.82	0.04	1774
NAT	80.80	1.73	0.02	7.26	0.02	3580
NES	86.59	8.93	0.15	57.67	0.24	4233
NON	81.68	4.73	0.08	21.08	0.14	2566
NPO	86.32	0.22	0.00	1.39	0.01	2634
NPT	52.29	12.41	0.17	13.60	0.17	3085
NSI	99.68	0.01	0.00	2.53	0.01	2401
OBW	47.17	30.68	0.22	27.40	0.25	2785
OFF	72.87	2.33	0.12	6.26	0.31	3401
OKO	94.39	1.81	0.00	30.50	0.01	4767
OSI	97.83	0.24	0.01	10.77	0.54	3624
OSO	61.21	2.68	0.00	4.23	0.02	3798
OWE	84.49	1.10	0.03	6.02	0.03	3911
PAU	93.15	26.23	0.15	356.78	0.45	5122
PCR	99.74	0.05	0.00	19.72	0.99	3741

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
PHI	92.93	1.13	0.01	14.87	0.07	4622
PON	99.99	0.00	0.00	9.53	0.11	4383
POS	82.65	7.06	0.11	33.65	0.08	4961
PSI	100.00	0.00	0.00	24.32	0.04	2108
PUN	82.58	3.96	0.04	18.78	0.06	4739
RHO	89.37	4.04	0.06	33.93	0.05	6202
RRO	83.92	1.10	0.02	5.73	0.08	3453
RSN	64.46	4.94	0.03	8.97	0.08	2540
RTE	79.58	1.92	0.03	7.47	0.04	3244
RTH	92.81	1.30	0.07	16.80	0.84	5127
RUT	86.41	1.87	0.04	11.87	0.04	3628
RWR	99.99	0.00	0.00	8.24	0.02	3001
RWY	22.68	49.65	0.01	14.56	0.01	1577
SAF	99.78	0.05	0.00	20.70	1.04	3730
SAO	82.56	8.39	0.42	39.74	1.99	6111
SAS	90.61	2.00	0.01	19.26	0.02	5460
SAT	95.29	1.75	0.06	35.38	0.06	4895
SAV	84.34	4.99	0.07	26.87	0.13	4965
SBE	84.09	18.77	0.25	99.17	0.17	6459
SBN	62.39	1.46	0.02	2.42	0.02	2374
SBS	86.94	11.93	0.60	79.39	3.97	6887
SBT	86.08	18.90	0.43	116.90	0.87	6758

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
SEW	90.98	2.79	0.12	28.12	0.22	4402
SFE	95.63	0.31	0.02	6.68	0.06	4901
SFF	98.41	0.26	0.01	15.74	0.03	5328
SFG	94.53	1.60	0.17	27.58	0.27	3991
SFH	81.01	5.98	0.30	25.53	1.28	3993
SFN	86.95	2.17	0.05	14.43	0.06	4531
SFO	76.93	4.59	0.23	15.30	0.76	4401
SFS	95.99	1.26	0.09	30.13	0.15	5431
SFV	85.89	40.50	2.41	246.50	12.44	3357
SFW	81.89	12.36	0.17	55.92	0.25	4742
SGT	84.65	3.53	0.06	19.48	0.10	3225
SIV	93.22	2.17	0.06	29.83	0.10	4630
SOD	99.68	0.02	0.00	5.88	0.01	4955
SOF	91.52	1.74	0.09	18.74	0.94	4671
SOS	81.73	1.94	0.02	8.68	0.01	3724
SSF	98.49	0.46	0.08	30.30	0.19	5606
SSY	84.73	1.93	0.03	10.70	0.09	3913
STF	98.17	0.32	0.04	16.93	0.04	5419
STI	93.76	2.42	0.12	36.33	1.82	5113
STO	99.32	0.26	0.01	37.71	1.89	3822
STT	92.34	2.35	0.12	28.36	1.42	4563
STW	93.15	2.05	0.04	27.87	0.10	4622

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
SVV	93.77	1.47	0.07	22.06	1.10	4311
SZR	73.56	3.43	0.03	9.54	0.08	2835
TER	96.23	1.46	0.05	37.26	0.03	4818
THO	49.79	2.28	0.01	2.26	0.01	2156
TOL	99.89	0.03	0.00	27.71	0.05	4173
TON	96.27	0.28	0.03	7.20	0.04	3305
TSC	72.61	94.40	4.72	250.24	12.51	5228
TUN	92.76	5.88	0.29	75.43	3.77	4199
UEI	97.68	0.44	0.05	18.41	0.17	4065
UFI	80.26	8.11	0.08	32.97	0.20	4755
UOS	92.82	0.64	0.02	8.23	0.04	3666
UOV	80.03	18.70	0.38	74.95	0.59	4197
UOZ	99.99	0.00	0.00	15.28	0.02	4532
USI	97.80	0.61	0.06	27.21	0.14	6568
UTL	86.74	6.94	0.09	45.35	0.14	5650
UWY	86.54	4.16	0.12	26.76	0.15	4415
VET	99.99	0.00	0.00	5.01	0.03	3612
VFI	76.69	6.23	0.31	20.51	1.03	5006
VNI	68.89	5.39	0.09	11.93	0.09	2121
VSV	52.17	6.47	0.04	7.06	0.06	1999
WEI	76.64	2.01	0.02	6.61	0.02	3310
YUG	88.81	0.55	0.01	4.37	0.04	2975

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Table S6 – continued from previous page

Name	S_{H_2O,H_2} / [%]	N_{H_2} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2}}$	N_{H_2O} / [molecules (unit cell)$^{-1}$]	$\sigma_{N_{H_2O}}$	V_{H_2} / [dm^3]
ZON	86.46	1.82	0.04	11.64	0.04	3985

Table S7: Si/Al ratio, helium void fraction (ϕ_{He}), pore limiting diameter (PLD), and largest cavity diameter (LCD) of each investigated zeolite type.

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
ABW	1.0	0.01	3.1	3.6
ACO	1.0	0.05	3.2	3.9
AEI	1.0	0.15	3.4	6.9
AEL	1.0	0.02	4.1	5.2
AEN	1.0	0.00	3.2	3.9
AET	1.0	0.11	7.2	7.8
AFG	1.0	0.06	2.1	5.8
AFI	1.0	0.11	7.0	7.6
AFN	1.0	0.04	3.1	4.8
AFO	1.0	0.03	4.3	5.0
AFR	1.7	0.20	6.6	7.8
AFS	1.0	0.21	5.6	9.1
AFT	1.0	0.16	3.3	7.1
AFV	1.5	0.14	3.1	6.4
AFX	1.0	0.16	3.3	7.1
AFY	1.0	0.19	5.5	7.4
AHT	1.0	0.00	2.1	3.4
ANA	1.0	0.00	2.0	3.7
APC	1.0	0.02	2.7	3.8
APD	1.0	0.01	3.2	4.2
AST	1.0	0.08	1.5	7.2
ASV	1.0	0.01	4.0	4.9

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Table S7 – continued from previous page

Name	Si/Al ratio	ϕ_{He}	PLD / [Å]	LCD / [Å]
ATN	1.0	0.05	3.7	5.5
ATO	1.0	0.03	5.1	5.3
ATS	1.0	0.15	6.4	6.6
ATT	2.0	0.10	3.4	4.9
ATV	1.0	0.00	3.0	3.9
AVL	1.3	0.13	3.2	6.6
AWO	1.0	0.03	3.3	4.5
AWW	2.0	0.12	3.8	6.9
BCT	1.0	0.01	2.2	2.8
BEA	1.5	0.18	5.6	6.1
BEC	1.5	0.22	5.9	6.2
BIK	2.0	0.01	3.1	3.8
BOF	2.0	0.05	4.2	5.2
BOG	1.6	0.16	6.5	7.5
BOZ	2.2	0.30	4.5	8.3
BPH	1.0	0.21	5.6	9.1
BRE	1.7	0.04	2.6	4.9
BSV	1.0	0.01	3.4	4.8
CAN	1.0	0.07	5.4	5.8
CAS	1.4	0.01	2.6	4.4
CDO	2.0	0.05	3.0	5.0
CFI	1.7	0.13	6.9	7.1
CGF	2.0	0.02	2.6	5.4

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
CGS	1.0	0.06	3.6	5.3
CHA	1.0	0.15	3.3	6.7
CSV	1.5	0.15	4.9	7.1
CZP	1.0	0.00	3.2	3.8
DAC	2.0	0.07	3.4	4.8
DDR	2.0	0.09	3.2	7.1
DFO	1.3	0.20	6.8	10.9
DFT	3.0	0.08	3.2	4.2
DOH	1.8	0.07	2.2	7.3
DON	1.4	0.13	7.7	8.2
EAB	1.0	0.10	3.1	6.6
EDI	4.0	0.15	3.0	4.9
EEI	2.1	0.09	2.2	6.2
EMT	1.0	0.28	7.0	11.0
EON	2.0	0.12	6.4	7.3
EPI	2.0	0.07	3.2	4.9
ERI	1.0	0.11	3.0	6.3
ESV	1.4	0.04	3.3	5.7
ETL	2.0	0.06	3.0	5.8
ETR	1.0	0.17	8.9	9.6
EUO	1.8	0.12	4.5	6.3
EZT	1.0	0.09	5.6	5.9
FAR	1.0	0.04	2.1	5.9

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
FAU	1.0	0.29	7.0	10.7
FER	2.0	0.06	4.3	5.4
FRA	1.0	0.07	2.3	6.0
GIS	1.0	0.05	2.9	4.6
GIU	1.0	0.04	2.2	5.9
GME	1.0	0.17	6.7	7.1
GON	1.3	0.04	4.9	5.7
GOO	1.0	0.02	2.6	3.9
HEU	2.0	0.08	3.3	5.2
IFO	1.0	0.13	7.0	7.4
IFR	1.7	0.11	6.0	6.6
IFW	1.5	0.18	5.2	7.2
IFY	1.4	0.09	3.4	6.4
IHW	1.9	0.07	3.3	6.1
IMF	2.2	0.10	4.9	6.7
IRN	1.4	0.16	3.2	8.6
IRR	1.6	0.39	11.7	13.9
ISV	1.5	0.21	5.8	6.4
ITE	1.7	0.14	3.8	7.8
ITG	1.5	0.14	5.9	6.4
ITH	1.7	0.08	4.7	6.3
ITR	1.7	0.09	4.7	6.0
ITT	1.6	0.33	11.6	12.8

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
ITW	1.4	0.04	3.5	4.2
IWR	1.3	0.17	5.5	6.9
IWS	1.6	0.24	6.3	7.6
IWV	1.9	0.24	6.6	8.1
IWW	1.7	0.14	5.8	6.6
JBW	2.0	0.02	3.3	3.9
JNT	1.0	0.00	1.4	4.0
JOZ	1.9	0.10	3.1	4.4
JRY	1.0	0.01	3.7	4.1
JSN	1.7	0.04	3.1	4.5
JSR	2.0	0.34	4.5	7.4
JST	2.0	0.19	3.3	4.9
JSW	1.0	0.02	2.2	5.0
KFI	1.0	0.18	3.6	10.2
LAU	2.0	0.06	3.7	5.5
LEV	1.3	0.11	3.1	6.4
LIO	1.0	0.03	1.9	5.6
LOS	1.0	0.05	2.2	5.9
LOV	2.0	0.07	3.4	4.3
LTA	1.0	0.25	3.8	10.2
LTF	2.1	0.12	7.1	7.8
LTJ	1.0	0.02	2.7	3.6
LTL	2.0	0.16	7.1	9.6

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
LTN	1.0	0.07	1.7	9.6
MAR	1.0	0.02	2.0	5.7
MAZ	2.0	0.13	7.1	7.7
MEI	1.4	0.21	6.5	7.7
MEL	2.0	0.10	4.8	6.9
MEP	1.9	0.04	1.4	5.0
MER	1.0	0.07	3.8	6.2
MFI	1.8	0.06	4.3	5.9
MFS	2.0	0.09	4.9	6.2
MON	3.0	0.10	3.1	3.8
MOR	2.0	0.11	6.0	6.2
MOZ	2.0	0.14	7.1	9.6
MRE	1.4	0.03	5.2	5.7
MSE	1.7	0.16	6.0	6.5
MSO	1.1	0.07	1.6	6.8
MTF	1.8	0.02	3.6	5.6
MTN	2.1	0.08	2.2	6.4
MTT	1.4	0.07	4.6	5.5
MTW	1.3	0.07	5.1	5.3
MVY	1.0	0.00	2.5	3.0
MWF	2.0	0.14	3.7	10.1
MWW	1.7	0.15	4.2	9.3
NAB	2.3	0.12	3.1	3.8

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
NAT	1.5	0.08	3.8	3.9
NES	2.0	0.16	4.7	6.2
NON	1.8	0.09	1.8	6.1
NPO	2.0	0.01	3.1	3.3
NPT	2.0	0.25	3.2	9.9
NSI	1.4	0.01	2.9	3.5
OBW	2.2	0.30	4.8	8.9
OFF	2.0	0.16	6.1	6.5
OKO	1.8	0.12	5.5	6.3
OSI	1.0	0.09	5.9	6.3
OSO	2.0	0.27	5.5	5.7
OWE	1.7	0.09	3.4	5.2
PAU	1.0	0.09	3.7	10.1
PCR	1.6	0.02	3.8	5.6
PHI	1.0	0.06	3.3	5.0
PON	1.0	0.03	3.9	4.5
POS	1.5	0.18	6.1	6.7
PSI	1.0	0.01	4.4	5.3
PUN	1.3	0.14	4.0	5.0
RHO	1.0	0.17	3.7	10.0
RRO	2.0	0.06	3.5	3.9
RSN	2.0	0.08	3.4	4.3
RTE	2.0	0.12	3.6	6.4

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
RTH	1.7	0.14	3.7	7.6
RUT	1.6	0.05	1.9	5.4
RWR	1.7	0.01	2.8	3.9
RWY	3.0	0.57	5.9	14.0
SAF	1.0	0.06	5.7	6.2
SAO	1.0	0.23	6.3	8.2
SAS	1.0	0.16	3.8	8.5
SAT	1.0	0.09	2.8	6.2
SAV	1.0	0.17	3.7	8.3
SBE	1.0	0.26	6.8	12.1
SBN	2.3	0.11	3.4	4.4
SBS	1.0	0.26	6.9	11.0
SBT	1.0	0.27	6.9	10.4
SEW	1.6	0.14	4.8	6.2
SFE	1.3	0.13	5.8	6.2
SFF	1.7	0.10	4.9	7.1
SFG	1.6	0.08	5.0	6.4
SFH	1.4	0.16	6.4	7.7
SFN	1.3	0.16	6.3	7.5
SFO	1.7	0.20	6.5	7.5
SFS	1.8	0.13	5.5	7.0
SFV	3.0	0.12	5.1	7.1
SFW	1.0	0.16	3.3	7.1

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
SGT	1.8	0.12	1.7	7.2
SIV	1.0	0.06	3.3	5.0
SOD	1.0	0.04	2.1	5.8
SOF	1.5	0.10	3.8	4.7
SOS	2.0	0.09	3.8	4.4
SSF	1.3	0.14	5.8	7.3
SSY	1.3	0.13	5.5	6.9
STF	1.7	0.13	5.0	7.2
STI	1.5	0.11	4.5	5.8
STO	1.5	0.07	5.6	6.4
STT	1.7	0.11	3.7	6.6
STW	1.5	0.11	4.5	4.9
SVV	1.3	0.04	1.5	6.0
SZR	2.0	0.10	4.3	5.6
TER	1.5	0.08	4.7	6.2
THO	2.3	0.13	3.3	4.5
TOL	1.0	0.02	1.9	5.6
TON	1.4	0.07	4.6	5.0
TSC	1.0	0.29	3.7	15.9
TUN	2.0	0.10	5.0	8.0
UEI	1.0	0.04	3.4	5.1
UFI	1.7	0.20	3.5	9.7
UOS	2.0	0.08	3.8	5.3

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Table S7 – continued from previous page

Name	**Si/Al ratio**	ϕ_{He}	**PLD** / [Å]	**LCD** / [Å]
UOV	1.8	0.17	5.8	6.6
UOZ	1.0	0.01	0.8	4.9
USI	1.0	0.12	5.8	6.3
UTL	1.8	0.20	7.1	8.7
UWY	1.6	0.14	5.6	8.4
VET	1.4	0.05	5.6	6.0
VFI	1.0	0.25	11.0	11.4
VNI	1.9	0.05	2.6	4.4
VSV	2.3	0.09	3.4	3.7
WEI	1.5	0.07	3.0	3.8
YUG	1.7	0.05	2.7	4.0
ZON	1.7	0.05	3.1	5.2

References

(S1) Martin-Calvo, A.; Parra, J. B.; Ania, C. O.; Calero, S. Insights on the Anomalous Adsorption of Carbon Dioxide in LTA Zeolites. *Journal of Physical Chemistry C* **2014**, *118*, 25460–25467.

(S2) Rick, S. W. A reoptimization of the five-site water potential (TIP5P) for use with Ewald sums. *Journal of Chemical Physics* **2004**, *120*, 6085–6093.

(S3) Deeg, K. S.; Gutiérrez-Sevillano, J. J.; Bueno-Pérez, R.; Parra, J. B.; Ania, C. O.; Doblaré, M.; Calero, S. Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. *Journal of Physical Chemistry C* **2013**, *117*, 14374–14380.

(S4) Castillo, J. M.; Silvestre-Albero, J.; Rodriguez-Reinoso, F.; Vlugt, T. J. H.; Calero, S. Water adsorption in hydrophilic zeolites: experiment and simulation. *Physical Chemistry Chemical Physics.* **2013**, *15*, 17374–17382.

(S5) Hens, R.; Rahbari, A.; Caro-Ortiz, S.; Dawass, N.; Erdős, M.; Poursaeidesfahani, A.; Salehi, H. S.; Celebi, A. T.; Ramdin, M.; Moultos, O. A.; Dubbeldam, D.; Vlugt, T. J. H. BRICK-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method. *Journal of Chemical Information and Modeling* **2020**, *60*, 2678–2682.

(S6) Rahbari, A.; Hens, R.; Ramdin, M.; Moultos, O. A.; Dubbeldam, D.; Vlugt, T. J. H. Recent advances in the continuous fractional component Monte Carlo methodology. *Molecular Simulation* **2020**, In Press, DOI: 10.1080/08927022.2020.1828585.

(S7) Lemmon, E. W.; Huber, M. L.; McLinden, M. O. NIST reference fluid thermodynamic and transport properties - REFPROP. *NIST standard reference database* **2002**, *23*, v7.