Supplementary Info

Post-synthetically treated ERI and SSZ-13 zeolites modified with copper as catalysts for NH_3-SCR-DeNO$_x$

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1. Experimental

1.1 Catalyst characterization

X-ray diffraction (XRD) patterns were captured using a HUBER G670 diffractometer (Rimsting, Germany). Cu-Kα radiation with a wavelength of 0.154 nm was utilized for the measurements. The samples underwent scanning within a diffraction angle range of 2θ spanning from 5° to 60°, with intervals of 0.005°.

Solid-state nuclear magnetic resonance (NMR) spectra were acquired using a Bruker Avance 750 spectrometer (Rheinstetten, Germany). The magnetic field strength was 17.6 T. Spectra were recorded at frequencies of 195.06 MHz for ^{27}Al and 148.67 MHz for ^{29}Si. The ^{27}Al experiments were conducted with a spinning frequency of 7 kHz and a recycle delay of 0.1 s. A pulse lasting 1 µs was employed, which corresponds to an approximate pulse angle of 30 °. For obtaining ^{29}Si spectra, direct excitation was employed, involving a 2.5 µs 90 ° pulse, a recycle delay of 10 s, and a spinning frequency of 7 kHz. Spectra were referenced using a 1 M $Al(NO_3)_3$ solution and TMS for ^{27}Al and ^{29}Si, respectively. Analysis of NMR spectra is done with the dmfit program. In all cases, Gaussian lines were employed to deconvolute the NMR spectra. In specific instances, the deconvolution of ^{27}Al spectra exhibited enhancement through the utilization of a chemical shift distribution employing the Czjzek model in dmfit [1], predominantly for the four-coordinated aluminum sites.

Nitrogen sorption isotherms were acquired at -196 °C employing a MicrotracBEL Corp. BELSORP-miniX instrument (Haan/Duesseldorf, Germany). Prior to measurement, ca. 0.1-0.2 g of the sample was subjected to activation at 250 °C and 1 Pa. The total pore volume was determined from the point where $p\ p_0^{-1} = 0.99$. The specific surface area was calculated using the Brunauer-Emmett-Teller (BET) method and the pore width distribution was derived from the adsorption branch of the nitrogen sorption isotherm

using the Barret-Joyner-Halenda (BJH) method. The micropore volume and specific surface area of micropores were determined utilizing the Harkins and Jura model through t-plot analysis.

Quantitative analysis of Al, Si, or Cu content within the samples was accomplished through inductively coupled plasma optical emission spectroscopy (ICP-OES) utilizing a Perkin Elmer Optima 8000 instrument (Rodgau, Germany). The samples (ca. 0.02 g) were dissolved in a mixture of HF (2 ml, 47-51 wt.-%, Sigma-Aldrich), HNO_3 (3 ml, 69 wt.-%, Sigma-Aldrich), and HCl (3 ml, 35 wt.-%, Sigma-Aldrich). The mixture was subjected to microwave radiation for 1 h at 200 °C. Prior to measurement, HF was eliminated by forming complexes with H_3BO_3 (12 ml, 99.99 wt.-%, Sigma-Aldrich) using microwave radiation for 5 min at 200 °C.

Temperature-programmed desorption of NH_3 (NH_3-TPD) profiles were acquired using a QMS MKS Cirrus 3 (Munich, Germany). Prior to the measurements, the sample (ca. 0.1 g) was pre-treated in a flow of pure helium (50 ml min^{-1}) at 500 °C for 0.5 h. After cooling down to 100 °C, the sample was saturated in a flow of 0.3 vol.-% NH_3 diluted in helium (50 ml min^{-1}) for 2 h. Afterwards, the sample was purged in a pure He for 3 h. NH_3 desorption was performed in a flow of pure helium up to 500 °C (heating rate of 10 °C min^{-1}, a total flow rate of 50 ml min^{-1}).

Temperature-programmed reduction of H_2 (H_2-TPR) profiles were acquired using a MicrotracBEL Corp., BelCat II (Osaka, Japan). Prior to measurements, the sample (ca. 0.05 g) was heated from room temperature to 300 °C (heating rate of 10 °C min^{-1}, 20 vol.-% O_2 diluted in Ar, total flow of 30 ml min^{-1}). The temperature was maintained at a constant level for 0.5 h. Afterward, the sample was cooled to 100 °C (pure Ar with a total flow of 20 ml min^{-1}). Then the sample was reduced with 5 vol.-% H_2 diluted in Ar in the temperature range between 100 to 800 °C (heating rate of 10 °C min^{-1}, a total flow rate

of 30 ml min^{-1}). A thermal conductivity detector (TCD) was employed to measure the H_2 consumption. After every experiment, a pulse calibration of the TCD was conducted. The H_2-TPR profiles were further analyzed through deconvolution using a Gaussian function, accomplished using the program OriginPro 9.1.

Diffuse reflectance UV-Vis (DR UV-Vis) spectra of the samples were recorded at room temperature with a Perkin Elmer Lambda 650S UV-Vis spectrometer (Rodgau, Germany). As a reference material spectralon® (PTFE, reflective value 99 %, Rodgau, Germany) was used. The experiments were conducted within the wavelength range of 200-850 nm, employing a step width of 1 nm and a slit width of 2 nm.

X-ray absorption spectroscopy (XAS) measurements were performed at the SuperXAS beamline, Swiss Light Source (SLS) of the Paul Scherrer Institute (Villigen, Switzerland). The incident photon beam from the storage ring was collimated by a Si-coated mirror and subsequently monochromatized by a liquid-cooled Si(111) channel-cut quick scanning monochromator. The measurement was conducted using a QEXAFS (Quick extended X-ray absorption fine structure) mode, which allowed for rapid collection of Cu K-edge XAS spectra in transmission mode (300 sec per sample). Copper-containing zeolites were prepared as pellets with a diameter of 10 mm, using optimal amounts for transmission measurements homogeneously mixed with cellulose. Cu foil spectra were collected simultaneously for internal energy calibration (edge energy, E_0 = 8979 eV). The obtained raw data underwent pre-processing using the ProQEXAFS software (Villigen, Switzerland) developed in-house. Standard XAS data reduction steps (i.e., subtraction of pre-edge and post-edge backgrounds, determination of the edge energy, and normalization of the data set to an edge jump of 1) were executed using the Athena software of the Demeter 0.9.26 package. The Fourier-transformed k^2-weighted EXAFS (extended X-ray absorption fine structure) spectra were prepared in the k range 0.31-1.21 nm^{-1}. The data presented have not undergone phase correction.

Electron paramagnetic resonance (EPR) measurements were conducted using a Bruker EMX micro spectrometer (X-band, 9.4 GHz, Rheinstetten, Germany) equipped with an ER 4119 HS resonator. Measurements at -196 °C were carried out using an Oxford Instruments He cryostat ESR 900 (Abingdon, UK). Spectral simulations were conducted using the EasySpin MATLAB simulation package (The Mathworks, Natick, MA, USA). The microwave power was adjusted to prevent any distortion in the line shape, and the modulation amplitude was set to 1 mT to prevent modulation broadening. Powder samples (ca. 0.03 g) were placed within an EPR quartz glass tube with an inner diameter of 3.8 mm and subsequently sealed directly. The activation procedure was conducted at 300 °C for a duration of 1 h under vacuum (10^{-4} – 10^{-5} Pa) for all samples.

The temperature-programmed isotopic exchange (TPIE) experiment was carried out in the Microactivity Reference unit (PID Eng & Tech, Madrid, Spain) equipped with a fixed-bed quartz reactor (ID: 8 mm, L: 340 mm) and using a QMS spectrometer (HPR-20 R&D, Hiden Analytical, Warrington, U.K.). Around 0.05 g of the sample was used for the tests, which was heated from room temperature up to 800 °C at the rate of 10 °C min^{-1}. The reaction mixture consisted of $c(^{18}O_2)$ = 3 vol.-%, c(Ar) = 5 vol.-% diluted in He with a total rate of 100 ml min^{-1}.

1.2 Catalytic experiments

The catalytic experiments were conducted within a house made fixed-bed quartz tube reactor (inner diameter (ID): 6 mm, length (L): 200 mm). Prior to the experiment, the catalyst (0.1 g, sieve fraction of 200-400 µm) was activated at 350 °C for 1.5 h under a flow of pure He (50 ml min^{-1}), and then cooled down to 50 °C. Following the aforementioned step, a simulated flue gas was introduced into the system. The flue gas, with a total flow rate of 120 ml min^{-1}, consisted of concentrations of c(NO) = 0.05 vol.-%, $c(NH_3)$ = 0.0575 vol.-%, $c(O_2)$ = 4 vol.-% and $c(H_2O)$ = 5 vol.-% diluted in He. The gas

hourly space velocity (GHSV) was set to be 30,000 h^{-1}. The reaction was conducted under atmospheric pressure and over a temperature range from 75 °C to 500 °C with an interval of 25-50 °C. At each temperature, the reaction was allowed to stabilize for a duration of 70-90 min. The gas leaving the reactor was purified by passing it through a gas-washing bottle filled with concentrated phosphoric acid. Analysis of the NO was performed using CLD 70 S Chemiluminescence Analyzer (Tutzing, Germany). The conversion of NO (X(NO)) was calculated according to the equation $X(NO) = ([c(NO)_{in}-c(NO)_{out}]/c(NO)_{in})\times100\%$, where: $c(NO)_{in}$ and $c(NO)_{out}$ - concentration of NO in the inlet and the outlet gas, respectively. The calculated conversion's experimental uncertainty was determined to be ±2 %, which was confirmed through repeated measurements of identical catalysts.

Comparative studies were achieved using a QMS MKS Cirrus 3 (Munich, Germany) mass spectrometer directly connected to the reactor outlet using a heated capillary. The pre-treatment of the materials was performed as above, only the composition of the gas mixture at the reactor inlet consisted of c(NO) = 0.1 vol.-%, $c(NH_3)$ = 0.1 vol.-%, $c(O_2)$ = 10 vol.-% diluted in He. The individual flow rates were controlled by Bronkhorst mass flow controllers (Veenendaal, The Netherlands). The total flow rate of the reaction mixture was 120 ml min^{-1}, while the GHSV was about 30,000 h^{-1}. The signal of the helium line served as the internal standard to compensate for small fluctuations in the operating pressure.

The conversion of NH_3 ($X(NH_3)$) was calculated using the following equation: $X(NH_3) = ([c(NH_3)_{in}-c(NH_3)_{out}]/c(NH_3)_{in})\times100\%$, where: $c(NH_3)_{in}$ and $c(NH_3)_{out}$ - concentration of NH_3 in the inlet and the outlet gas, respectively. In the NH_3-SCR-DeNO$_x$ and NH_3-SCO, only N_2 was detected among N-containing products.

The turnover frequency (TOF) values for NH_3-SCR-DeNO$_x$ were calculated by the following equation: TOF (s^{-1}) = $(c(NO)\times X(NO)\times F)/(m/m_W)$, where c(NO), X(NO) and F are

concentration of NO (mol ml^{-1}), NO conversion (%), volumetric flow rate (ml s^{-1}), respectively. Also, m and m_W are the copper loading (g) on the catalyst and the molecular weight (63.54 g mol^{-1}) of copper, respectively.

The standard NH_3-SCR-$DeNO_x$ reaction on Cu-containing zeolites can be considered as a first-order reaction with respect to NO. According to the first-order power-law equation: $-R_{SCR} = k_a \times c(NO)$, in which, k_a (ml g^{-1} s^{-1}) represents the apparent rate constant. The correlation between k_a and NO conversion (X(NO)) is expressed as follows: $k_a = -(F/(c(NO) \times W)) \ln(1-X(NO))$ where, F (mol s^{-1}) is the molar NO feed rate, c(NO) (mol ml^{-1}) is the concentration of NO, W (g) is the catalyst amount and X(NO) is NO conversion (%). The apparent activation energy (E_a) was calculated from the slope of linear regression derived from the Arrhenius equation $k_a = A \cdot \exp(-E_a R^{-1}T^{-1})$. To minimize the influence of heat generated from the exothermic reaction as well as the mass transfer issue, the measurements and following calculations were performed for data points with conversion lower than 25 % (in the three-point linear regression model).

1.3 *In situ* investigations

The FT-IR spectra were recorded with an Invenio-X spectrometer (integrated with MCT detector; Ettlingen, Germany) with a spectral resolution 2 cm^{-1}. Before conducting measurements, all samples were prepared in the shape of self-supporting discs (ca. 5 mg^{-1} cm^2) and subjected to *in situ* treatment within a custom-made quartz IR cell. This treatment occurred at 350 °C under high vacuum (10^{-5} mbar) for a duration of 1 h. Following the cooling process to 125 °C, the catalysts were exposed to a mixture consisting of NH_3, NO, O_2, and H_2O ($c(NH_3)$:c(NO):$c(O_2)$:$c(H_2O)$ = 4:4:1:8). Spectra were gathered over the subsequent 60 min reaction period, with a frequency of one spectrum acquired every 30 s during the course of the reaction. The plots were generated using

the OPUS 3D software from Bruker Optics (Ettlingen, Germany) and OriginPro9.1 (OriginLab Corp., Northampton, MA, USA).

For an *in situ* DR UV-Vis, a 0.1 g sample (sieve fraction of 150-300 µm), was placed in a quartz tube reactor (ID: 4 mm, L: 30 cm, with a height of the catalytic bed of 2 cm). The same reaction condition was applied as in the catalytic experiments described above. Prior to measurements, the catalyst was heated to 300 °C in pure He flow for 0.5 h. Subsequently, the reactor was cooled down to 75 °C, and the reaction mixture was introduced. The reactor was then gradually heated up to 500 °C, with temperature intervals of 25-50 °C. During each step, the temperature was maintained for 0.5 h while continuously monitoring the composition of the product gas using a Pfeiffer OmniSTAR GDS320 mass spectrometer (Asslar, Germany). DR UV-Vis spectra were gathered throughout the entirety of the experiment using an Avantes AvaSpec-ULS2048XL-EVO (Apeldoorn, The Nehterlands) spectrometer using a Avantes AvaLight-DH-S light source (including both a deuterium and halogen lamp). A custom-made reflection probe optical fiber with a high-OH fused silica core (diameter of 100 µm) was used for light collection, using polytetrafluoroethylene powder in a separate reactor as standard for 100 % reflectance. Spectra were captured at intervals of 60 s during the course of the reaction.

2. Results

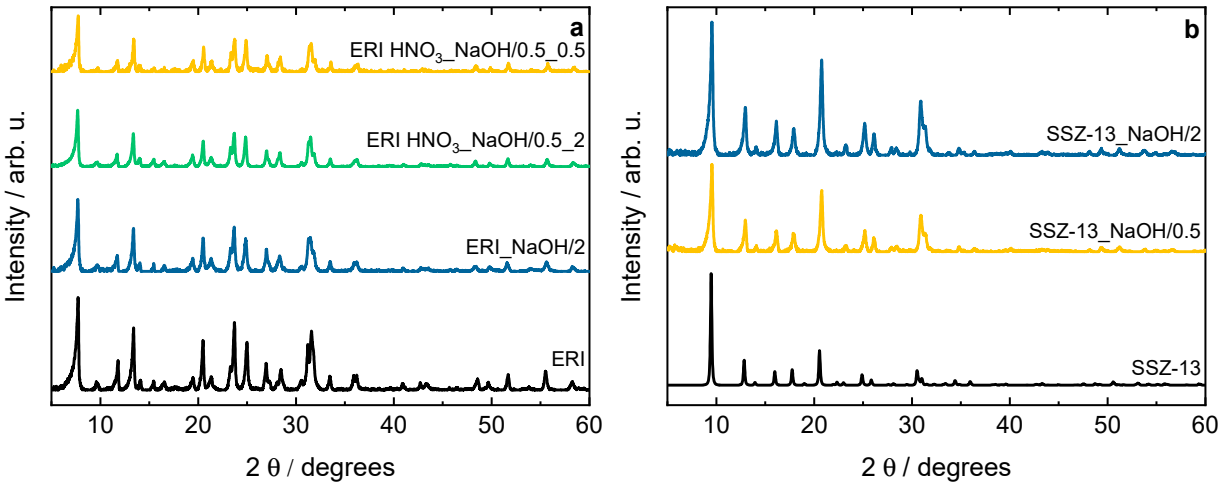


Figure S1: XRD patterns of the parent and post-modified form of a) ERI and b) SSZ-13 samples.

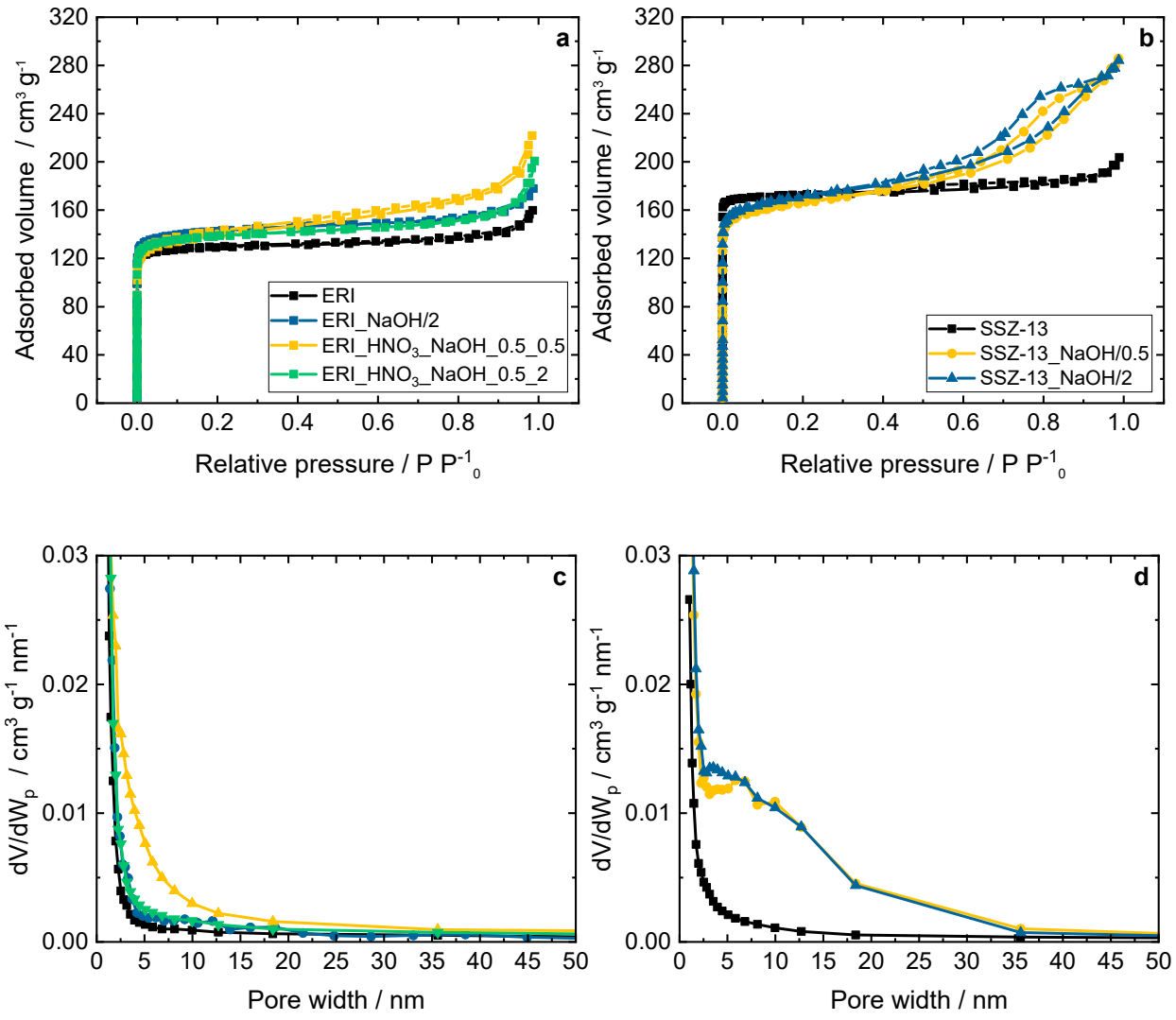
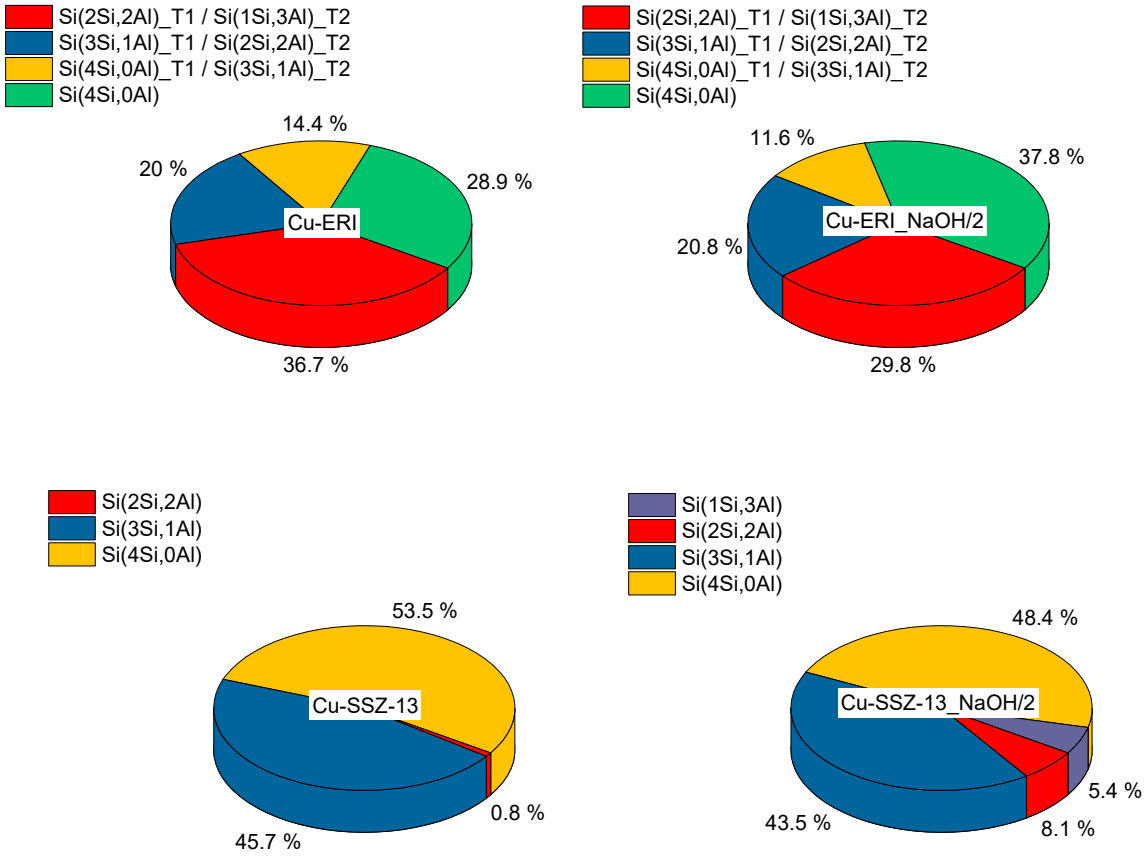


Figure S2: a,b) N_2 sorption isotherms collected at -196 °C and c,d) BJH pore width distribution of ERI, SSZ-13 samples; a,c) and b,d) sample labels are identical.

Table S1: The results of the textural properties of the parent and post-modified form of ERI, SSZ-13 samples: specific surface area ($A_{s(BET)}$), micropore pore volume ($V_{(MIC)}$), mesopore pore volume ($V_{(MES)}$), total pore volume ($V_{(TOT)}$) and average pore width (d_{Wp}).

Sample	$A_{s(BET)}$ / $m^2\,g^{-1}$	$V_{(MIC)}$ / $cm^3\,g^{-1}$	$V_{(MES)}$ / $cm^3\,g^{-1}$	$V_{(TOT)}$ / $cm^3\,g^{-1}$	d_{Wp} / nm
ERI	525	0.19	0.04	0.24	2.7
ERI_HNO_3_ NaOH/0.5_0.5	532	0.19	0.15	0.34	3.2
ERI_HNO_3_ NaOH/0.5_2	551	0.20	0.11	0.31	3.7
ERI_NaOH/2	568	0.21	0.04	0.28	2.7
SSZ-13	716	0.26	0.06	0.32	4.0
SSZ-13_NaOH/0.5	642	0.21	0.23	0.44	5.0
SSZ-13_NaOH/2	660	0.19	0.25	0.44	4.5

a



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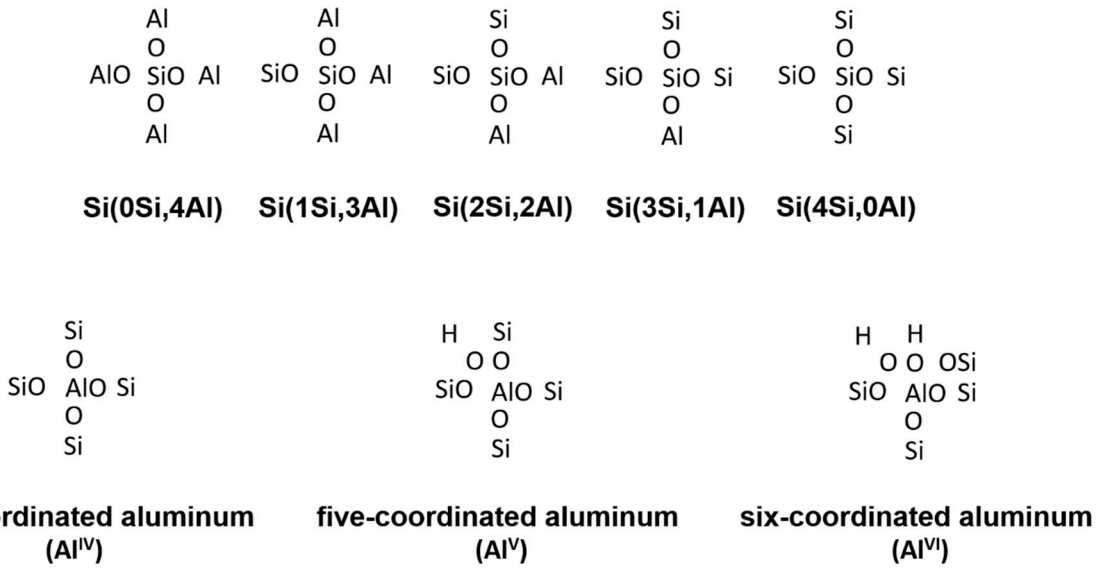

Figure S3: a) Contribution of different Si coordination to the area of the ^{29}Si NMR spectra of Cu-containing ERI and SSZ-13 samples and b) a schematic diagram of the coordination environment of Si and Al.

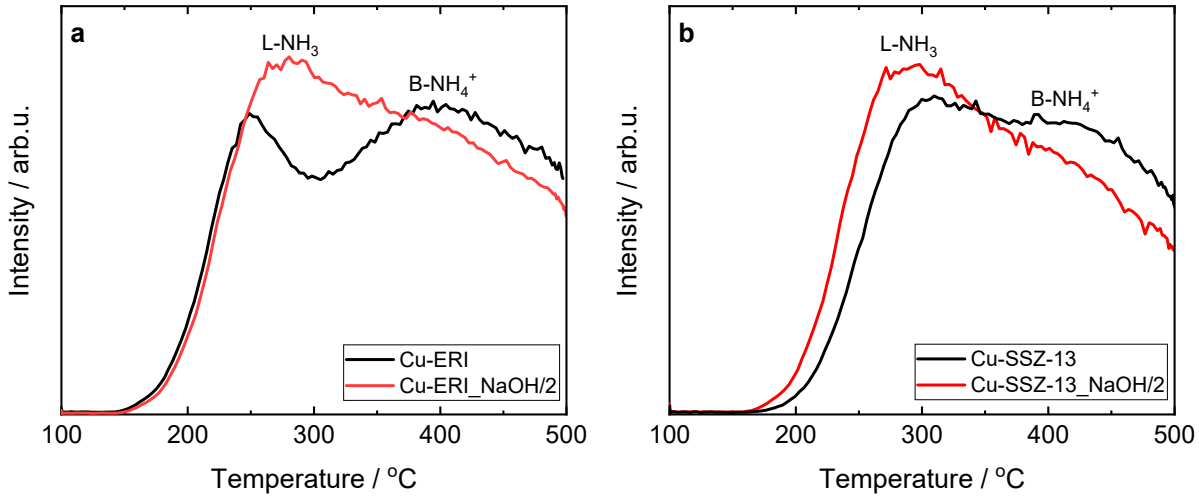

Figure S4: Results of the TPD-NH_3 over a) Cu-containing ERI and b) SSZ-13 samples.

Table S2: Deconvolution of the ^{29}Si MAS NMR spectra.

Sample	Assignment	Chemical shift / ppm (Rel. area / %)
Cu-ERI	Si(2Si,2Al)_T1 / Si(1Si,3Al)_T2	-98.8 (36.7)
	Si(3Si,1Al)_T1 / Si(2Si,2Al)_T2	-102.2 (20.0)
	Si(4Si,0Al)_T1 / Si(3Si,1Al)_T2	-106.9 (14.4)
	Si(4Si,0Al)_T2	-109.6 (28.9)
Cu-ERI_NaOH/2	Si(2Si,2Al)_T1 / Si(1Si,3Al)_T2	-98.8 (29.8)
	Si(3Si,1Al)_T1 / Si(2Si,2Al)_T2	-102.7 (20.8)
	Si(4Si,0Al)_T1 / Si(3Si,1Al)_T2	-107.4 (11.6)
	Si(4Si,0Al)_T2	-109.6 (37.8)
Cu-SSZ-13	Si(2Si,2Al)	-98.7 (0.8)
	Si(3Si,1Al)	-105.1 (45.7)
	Si(4Si,0Al)	-110.8 (53.5)
Cu-SSZ-13_NaOH/2	Si(1Si,3Al)	-93.9 (5.4)
	Si(2Si,2Al)	-99.0 (6.3)
	Si(3Si,1Al)	-104.9 (41.7)
	Si(4Si,0Al)	-110.5 (46.6)

T1, T2 – Si sites

Table S3: Deconvolution of the ^{27}Al MAS NMR spectra.

Sample	Assignment	Chemical shift / ppm (Rel. area / %)
Cu-ERI	Al^{IV}	62.8 (91.5)
	Al^{IV}	55.3 (7.1)
	Al^{V}	19.6 (1.4)
Cu-ERI_NaOH/2	Al^{IV}	62.1 (82.5)
	Al^{IV}	56.0 (8.3)
	Al^{V}	23.3 (5.1)
	Al^{VI}	1.4 (4.0)
Cu-SSZ-13	Al^{IV}	60.8 (96.9)
	Al^{VI}	0.3 (3.1)
Cu-SSZ-13_NaOH/2	Al^{IV}	61.0 (89.4)
	Al^{V}	37.4 (5.5)
	Al^{VI}	2.1 (5.1)

Al^{IV} – four-coordinated aluminum

Al^{V} – five-coordinated aluminum

Al^{VI} – six-coordinated aluminum

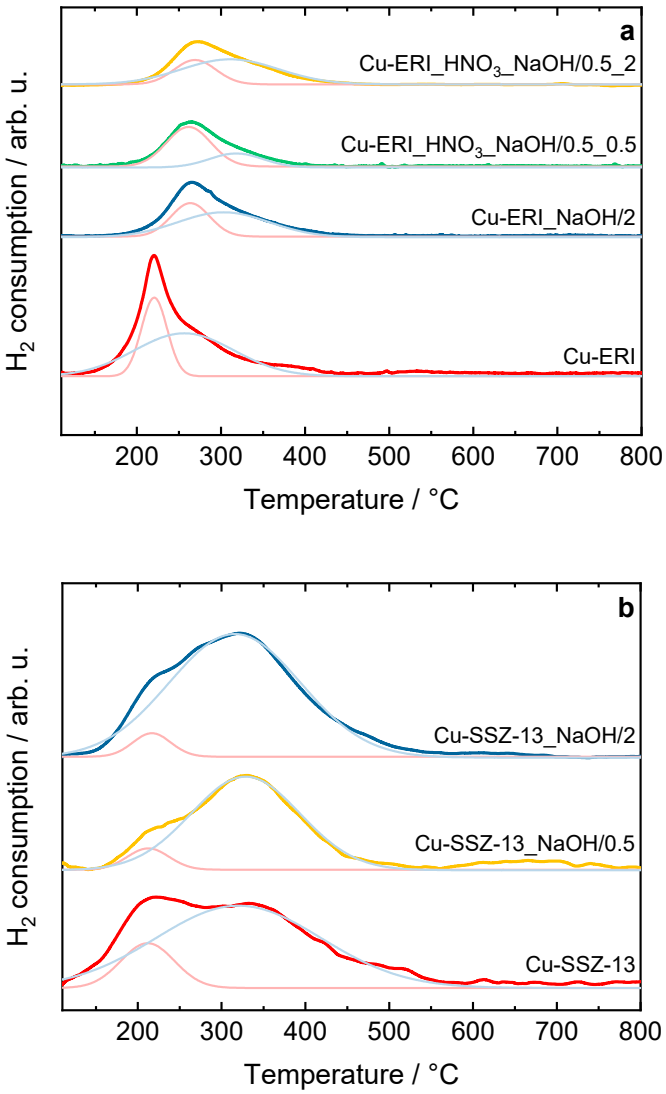

Figure S5: Deconvoluted H_2-TPR profiles of a) Cu-containing ERI and b) Cu-containing SSZ-13 samples.

Table S4: Contribution of the different peaks after deconvolution of H_2-TPR profiles.

Sample	Peak area / %	Peak area / %
Cu-ERI	23	77
Cu-ERI_HNO_3_ NaOH/0.5_0.5	63	37
Cu-ERI_HNO_3_ NaOH/0.5_2	32	68
Cu-ERI_NaOH/2	37	63
Cu-SSZ-13	19	81
Cu-SSZ-13_NaOH/0.5	13	87
Cu-SSZ-13_NaOH/2	8	92

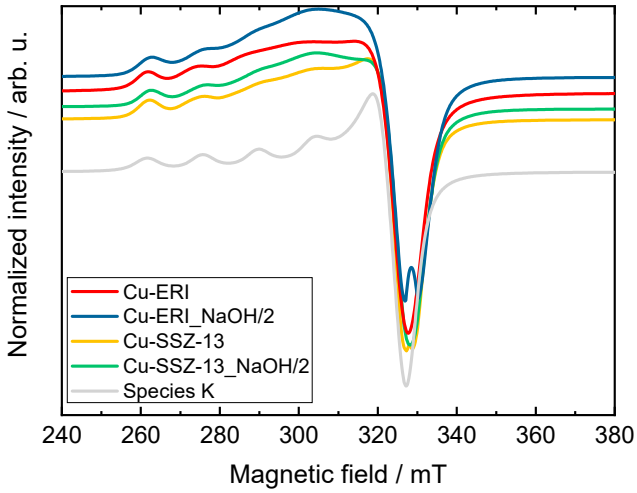

Figure S6: EPR spectra of the hydrated Cu-containing ERI and SSZ-13 samples recorded at -196 °C.

Table S5: Spin Hamiltonian parameters used for spectral simulation of Cu-containing zeolite samples before and after activation at 300 °C for 1 h under vacuum.

Cu species	$g_{xx,yy}$	g_{zz}	$A_{xx,yy}$ / MHz	A_{zz} / MHz	w_{pp} / mT	Assignment
K	2.070± 0.006	2.380 ± 0.006	30 ± 5	460 ± 5	3.0 ± 0.2	$[Cu(H_2O)_6]^{2+}$
L	2.070± 0.006	2.380 ± 0.006	30 ± 5	420 ± 5	3.0 ± 0.2	isolated Cu^{2+} (6MR in CHA cage)
M	2.070 ± 0.006	2.330 ± 0.006	30 ± 5	450 ± 5	3.0 ± 0.2	isolated Cu^{2+} (CHA cage)
N	2.070 ± 0.006	2.320 ± 0.006	30 ± 5	470 ± 5	3.0 ± 0.2	Cu^{2+} square pyramidal
O	2.070 ± 0.006	2.280 ± 0.006	30 ± 5	545 ± 5	3.0 ± 0.2	Cu^{2+} square planar
P	2.070 ± 0.006	2.390 ± 0.006	30 ± 5	390 ± 5	3.0 ± 0.2	isolated Cu^{2+} (octahedrally distorted)

Table S6: Composition in percentage for different Cu species in activated Cu-containing zeolite samples obtained from the spectral simulations using EasySpin [1].

Sample	L	M	N / %	O	P
Cu-ERI	0	0	10	0	90
Cu-ERI_ NaOH/2h	0	0	60	0	40
Cu-SSZ-13	60	40	0	0	0
Cu-SSZ-13_NaOH/2h	60	40	0	0	0

*The uncertainty of 5 % has been estimated during spectral simulation.

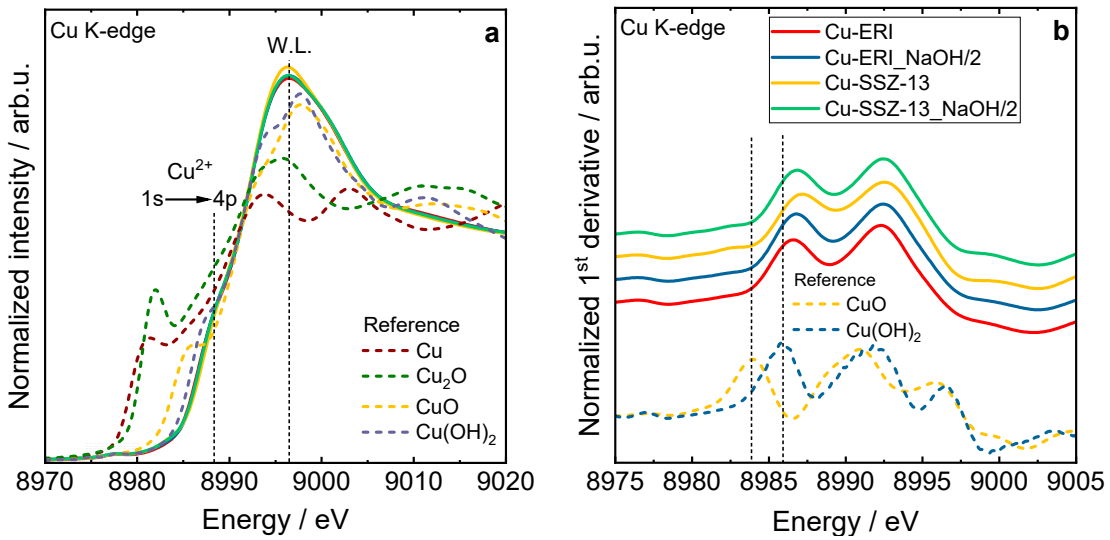

Figure S7: a,b) XANES spectra of Cu-containing zeolite samples with copper references, a) and b) sample labels are identical.

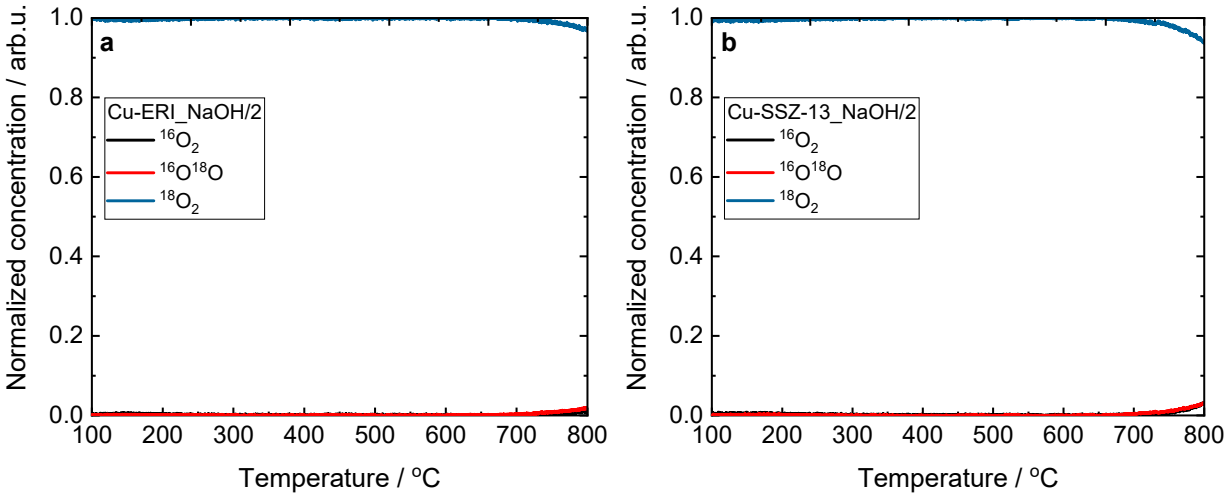

Figure S8: Results of the TPIE experiment obtained for a) Cu-ERI_NaOH/2 and b) Cu-SSZ-13_NaOH/2.

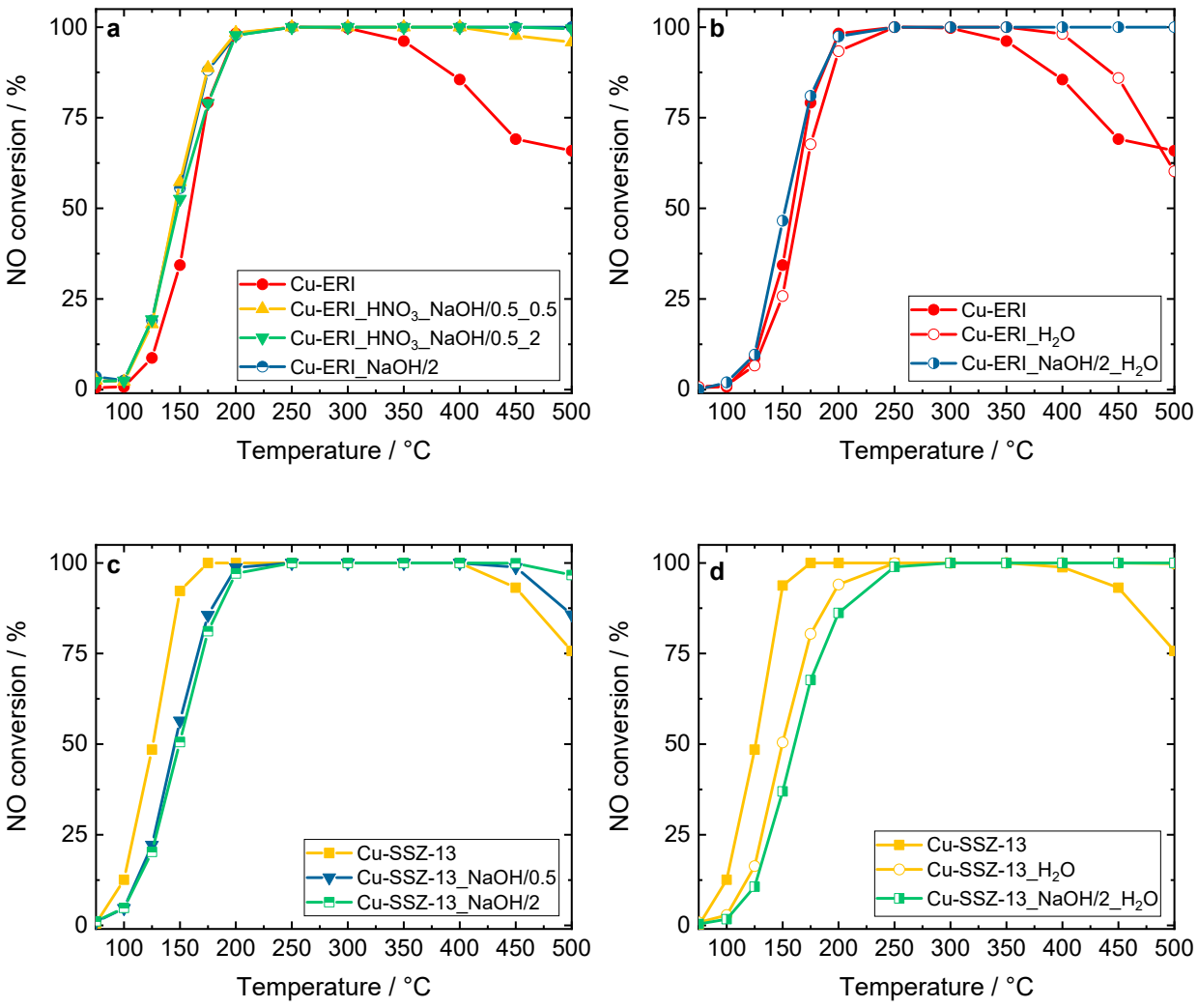

Figure S9: NO conversion of the Cu-containing ERI and SSZ-13 samples: a,c) without H_2O in the feed, b,d) in the presence of H_2O in the feed. Reaction conditions: m_K = 0.1 g, c(NO) = 0.05 vol.-%, c(NH_3) = 0.0575 vol.-%, c(O_2) = 4 vol.-%, (c(H_2O) = 5 vol.-% when used), He balance, F_{TOT} = 120 ml min^{-1}, GHSV = 30,000 h^{-1}.

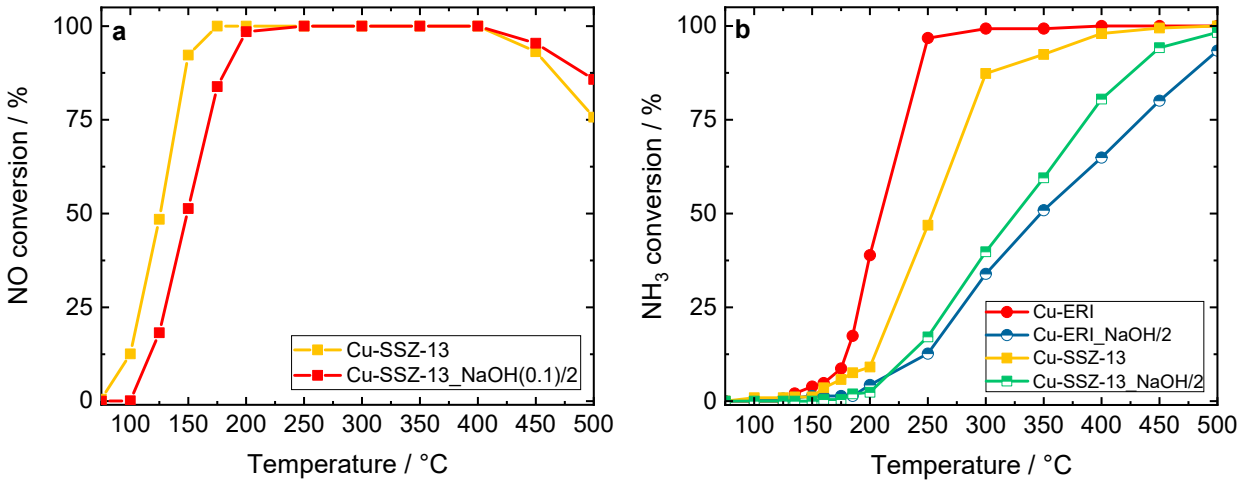

Figure S10: a) NO conversion of Cu-containing SSZ-13 sample (based on support modified with a 0.1 M NaOH solution) and b) NH_3 conversion*. Reaction conditions: m_K = 0.1 g, *c*(NO) = 0.05 vol.-%, *c*(NH_3) = 0.0575 vol.-%, *c*(O_2) = 4 vol.-%, (*c*(H_2O) = 5 vol.-% when used), He balance, F_{TOT} = 120 ml min^{-1}, GHSV = 30,000 h^{-1}. *Reaction conditions: m_K = 0.1 g, *c*(NH_3) = 0.1 vol.-%, *c*(O_2) = 10 vol.-%, He balance, F_{TOT} = 120 ml min^{-1}, GHSV = 30,000 h^{-1}.

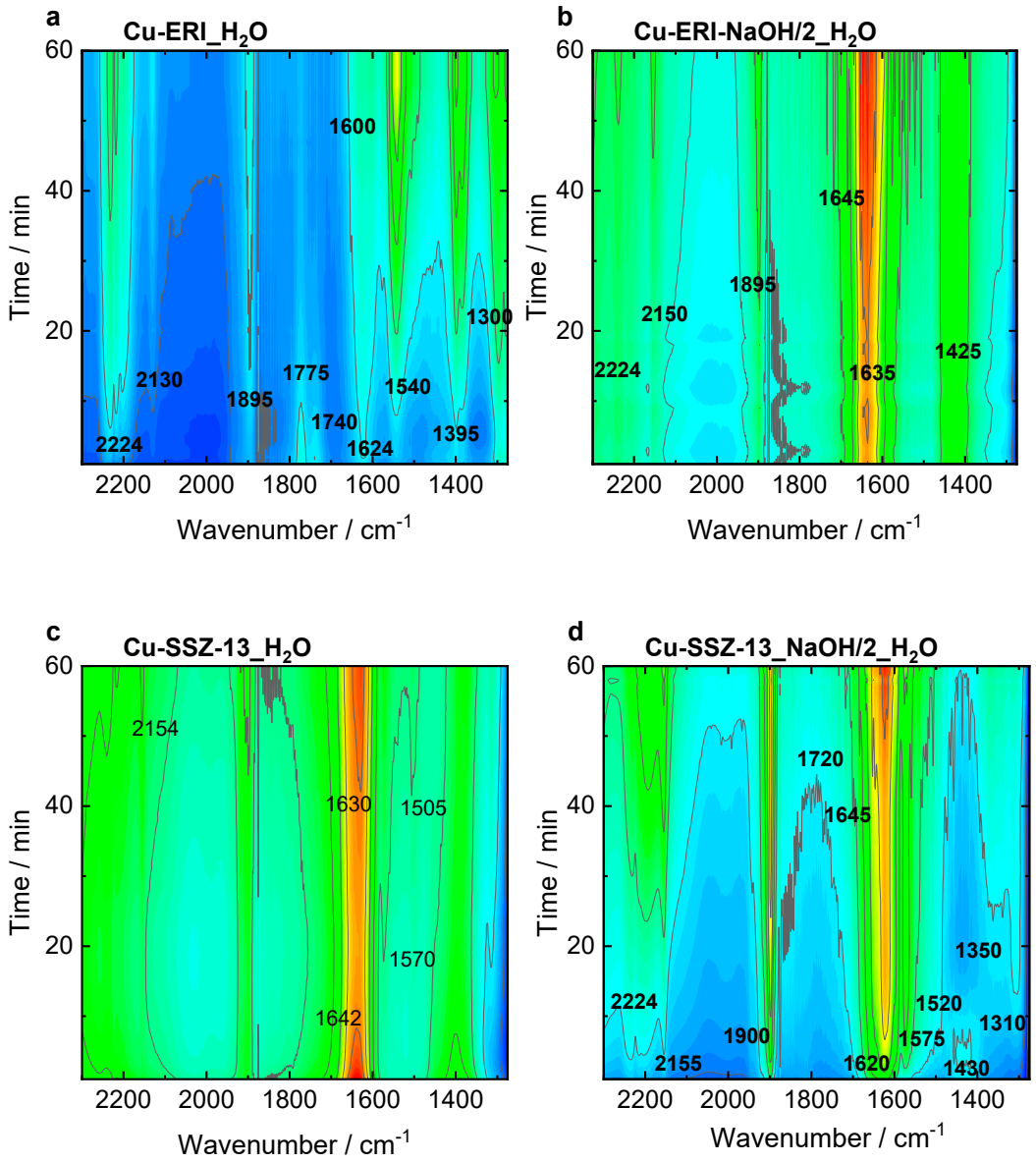

Figure S11: *In situ* FT-IR spectra of a,b) Cu-containing ERI and c,d) Cu-containing SSZ-13 samples, recorded during NH_3-SCR-DeNO$_x$ at 125 °C. Reaction conditions: m_K = 0.1 g, c(NO) = 0.1 vol.-%, c(NH_3) = 0.1 vol.-%, c(O_2)= 10 vol.-%, c(H_2O) = 5 vol.-%, He balance, F_{TOT} = 120 ml min^{-1}.

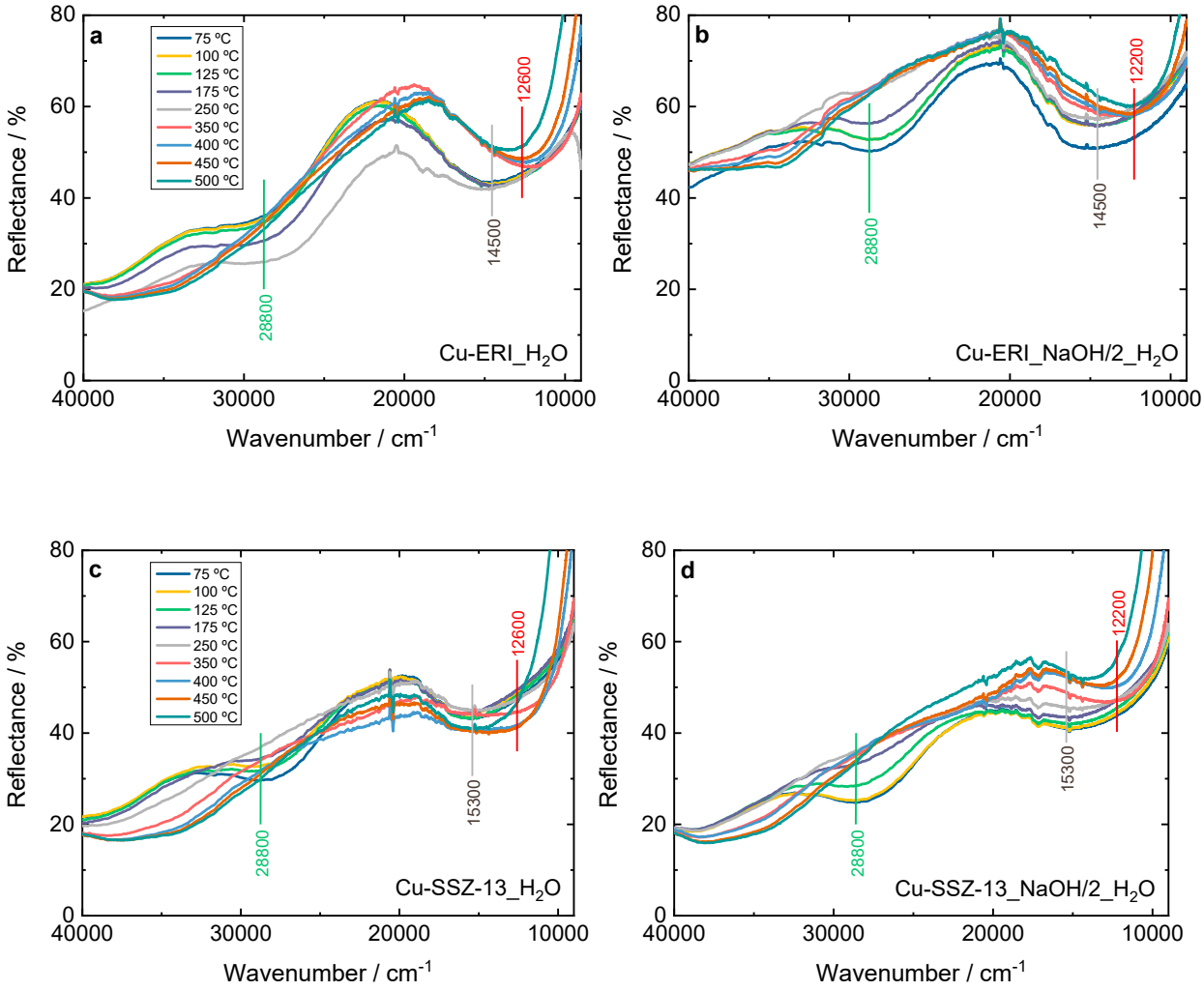

Figure S12: *In situ* DR UV-Vis DR spectrum of a,b) Cu-containing ERI and c,d) Cu-containing SSZ-13 samples during NH_3-SCR-DeNO$_x$ at different temperatures. Reaction conditions: m_K = 0.1 g, *c*(NO) = 0.1 vol.-%, *c*(NH_3) = 0.1 vol.-%, *c*(O_2)= 10 vol.-%, *c*(H_2O) = 5 vol.-%, He balance, F_{TOT} = 120 ml min^{-1}; a,b) and c,d) sample labels are identical.

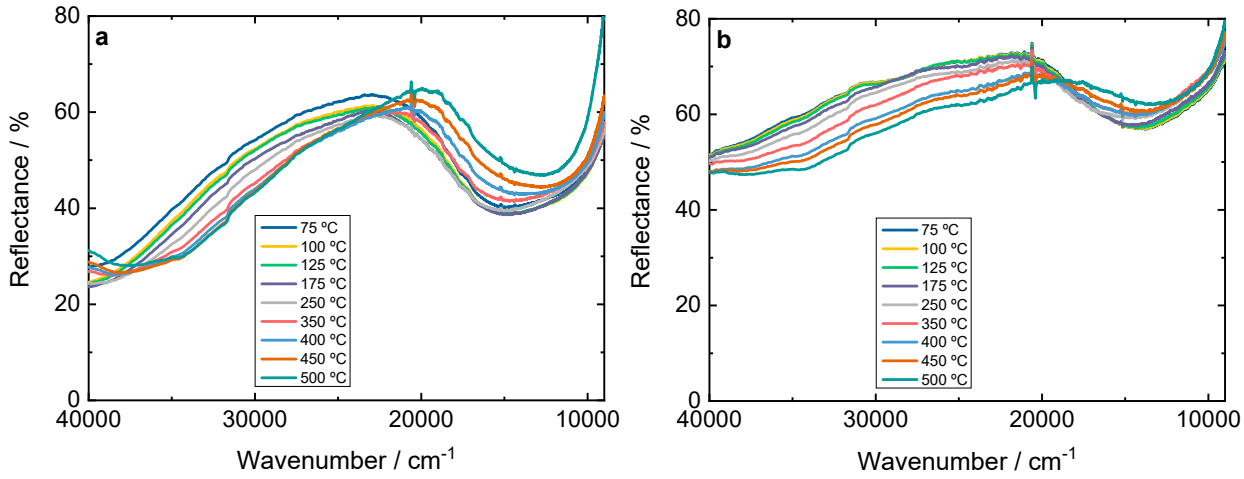

Figure S13: *In situ* DR UV-Vis spectrum of a) Cu-ERI_NaOH/2, and b) Cu-SSZ-13_NaOH/2 applied to the NH_3-SCO at different temperatures. Reaction conditions: m_K = 0.1 g, $c(NH_3)$ = 1000 ppm, $c(O_2)$= 10 vol.-%, He balance, F_{TOT} = 120 ml min^{-1}.