

## Supplementary Material

### Enhanced Hydrothermal Stability and SO<sub>2</sub>-tolerance of Cu–Fe Modified AEI Zeolite Catalysts in NH<sub>3</sub>-SCR of NO<sub>x</sub>

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#### 1. Characterization

The copper and iron contents in the Cu/Fe-AEI catalysts were determined by inductively coupled plasma atomic emission spectroscopy (ICP-AES, Optima 2000 DV, USA).

X-ray powder diffraction patterns (XRD) were obtained on an X-ray diffractometer (Rigaku D-Max Rotaflex, Japan) using Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ).

<sup>27</sup>Al MAS NMR spectra were acquired on the Agilent DD2-500 MHz spectrometer at 130.2 MHz using a 4 mm MAS NMR probe with a spinning rate of 14 kHz. Chemical shifts were referenced to 1% Al(NO<sub>3</sub>)<sub>3</sub> aqueous solution. The spectra were accumulated for 200 scans with  $\pi/12$  flip angle and 2 s pulse delay.

NH<sub>3</sub> temperature-programmed desorption (NH<sub>3</sub>-TPD) was carried out on a chemisorption analyzer (Finesorb-3010C, FINETEC Instruments, China). Before the measurements, the sample (50 mg) was pretreated in He stream at 400 °C and cooled down to the desired temperatures. NH<sub>3</sub> (500 ppm in N<sub>2</sub>, 30 mL/min) was introduced at 100 °C for 1 h, followed by He purging for 2 h, then the temperature was ramped from 100 to 700 °C at a rate of 10 °C/min.

H<sub>2</sub>-TPR experiments were conducted on a chemisorption analyzer (Finesorb-3010C, FINETEC Instruments, China). Typically, about 50 mg of catalyst sample was pretreated under pure argon (Ar) at 300 °C for 1 h and then cooled down to 30 °C. Then, the catalyst was heated to

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700 °C at 10 °C/min in a 5% H<sub>2</sub>/Ar at a flow rate of 50 mL/min.

The electron paramagnetic resonance (EPR) of the samples was recorded at -173 °C using a Bruker E500 spectrometer, where all the catalysts were placed in quartz tubes for the measurements.

In situ DRIFTS experiments were carried out in an environmental temperature chamber (PIKE Technologies), using a Thermo Fisher Nicolet iS10 spectrometer equipped with an MCT detector. All samples were dehydrated under a 10% O<sub>2</sub>/N<sub>2</sub> flow at 300 °C for 30 min, and then cooled to room temperature. After the background spectra were collected under pure N<sub>2</sub>, 500 ppm NO or NH<sub>3</sub> in N<sub>2</sub> was introduced. The spectra were collected in the wavenumber range of 4000–650 cm<sup>-1</sup> by accumulating 64 scans until stable. Nicolet OMNIC software was used to convert the absorbance data into Kubelka–Munk format.

The thermal gravimetric analysis (TGA) experiments were conducted using a SDT-Q600 analyzer (TA Instruments, USA). The sample (15 mg) was subjected to air at a flow rate of 100 mL/min, and the cycle was programmed with a temperature increase of 10 °C/min up to a maximum temperature of 850 °C.

UV-vis spectra were collected in the range of 190–800 nm on a JASCO V-550 spectrometer equipped with an integrating sphere coated with BaSO<sub>4</sub>.

## 2. Results

Table S1 The amount of ammonium sulfate obtained from TG results.

Sample	The amount of ammonium sulfate
Fe0.17-AEI	4%
Cu0.41-AEI	7%
Cu0.42/Fe0.16-AEI	3%

Table S2 H<sub>2</sub>-consumption of the regeneration catalysts obtained from Fig. S9.

Samples	H <sub>2</sub> -consumption (μmol/g)				
	CuO <sub>x</sub>	Z-CuOH <sup>+</sup>	Fe <sup>3+</sup> or Cu <sup>2+</sup> at 6MR	CuSO <sub>4</sub>	FeO <sub>x</sub>
Fe-AEI-Regenerated	0	0	5	0	17
Cu-AEI-Regenerated	3	15	18	23	0
Cu/Fe-AEI-Regenerated	10	43	44	19	19

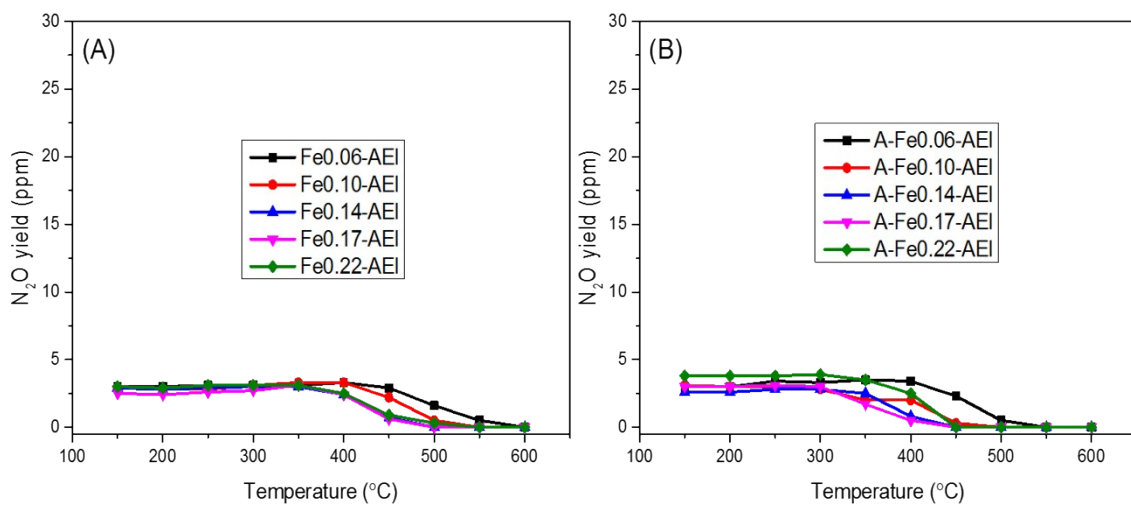


Fig. S1  $N_2O$  yield as a function of temperature on various Fe-AEI catalysts: (A) fresh and (B) hydrothermally aged. Reaction conditions: 500 ppm NO, 500 ppm  $NH_3$ , 10%  $O_2$ , 5%  $H_2O$ , and  $N_2$  balance; GHSV: 80000  $h^{-1}$ .

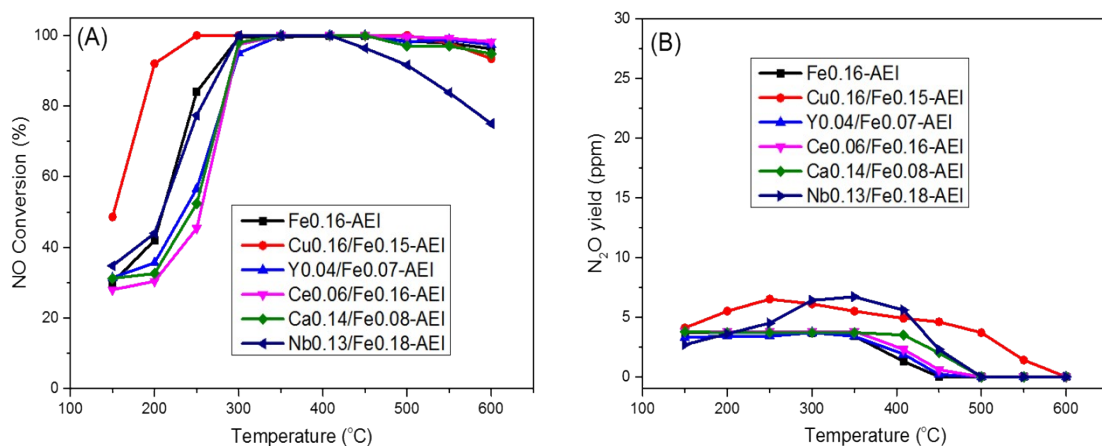


Fig. S2 NO conversion (A) and  $N_2O$  yield (B) as a function of temperature on Fe-AEI catalysts modified with various metal elements. Reaction conditions: 500 ppm NO, 500 ppm  $NH_3$ , 10%  $O_2$ , 5%  $H_2O$ , and  $N_2$  balance; GHSV: 80000  $h^{-1}$ .

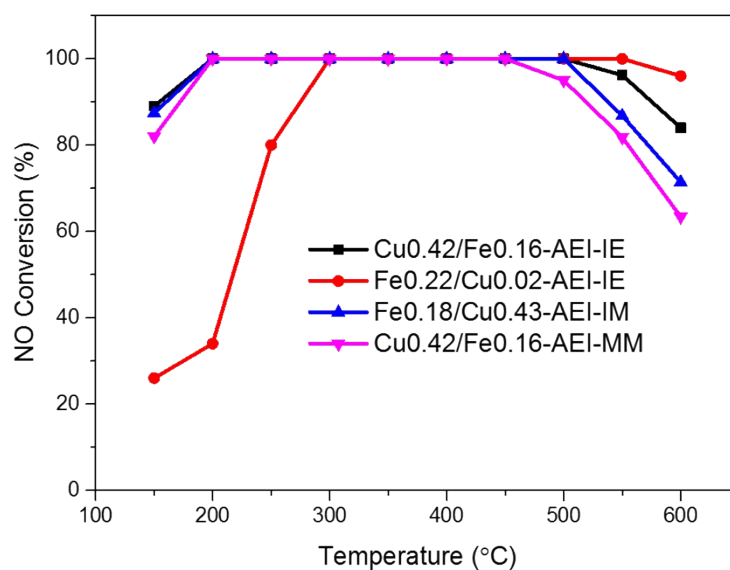


Fig. S3 NO conversion as a function of temperature on catalysts prepared by different methods. Reaction conditions: 500 ppm NO, 500 ppm NH<sub>3</sub>, 10% O<sub>2</sub>, 5% H<sub>2</sub>O, and N<sub>2</sub> balance; GHSV: 80000 h<sup>-1</sup>.

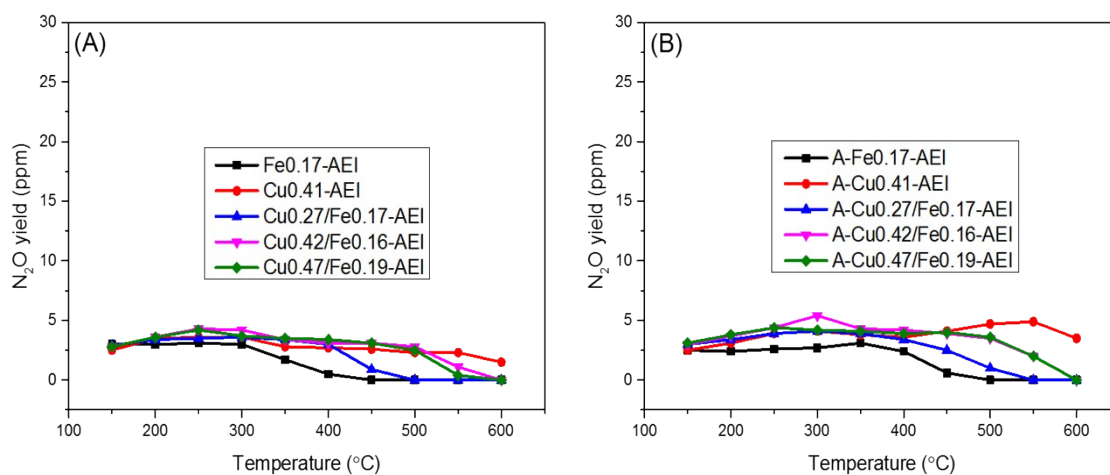


Fig. S4 N<sub>2</sub>O yield as a function of temperature on various Cu/Fe-AEI catalysts: (A) fresh and (B) hydrothermally aged. Reaction conditions: 500 ppm NO, 500 ppm NH<sub>3</sub>, 10% O<sub>2</sub>, 5% H<sub>2</sub>O, and N<sub>2</sub> balance; GHSV: 80000 h<sup>-1</sup>.

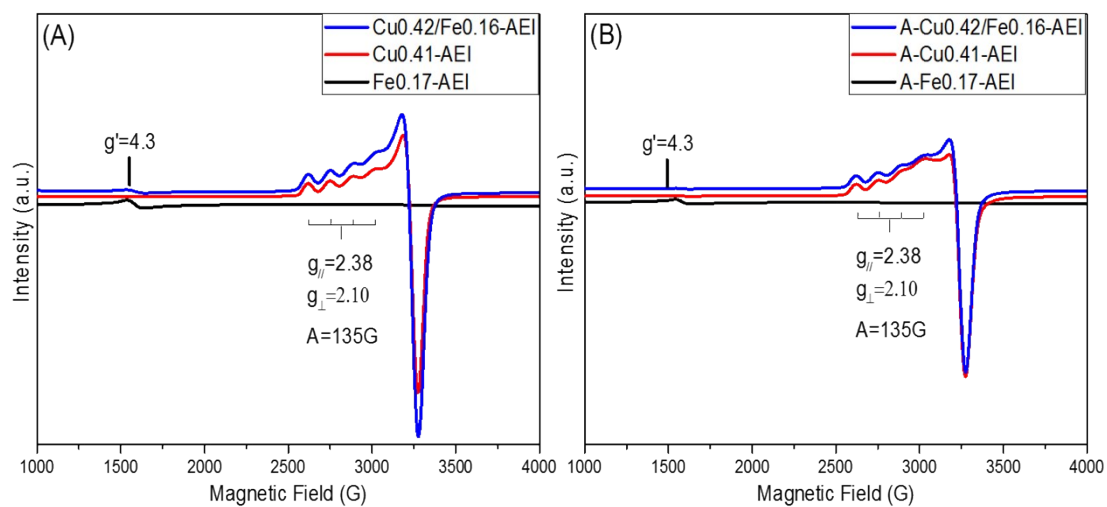


Fig. S5 EPR spectra of Fe-AEI, Cu-AEI and Cu /Fe-AEI catalysts at -173 °C: fresh (A) and hydrothermally aged (B)

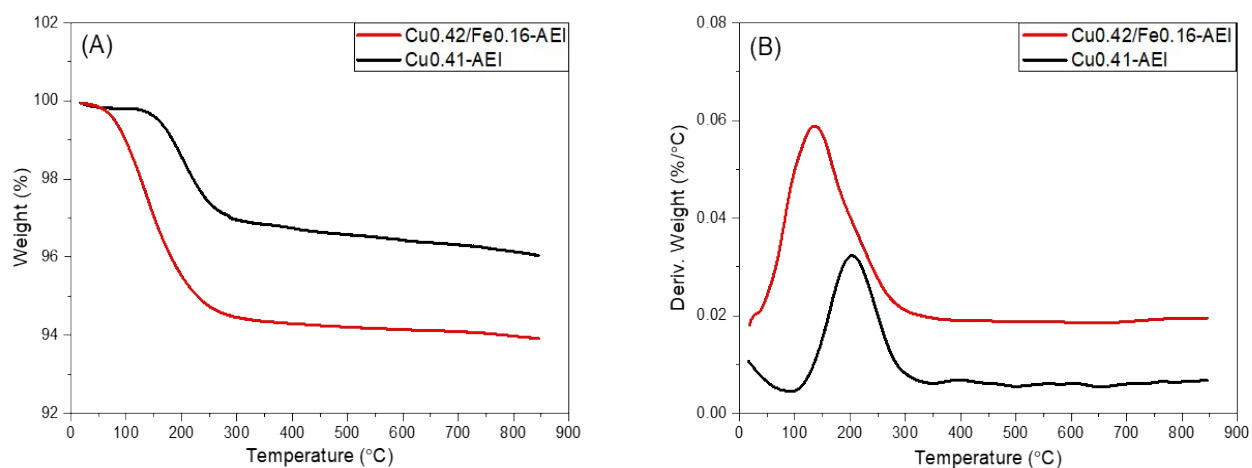


Fig. S6 TG (A) and DTG (B) profiles of regenerated catalysts after sulfur resistance tests.

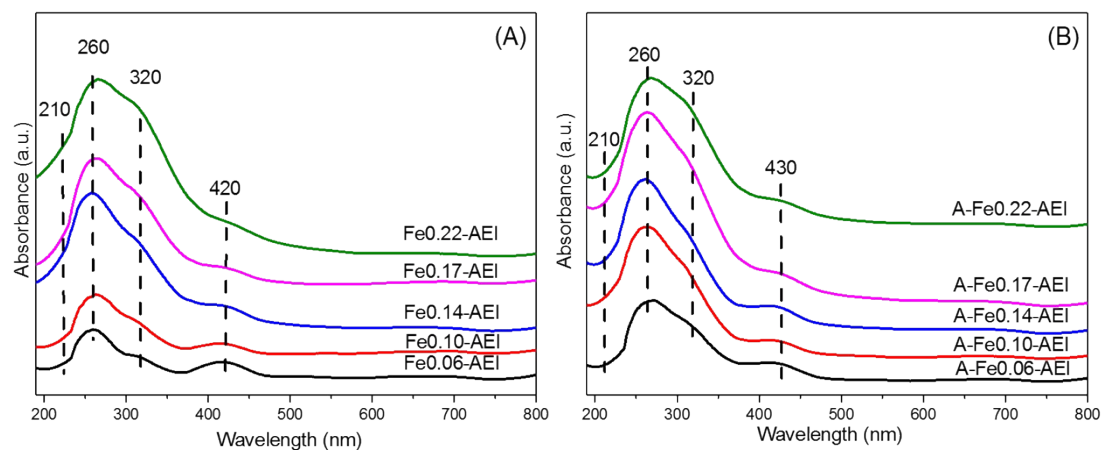


Fig. S7 UV-Vis spectra of Fe-AEI catalysts: fresh (A) and hydrothermally aged (B).

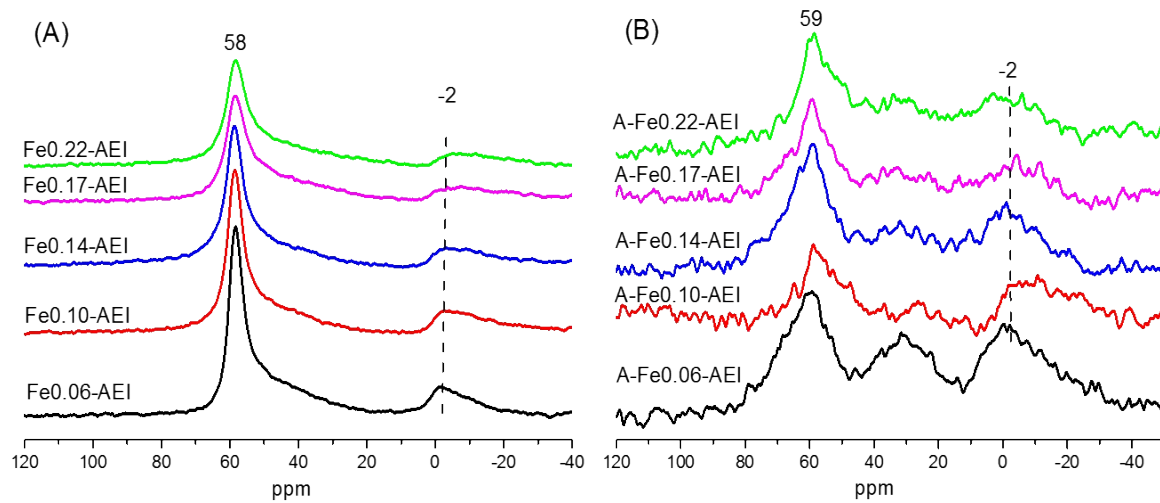


Fig. S8  $^{27}\text{Al}$  MAS NMR spectra of Fe-AEI catalysts: fresh (A) and hydrothermally aged (B).

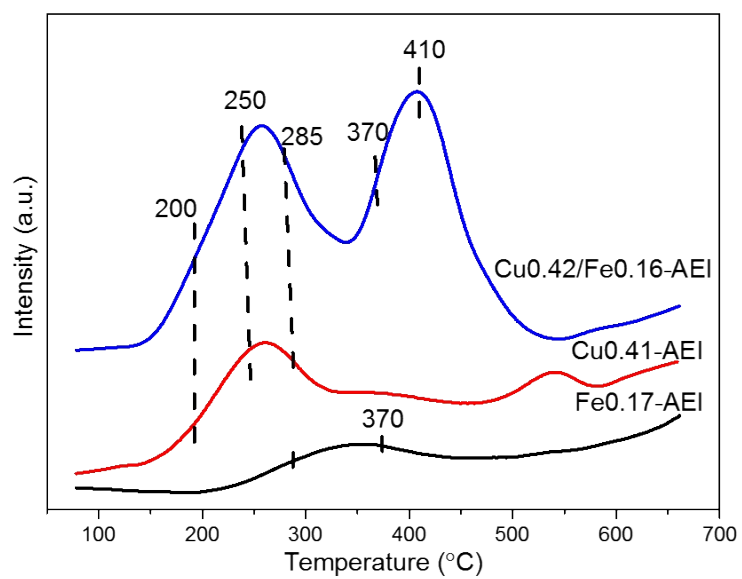


Fig. S9 H<sub>2</sub>-TPR profiles of the regenerated catalysts.