

Supporting information

The Role of Impregnated Sodium Ions in Cu/SSZ-13 NH₃-SCR Catalysts

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1. DRIFTS upon NH₃ desorption at different temperatures over fresh Cu/SSZ-13

Diffuse reflectance infrared Fourier transform spectra (DRIFTS) were measured on a Nicolet 6700 spectrometer. The pretreatment at 250 °C for 1 h was executed to remove the adsorbed water and clean the surface before the measurement. NH₃ chemisorption was operated at 100 °C in 500 ppm NH₃/N₂ (50 mL/min). After being saturated with NH₃, the flow was switched to N₂, and the sample was heated up to 600 °C at a rate of 10 °C /min in the N₂ flow. The DRIFTS results of F-Cu are shown in Figure S1.

For fresh Cu/SSZ-13 catalysts, the negative band at ≈ 896 and 954 cm^{-1} was assigned to Cu²⁺ in 6MR and [Cu(OH)]⁺ in 8MR, respectively. When the adsorption temperature increased from 100 to 400 °C, the bands at 896 and 954 cm^{-1} gradually weakened and did not change at last, which revealed that no NH₃ desorbed from Cu/SSZ-13 when the temperature was higher than 400 °C. This process corresponded to the release of NH₃ in the peak (A) of the NH₃-TPD profiles (Figure 2a in the manuscript).

The bands at 3604 and 3576 cm^{-1} were assigned to NH₃ adsorbed on Brönsted acid sites. The bands at 3604 and 3576 cm^{-1} were obvious when temperature was 400 °C. With further increasing temperature, the bridged OH groups generally came out. This again confirmed that the peak (B) in the NH₃-TPD process (Figure. 2a in the manuscript) was assigned to ammonia adsorbed at Brönsted acid sites.

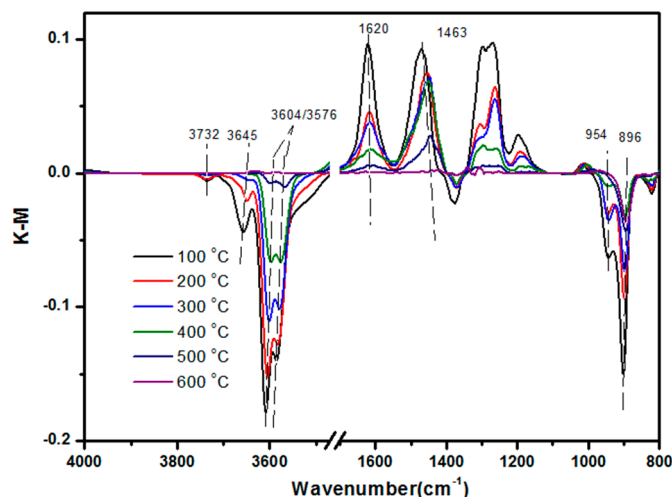


Figure S1. DRIFTS spectra of NH₃-TPD over Cu/SSZ-13 catalysts.

2. XRD results

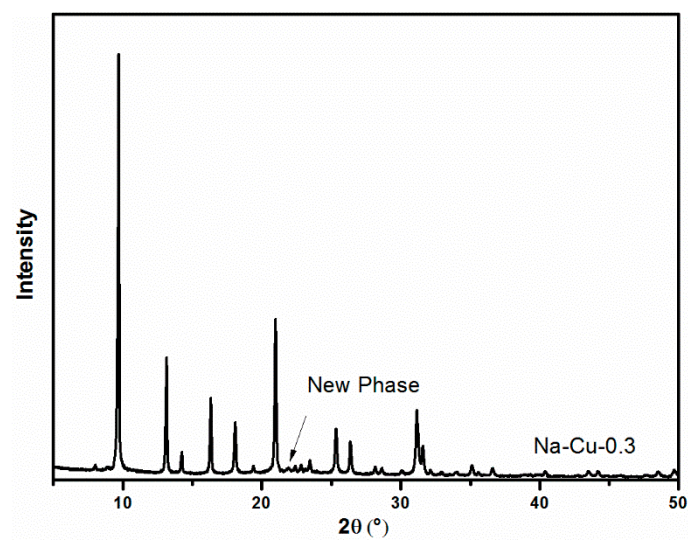


Figure S2. XRD results of Na-Cu-0.3 after hydrothermal aging at 750 °C for 16 h.