Supporting information

Quantitative determination of the Cu species, acid sites and NH_3-SCR mechanism on Cu-SSZ-13 and H-SSZ-13 at low temperatures

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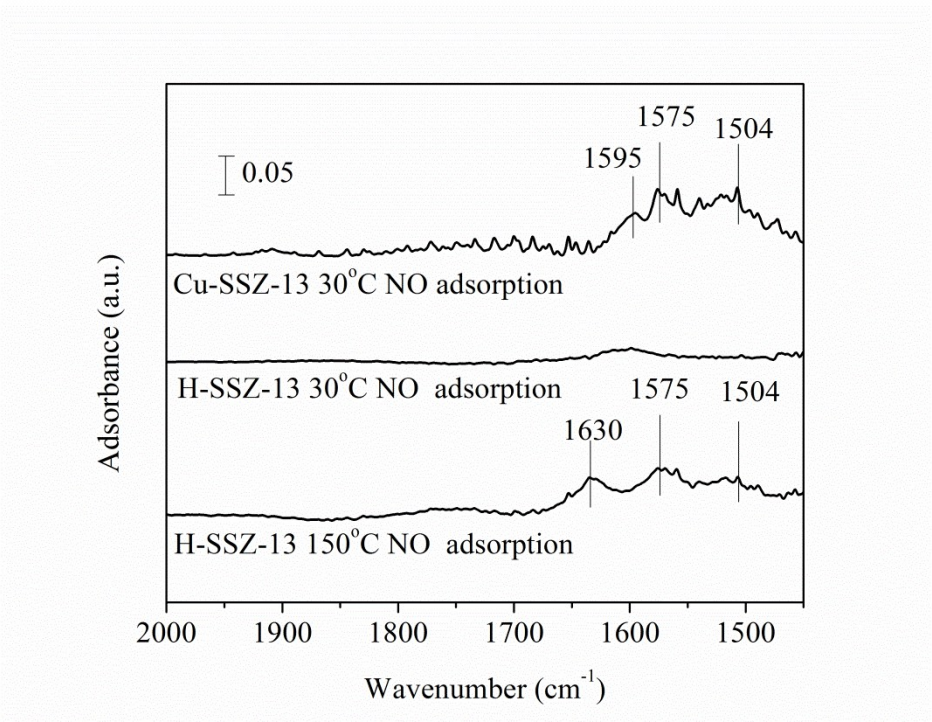

Figure S1 In situ DRIFT spectra of species on Cu-SSZ-13 and H-SSZ-13 after NO adsorption.

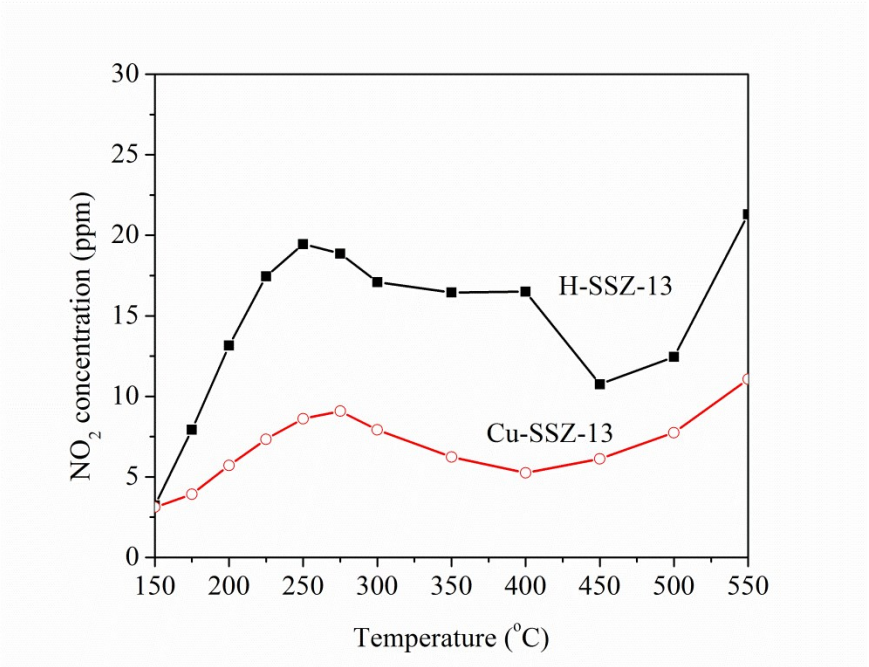

Figure S2 NO_2 formation during NO oxidation on Cu-SSZ-13 and H-SSZ-13. Reaction conditions: 500 ppm NO and 5% O_2, with N_2 balance; 500 mL/min gas flow rate.

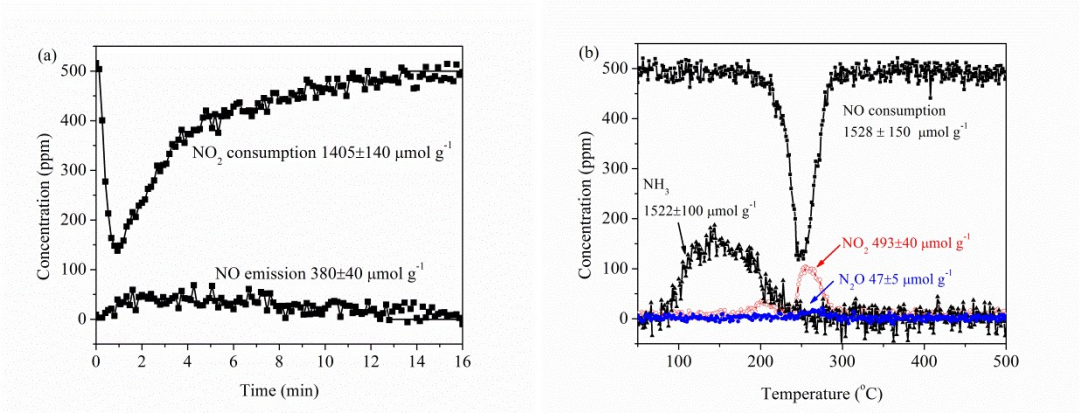

Figure S3 (a) Adsorption of NO_2 on Cu-SSZ-13 pretreated by NH_3 at 30°C and (b) TPSR in NO/N_2 of Cu-SSZ-13 pretreated by 500 ppm NH_3 and then 500 ppm NO_2 at 30°C.

Following experiment was conducted to study if the reaction mechanism changes with the change of the adsorption: NH_3 was adsorbed on Cu-SSZ-13 firstly, and then NO_2 was introduced into the reactor. Afterwards, TPSR in NO/N_2 was conducted, and the results are shown in **Figure S3**.

The amount of NH_3 adsorbed on fresh Cu-SSZ-13 was 3829 μmol g^{-1} (**Figure 6a**), and the subsequent NO_2 adsorption resulted in 1405 μmol g^{-1} NO_2 consumption and 380 μmol g^{-1} NO evolution. Thus, the nitrate adsorbed on Cu-SSZ-13 was 1405 – 380 = 1025 μmol g^{-1}. Since the amounts of weakly adsorbed NH_3 and nitrates were 721 and 456 μmol g^{-1}, respectively, the remaining amounts of NH_3 and nitrates on Cu-SSZ-13 could be calculated to be 3829 – 721 = 3108 μmol g^{-1} and 1025 – 456 = 569 μmol g^{-1}, respectively. During TPSR, the amounts of NO consumption, NO_2, N_2O and NH_3 evolution were 1528, 493, 47 and 1522 μmol g^{-1}, respectively. Therefore, it can be concluded that 3108 – 1522 = 1586 μmol g^{-1} NH_3 and 569 μmol g^{-1} nitrates could reacted with 1528 μmol g^{-1} NO at the ratios of NO/NH_3 1/1 (1035/1035), NO/NH_4NO_3/(NO_2 emission) 1/1/1 (493/493/493), and NH_4NO_3/(N_2O emission) 1/1 (47/47), and following reactions took place:

$$2NO + 2NH_3\text{-adsorbed} + (Z^-Cu^{2+})_2\text{-}O_2 \rightarrow 2N_2 + 3H_2O + Z^-Cu^{2+}\text{-}O\text{-}Cu^{2+}Z^- \quad (27)$$

$$2NO + 2NH_3\text{-adsorbed} + Z^-Cu^{2+}\text{-}O\text{-}Cu^{2+}Z^- \rightarrow 2N_2 + 3H_2O + 2\,Z^-Cu^+ \quad (28)$$

$$4NO + 4NH_3\text{-adsorbed} + Z^-Cu^{2+}O_2\bullet \rightarrow 4N_2 + 6H_2O + Z^-Cu^+ \quad (29)$$

$Z\text{-}ONH_4NO_3\text{-}Z + NO \rightarrow N_2 + NO_2 + 2H_2O + Z\text{-}O + Z$ (24)

$Z\text{-}ONH_4NO_3\text{-}Z \rightarrow N_2O + 2H_2O + Z\text{-}O + Z$ (23)

The mechanism was the same as that concluded from **Figure 10a**, i.e., the results of TPSR of Cu-SSZ-13 in NO pretreated by NO_2 and then NH_3, indicating that the reaction mechanism was not affected by the adsorption order. It should be noted that more NH_3 adsorbed on the fresh Cu-SSZ-13 catalyst than on NO_2-pretreated Cu-SSZ-13 (**Figure S3a**), and thus, the amount of NH_3 desorption in **Figure S3b** was higher than that in **Figure 10a**. The amount of NO_2 adsorbed on NH_3-pretreated Cu-SSZ-13 was smaller than that on fresh Cu-SSZ-13 (**Figure 6a**), leading to lower amounts of NO_2 and N_2O emission.