

## SUPPLEMENTARY INFORMATION

### **The Effect of Synthesis Methods on Cu species and Active Sites over Cu/SAPO-34 for NH<sub>3</sub>-SCR reaction**

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## 1. NH<sub>3</sub>-TPD experiment

Temperature programmed desorption (NH<sub>3</sub>-TPD) experiments were performed in the same reactor for the SCR activity test and the same sample weight were packed. Prior to the experiments, the catalysts were pre-oxidized at 500 °C for 30 min in 5 % O<sub>2</sub>/N<sub>2</sub>, and then 500 ppm NH<sub>3</sub>/N<sub>2</sub> was purged until the outlet NH<sub>3</sub> concentration was stable at 80 °C. After that, the catalysts were purged with N<sub>2</sub> to remove any weakly absorbed NH<sub>3</sub> at 80 °C. When NH<sub>3</sub> concentration was lower than 5 ppm, the catalysts were heated from 80 °C to 550 °C at a ramping rate of 10 °C /min. The outlet NH<sub>3</sub> concentrations were analysed by a Fourier Transform Infrared (FTIR) spectrometer (MKS-2030) which equipped with a 5.11 m gas cell.

## 2. The result and discussion

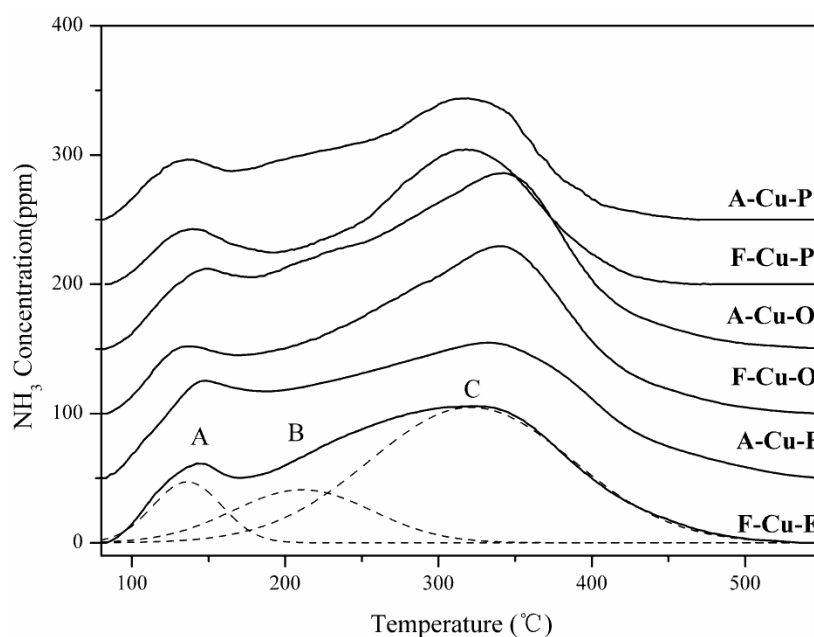


Fig.1 NH<sub>3</sub>-TPD profiles for Cu/SAPO-34 with various Cu/SAPO-34 and H-SAPO. The NH<sub>3</sub>-TPD experiment was ramped from 80 °C to 550 °C at a rate of 10 °C/min. “Dash line” represents for the fitting results.

NH<sub>3</sub>-TPD was carried out to detect the number and strength of acid sites in catalyst and the results are displayed in Fig.1. In the entire desorption temperature range, all samples

show two distinct desorption regions at 130–150 °C and 330–360 °C which can be deconvoluted into three peaks (A, B and C). The low-temperature (LT) desorption peak (A and B) are attributed to weakly adsorbed NH<sub>3</sub> or ammonium species adsorbed at Lewis acid sites<sup>1,2</sup>. The high-temperature peak C is possibly assigned to the structural Brønsted acid sites referred to strong acidity<sup>1,3</sup>.

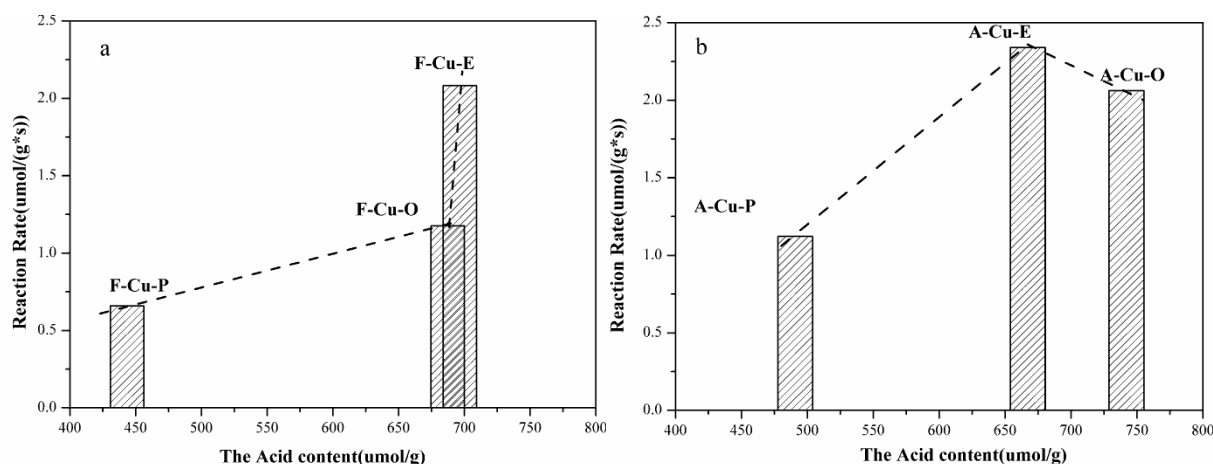


Fig.2 Relationship between the acid content of Cu/SAPO-34 and the SCR reaction rate at 200°C. (a) Fresh samples (b) Aged samples

In order to investigate the effect of acidity on the SCR activity over different synthesis methods, the acid content (calculated by NH<sub>3</sub>-TPD) and the SCR reaction rate at 200°C were studied and the results were shown in Fig.2. For the fresh samples, the F-Cu-E and F-Cu-O sample have almost the same acid content, but the SCR reaction rate on the F-Cu-E is almost twice of that on F-Cu-O. In addition, although the acid content of A-Cu-O is more than that of F-Cu-O sample, the SCR reaction rate is lower. All above results indicates that the acidity does not strongly affect the SCR activity of the Cu/SAPO-34 catalyst.

#### Reference:

- 1 G.V.A. Martins, G. Berlier, C. Bisio, S. Coluccia, H.O. Pastore, L. Marchese, *Journal of Physical Chemistry C*, 2008, **112**, 7193.
- 2 L. Ma, Y. Cheng, G. Cavataio, R.W. McCabe, L. Fu, J. Li, *Chemical Engineering Journal*, 2013, **225**, 323
- 3 B. Onida, Z. Gabelica, J. Lourenco, E. Garrone, *Journal of Physical Chemistry*, 1996, **100**, 11072