

1 **Supporting Information for the manuscript “Excellent performance**
2 **of one-pot synthesized Cu-SSZ-13 catalyst for the selective catalytic**
3 **reduction of NO_x with NH₃”**
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18 **1. NH₃-SCR performance of Cu_{3,8}-SSZ-13 in the high temperature range**

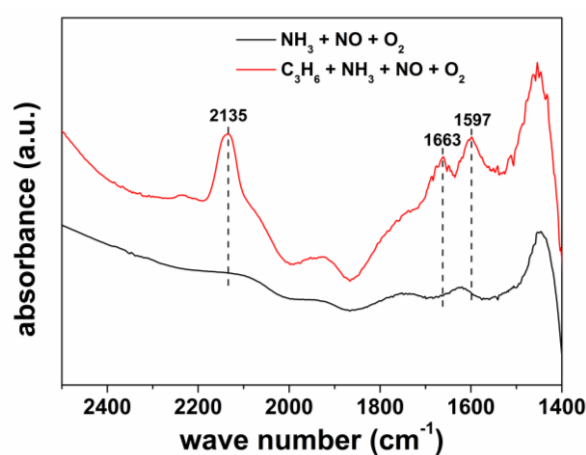
19 **Table S1 NH₃-SCR performance of Cu_{3,8}-SSZ-13 in the high temperature range.**

	Temperature (°C)		
	600	650	700
NO _x conversion (%)	86.3	74.8	52.6
N ₂ selectivity (%)	99.2	98.9	99.3

20 It was observed that deNO_x catalytic activity of the catalyst decreased with the

1 increase of reaction temperature. However, NO_x conversion exceeding 70% was
2 achieved with GHSV at $400,000 \text{ h}^{-1}$ at temperatures lower than $650 \text{ }^\circ\text{C}$. In addition,
3 excellent N_2 selectivity (nearly 100%) was kept even the temperature was as high as
4 $700 \text{ }^\circ\text{C}$. The results indicated that the catalyst could also maintain good NH_3 -SCR
5 performance in such high temperature range.

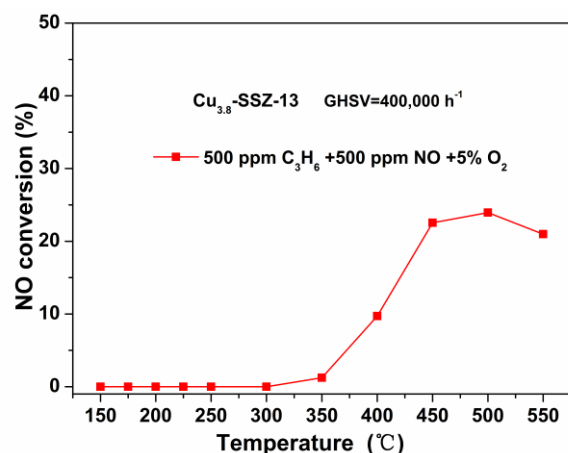
6 2. The effect of C_3H_6 on NH_3 -SCR reaction for $\text{Cu}_{3.8}$ -SSZ-13 catalyst



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8 **Figure S1. Comparison of species adsorbed on catalyst surface with different feed gas at 300**
9 **$^\circ\text{C}$.**

10 The *in situ* DRIFTS experiments were carried out to confirm the effect of C_3H_6 at
11 $300 \text{ }^\circ\text{C}$. In “standard SCR” condition, few species were recorded on catalyst surface.
12 However, much species deserved in the presence of C_3H_6 . The peaks of 1597 and
13 1663 cm^{-1} could be assigned to carboxylate and acrolein, respectively [1-2]. Both of
14 them should be caused by the oxidation of C_3H_6 . The peak of 2135 cm^{-1} was assigned
15 to CO-Cu^+ aroused from the reaction between $-\text{NCO}$ and NO , meaning some Cu
16 species were occupied and could not participate in NH_3 -SCR reaction [1,3]. The
17 above three species were all related to the partial oxidation of C_3H_6 strongly. Thus,
18 C_3H_6 partial oxidation poisoned the catalysts severely around $300 \text{ }^\circ\text{C}$.

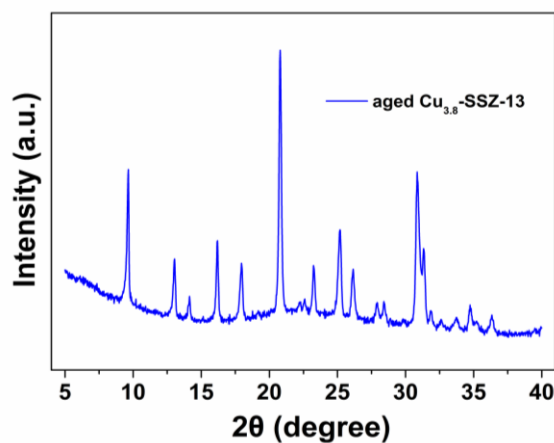


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2 **Figure S2. C₃H₆-SCR activity of Cu_{3.8}-SSZ-13 catalyst. Reaction conditions: [NO] = [C₃H₆] =**
 3 **500 ppm, [O₂] = 5 vol.%, N₂ balance and GHSV = 400,000 h⁻¹.**

4 As shown in Figure S2, the NO_x conversion was relatively low over Cu_{3.8}-SSZ-13
 5 when C₃H₆ was used as reducing agent. NO_x was converted obviously when
 6 temperature was higher than 300 °C. The phenomenon was consistent with the results
 7 that the NH₃-SCR activity increased in the high temperature range in the presence of
 8 C₃H₆ (> 300 °C).

9 3. XRD profile of aged Cu_{3.8}-SSZ-13 catalyst



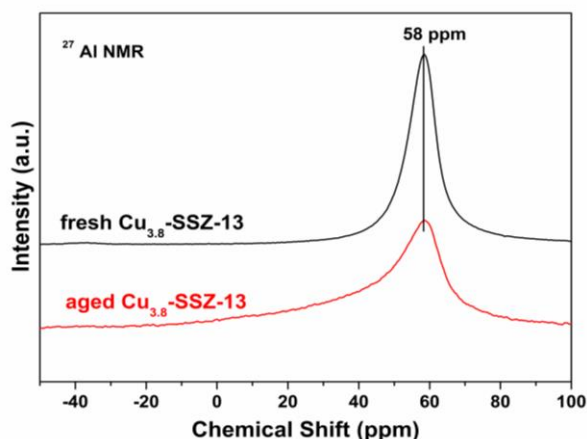
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11 **Figure S3. XRD profile of aged Cu_{3.8}-SSZ-13 catalyst.**

12 The catalyst still maintained zeolite structure after severe hydrothermal aging
 13 treatment even a few amount of amorphous phase appeared.

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1 4. ²⁷Al NMR profiles of fresh and aged Cu_{3.8}-SSZ-13 catalyst



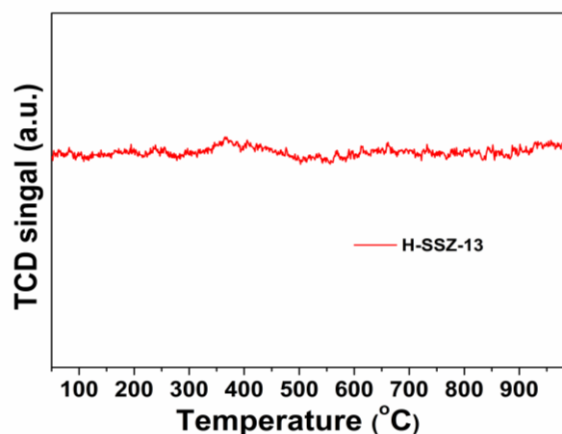
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3 **Figure S4.** ²⁷Al NMR profile of fresh and aged Cu_{3.8}-SSZ-13 catalyst.

4 Solid state ²⁷Al MAS NMR spectra were collected on a Bruker AVANCE III
5 400MHz WB Solide-State NMR spectrometer with operating at the spectral frequency
6 of 104.29 MHz. A relaxation delay 1 s was applied to collect single pulse spectra. All
7 measurements were performed at room temperature, and Al(NO₃)₃ were used as
8 external references, respectively. The ²⁷Al NMR results of Cu_{3.8}-SSZ-13 catalyst
9 before and after hydrothermal treatment were shown below.

10 The chemical shift of 58 ppm was resulted by the Al atom in the framework, which
11 has a 4-fold coordination (Al^{IV}). However, if Al atom was removed from the zeolite
12 framework, the atom can be located outside the lattice, showing a 6-fold-type
13 coordination (Al^{VI}) with much lower chemical shift in ²⁷Al NMR spectra [4].
14 Compared with fresh Cu_{3.8}-SSZ-13 catalyst, the intensity area of Al^{IV} in the aged
15 sample decreased greatly, and a broad peak at *ca.* 15 ppm appeared. The results
16 indicated that dealumination occurred during the hydrothermal treatment.

1 5. H₂-TPR profile of H-SSZ-13



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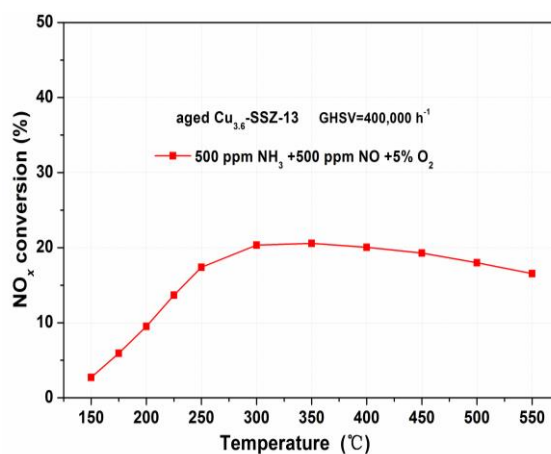
Figure S5. H₂-TPR profile of H-SSZ-13.

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There was no H₂ consumption for H-SSZ-13 sample.

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6. NH₃-SCR performance of aged Cu_{3,6}-SSZ-13 catalyst



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Figure S6. NH₃-SCR performance of aged Cu_{3,6}-SSZ-13 catalyst.

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After hydrothermal aging at 750 °C for 16 h, the aged Cu_{3,6}-SSZ-13 sample showed

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poor NH₃-SCR performance. The highest NO_x conversion was only *ca.* 20%. Thus,

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Cu_{3,6}-SSZ-13 catalyst showed much lower hydrothermal stability.

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1 **References**

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