

Supporting information

**Exploring the role of V_2O_5 in the reactivity of NH_4HSO_4 with NO on
 V_2O_5/TiO_2 SCR catalysts**

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Figure captions

Fig. S1. XRD patterns of the series V/Ti catalysts

Fig. S2. FTIR spectra of the series V/Ti catalysts

Fig. S3. *In situ* DRIFTS study of the NH_4HSO_4 decomposition behavior over the V4/Ti catalyst surface

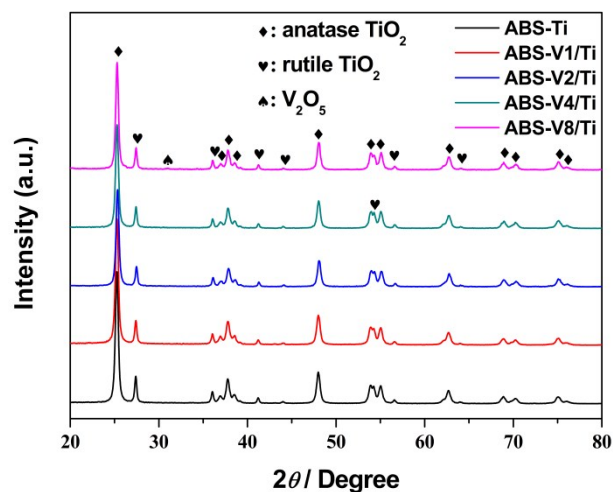


Fig. S1. XRD patterns of the series V/Ti catalysts

The XRD patterns of the series catalysts are presented in Fig. S1. All the diffraction peaks of the samples with V content lower than 8 wt% could be indexed to anatase TiO₂ and rutile TiO₂ phases. The absence of V₂O₅ and NH₄HSO₄ crystallites suggests that vanadium and sulfate species are highly dispersed, which exist in an amorphous state on the TiO₂ surface. Given increases in V₂O₅ content to 8 wt%, new diffraction peaks indexed to V₂O₅ phase appear, indicating that V loading is beyond the theoretical monolayer coverage on the TiO₂ support.¹

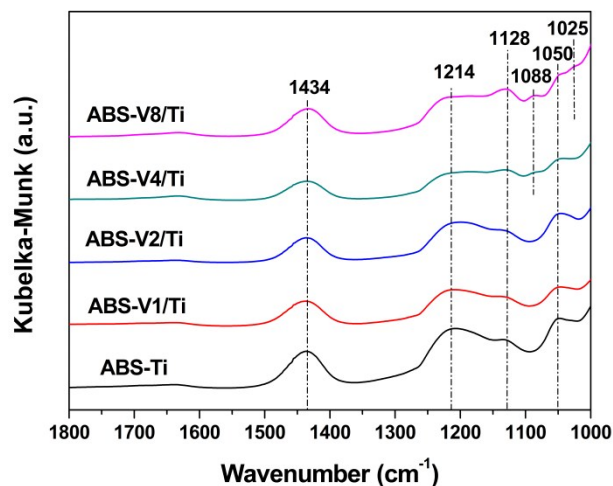


Fig. S2. FTIR spectra of the series V/Ti catalysts

In the case of the NH_4HSO_4 -deposited samples, the characteristic peaks attributed to bidentate SO_4^{2-} at 1214, 1128, 1050 cm^{-1} are generated, which are assigned to the ν_3 vibrations of bidentate SO_4^{2-} in C_{2v} symmetry (Fig. S2). The bands at 1214 and 1128 cm^{-1} appear because of asymmetric and symmetric stretching of the S=O vibrations.^{2, 3} In the meantime, the peak at 1050 cm^{-1} is related to the asymmetric S-O stretching vibrations. Given an increase in V_2O_5 content, new bands centered at 1088 and 1025 cm^{-1} , which could be related to the stretching of the S-O vibrations in pure NH_4HSO_4 , appear.^{4, 5} The presence of vanadium species leads to a deficit in TiO_2 surface basic sites, thereby allowing the appearance of pure NH_4HSO_4 phase. Combined with the XRD patterns in Fig. S1, NH_4HSO_4 might exist in the amorphous state.

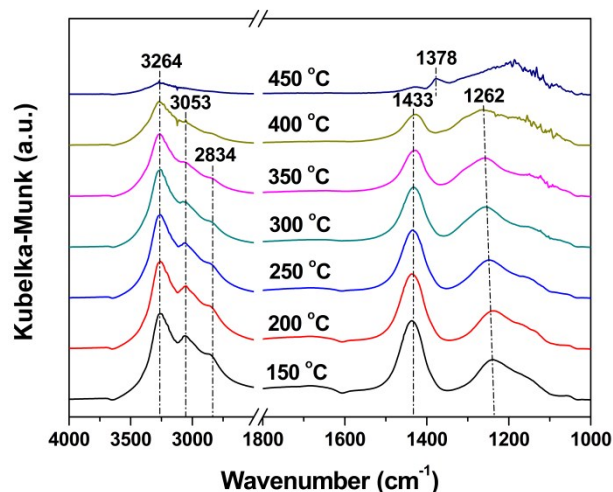


Fig. S3. *In situ* DRIFTS study of the NH₄HSO₄ decomposition behavior over the V₄/Ti catalyst surface

In situ DRIFTS was conducted to investigate the detailed NH₄HSO₄ decomposition behavior on the catalyst surface. As is shown in Fig. S3, characteristic IR peaks centered at 1242 and 1433 cm⁻¹ attributed to bidentate SO₄²⁻ and NH₄⁺ appear when the temperature is 100 °C.^{6, 7} In the meantime, the bands at 2834, 3050, 3262 cm⁻¹, assigned to the stretching vibrations of N-H in NH₄⁺ also come out.⁸ With increasing temperature, the peak related to bidentate SO₄²⁻ undergoes a blue shift, together with the occurrence of a decrease in the intensity of the bands attributed to sulfate and ammonium species. In addition, characteristic IR peak centered at 1378 cm⁻¹ attributed to tridentate SO₄²⁻ comes out at a temperature of 450 °C, which might be due to the transformation of sulfate species from (M₂SO₄)H structure to (M-O)₃=O one.⁹

Tables

Table S1

N₂ adsorption results of the series V/Ti catalysts

Samples	BET (m ² g ⁻¹)	Pore volume (cm ³ g ⁻¹)
ABS-Ti	30	0.22
ABS-V1/Ti	30	0.23
ABS-V2/Ti	28	0.23
ABS-V4/Ti	24	0.22
ABS-V8/Ti	28	0.19

Reference

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