

Electronic Supplementary Information

Improved NH₃-SCR activity by the cooperation of FeVO₄ and CeO₂ nanosheets catalyst: Structure and mechanism

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1. Preparation steps of FeVO₄, CeO₂-S and CeO₂-P

FeVO₄ was synthesized by a modified hydrothermal method. In a typical procedure, 6 mmol NH₄VO₃ and 6 mmol Fe(NO₃)₃·9H₂O were dissolved in 30 ml deionized water respectively, and NH₄VO₃ solution was heated to 80 °C to accelerate its dissolving. NH₄VO₃ solution was added to the Fe(NO₃)₃ solution at a constant stirring rate of 800 rpm. The pH of the above solution was adjusted to 2 by dropping dilute nitric acid or ammonia water and it was filled to 75 mL with deionized water. After 3 h of stirring, the solution was transferred to a Teflon-lined stainless-steel autoclave and remained for 6 h at 180 °C. After cooling to room temperature, the precipitates were centrifuged and then dried at 60 °C for 12 h, the dried mixtures were calcined at 500 °C in air for 5 h.

CeO₂ nanosheets (named as CeO₂-S) were prepared by precipitation method. 1.39 g Ce(NO₃)₃·6H₂O and 0.75 g NH₄HCO₃ were dissolved in 200 mL deionized water, respectively. Then, the NH₄HCO₃ solution was quickly poured into the Ce(NO₃)₃

solution, and the mixed solution was stirred for 30 min. After that, it was left at room temperature for 15 h. After centrifugation, the sample was dried at 60 °C for 12 h. The dried sample was heated to 450 °C at a rate of 2 °C/min in muffle furnace, and kept at 450 °C for 4 h. CeO₂ nanoparticles (named as CeO₂-P) as comparison samples were also prepared by precipitation method. 1 mol/L Ce(NO₃)₃ solution and 1 mol/L ammonia solution were prepared, and the ammonia solution was dropped into the Ce(NO₃)₃ solution at a rate of 3 mL/min under intense stirring until pH = 10. After 1.5 h of stirring, the solution was left standing for 3 h. The precipitate was collected by centrifugation, then dried and calcined as described above.

2. Tables

Table S1. Specific surface area and S content of fresh and used 10%FeV/CeO₂-S after SO₂ resistance test.

| | S_{BET} | S element content detected by XRF |
|-------|------------------------|-----------------------------------|
| Fresh | 53.6 m ² /g | — |
| Used | 7.9 m ² /g | 0.5 wt.% |

Table S2. The average grain size of the prepared catalysts calculated by Scherrer equation.

| Sample | Grain size (nm) |
|----------------------------|-----------------|
| CeO ₂ -P | 12.1 |
| CeO ₂ -S | 7.1 |
| CeO ₂ -S-500 | 8.5 |
| 5%FeV/CeO ₂ -S | 7.4 |
| 10%FeV/CeO ₂ -S | 8.1 |
| 10%FeV/CeO ₂ -P | 11.6 |
| 15%FeV/CeO ₂ -S | 8.0 |
| 20%FeV/CeO ₂ -S | 9.5 |

3. Figures

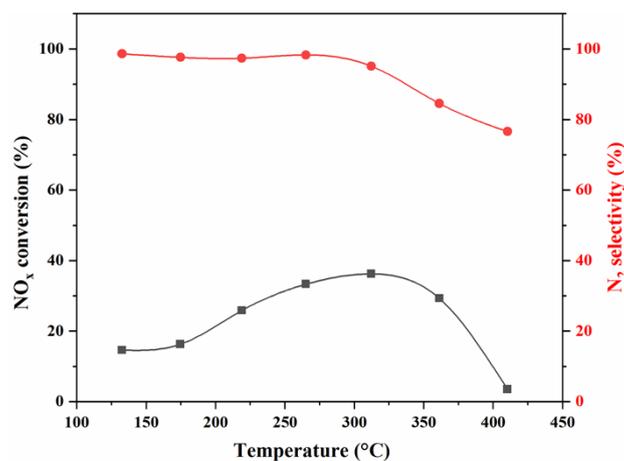


Fig. S1 NO_x conversion and N₂ selectivity of CeO₂-S. Reaction conditions: [NO] = 500 ppm, [NH₃] = 500 ppm, [O₂] = 5 vol.%, balance N₂, 150 mg catalyst, GHSV = 80,000 mL · g⁻¹ · h⁻¹.

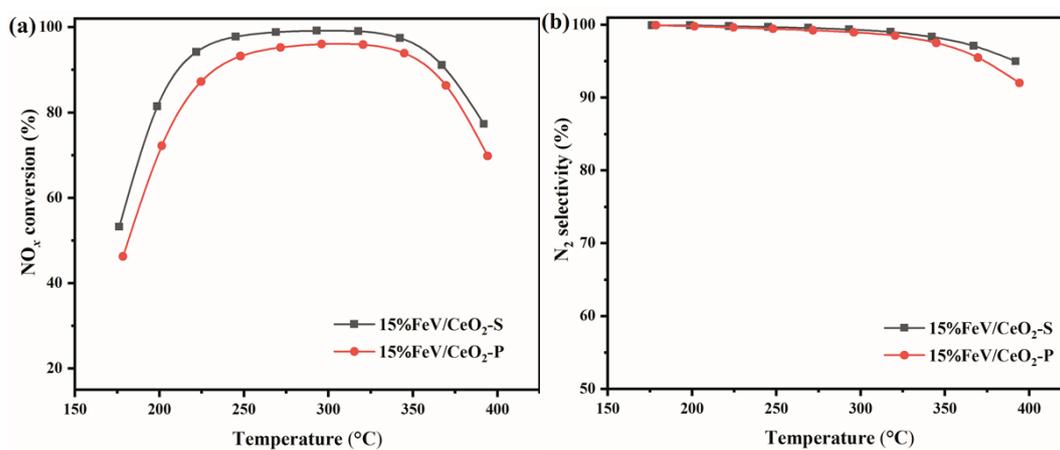


Fig. S2 (a) NO_x conversion and (b) N₂ selectivity of 15%FeV/CeO₂-S and 15%FeV/CeO₂-P. Reaction conditions: [NO] = 500 ppm, [NH₃] = 500 ppm, [O₂] = 5 vol.%, balance N₂, 150 mg catalyst, GHSV = 80,000 mL · g⁻¹ · h⁻¹.

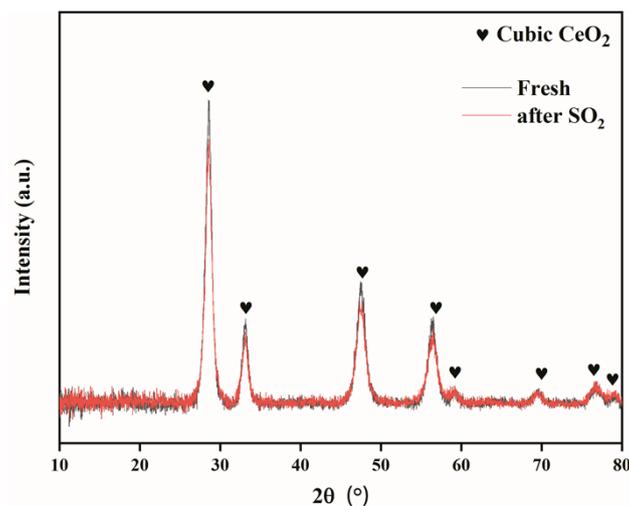


Fig. S3 XRD patterns of fresh 10%FeV/CeO₂-S and 10%FeV/CeO₂-S poisoned by SO₂.

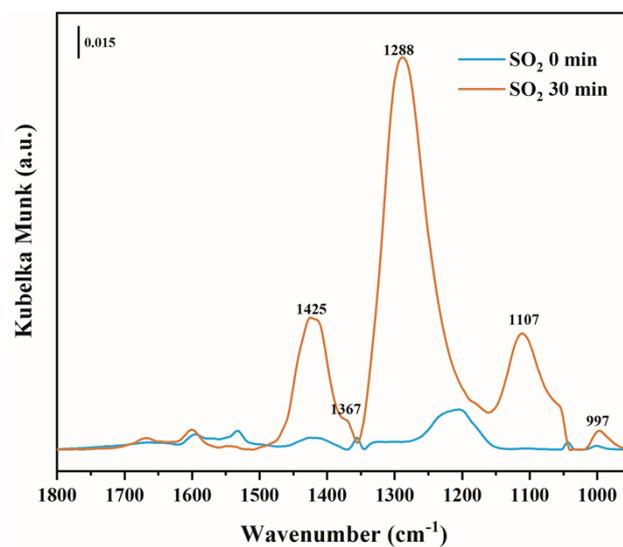


Fig. S4 In situ DRIFTS spectra of SO₂ + O₂ adsorption after the reaction between NO_x species and NH₃ over 10%FeV/CeO₂-S catalyst.

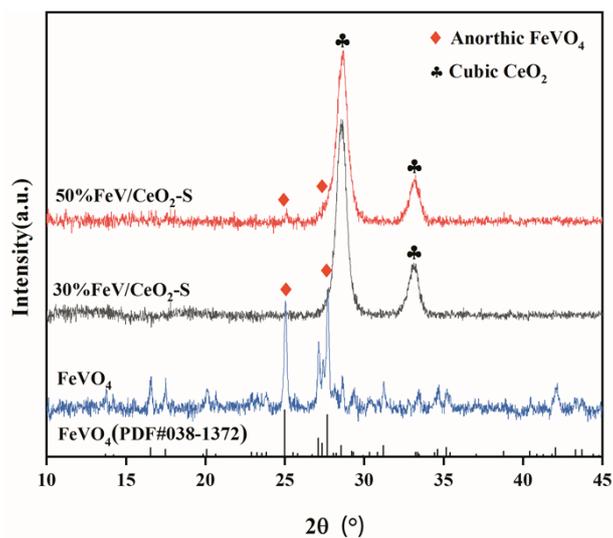


Fig. S5 XRD patterns of FeVO_4 , $30\%\text{FeV}/\text{CeO}_2\text{-S}$ and $50\%\text{FeV}/\text{CeO}_2\text{-S}$ catalysts.

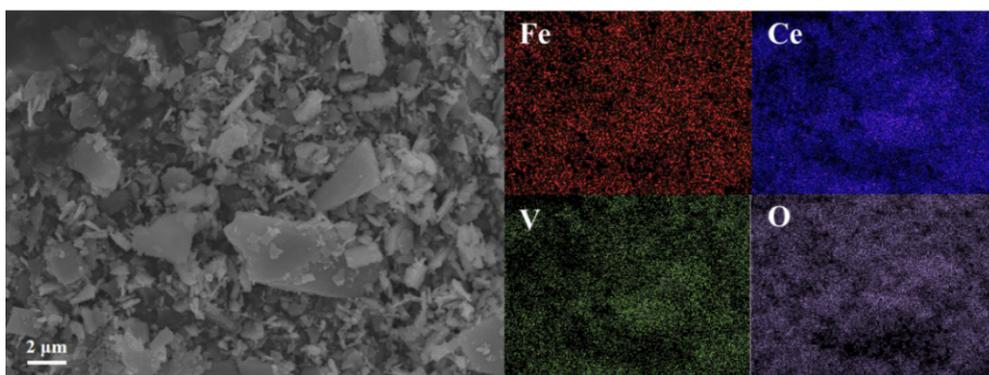


Fig. S6 EDS-mapping images of $10\%\text{FeV}/\text{CeO}_2\text{-S}$.

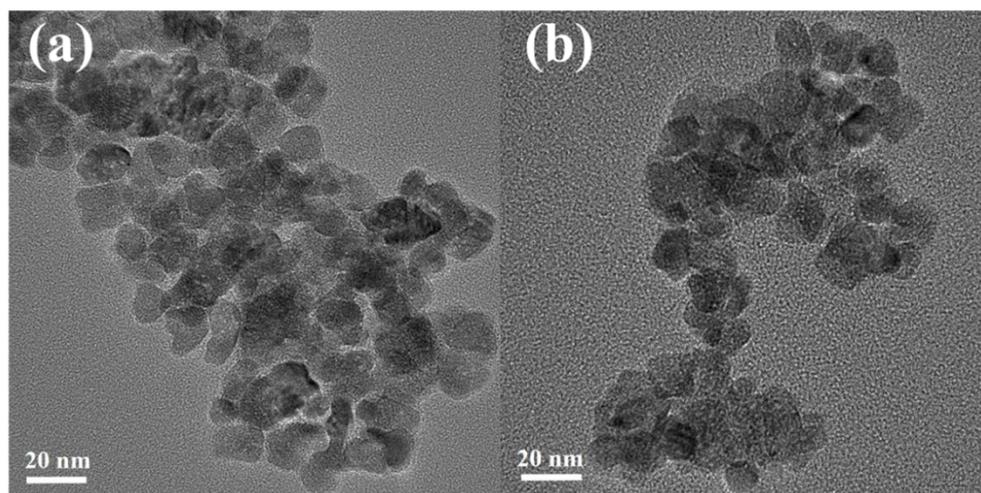


Fig. S7 TEM images of (a) $\text{CeO}_2\text{-P}$ and (b) $10\%\text{FeV}/\text{CeO}_2\text{-P}$ catalysts.

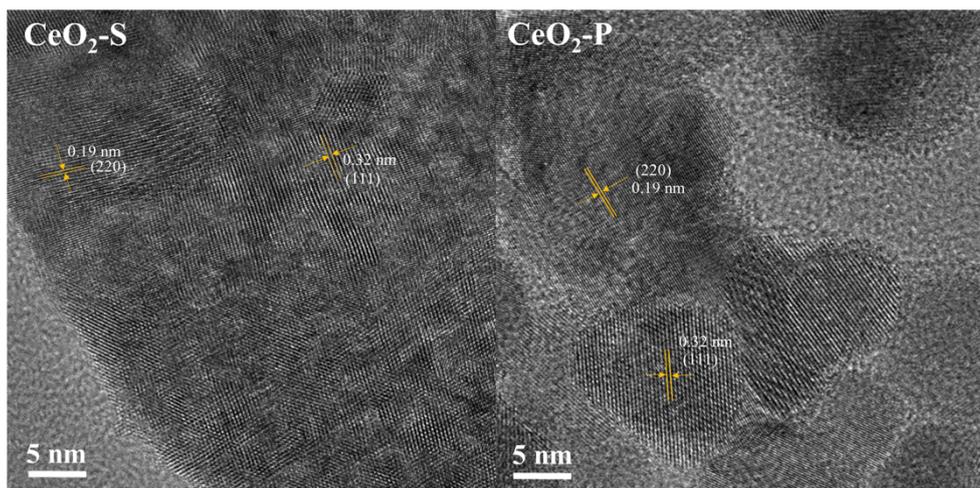


Fig. S8 HR-TEM images of $\text{CeO}_2\text{-S}$ and $\text{CeO}_2\text{-P}$ catalysts.

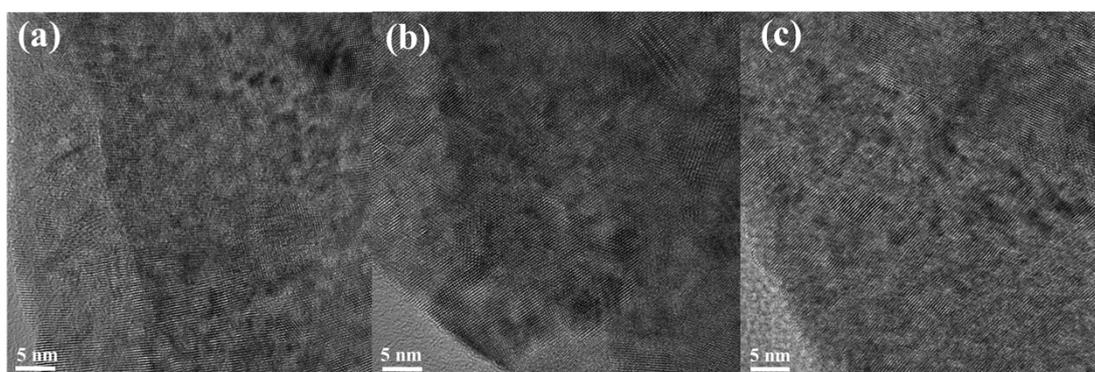


Fig. S9 HR-TEM images of $\text{CeO}_2\text{-S}$ catalysts.

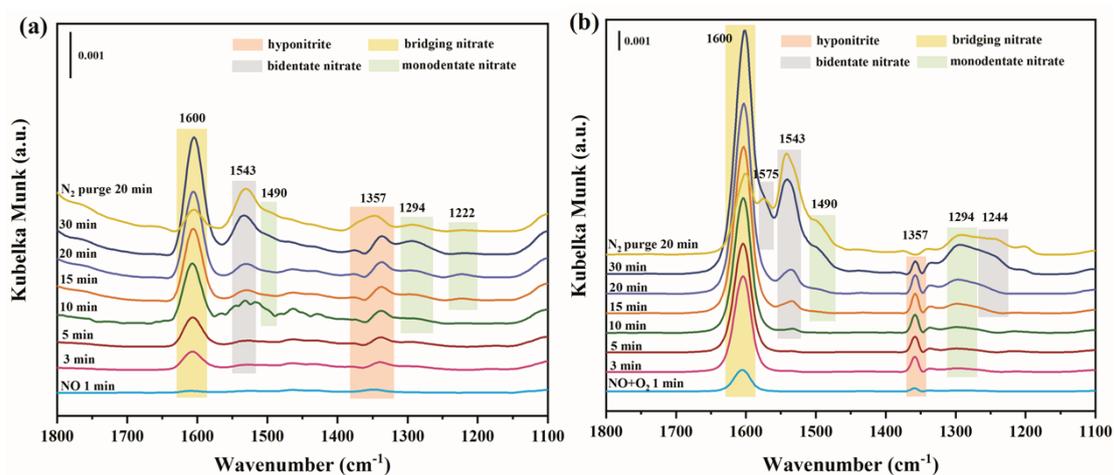


Fig. S10 *In situ* DRIFT spectra of 10%FeV/ $\text{CeO}_2\text{-S}$ obtained during exposure to (a) 500 ppm NO for 30 min followed by 20 min N_2 purge, and (b) 500 ppm NO + 5% O_2 for 30 min followed by 20 min N_2 purge at 250 °C.

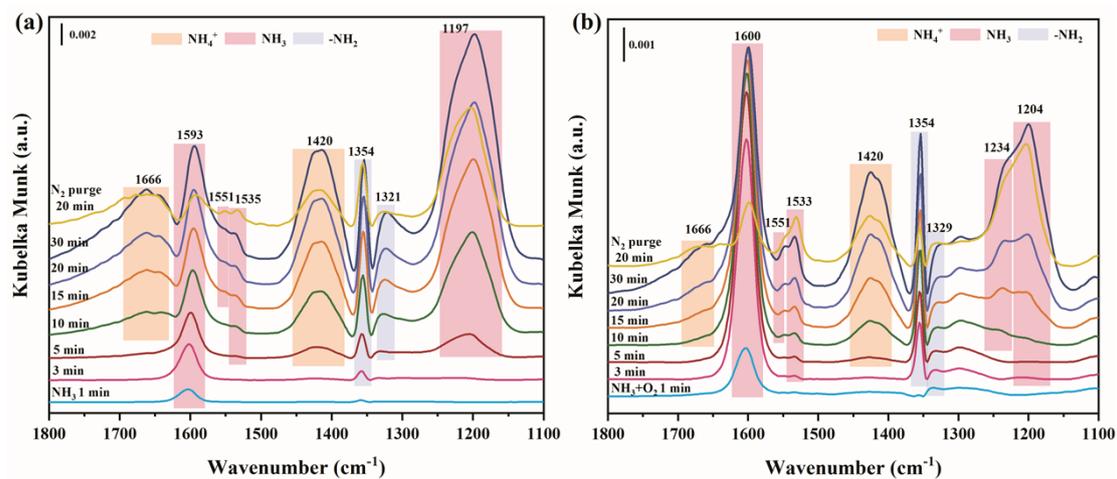


Fig. S11 *In situ* DRIFT spectra of 10%FeV/CeO₂-S obtained during exposure to (a) 500 ppm NH₃ for 30 min followed by 20 min N₂ purge, and (b) 500 ppm NH₃ + 5% O₂ for 30 min followed by 20 min N₂ purge at 250 °C.

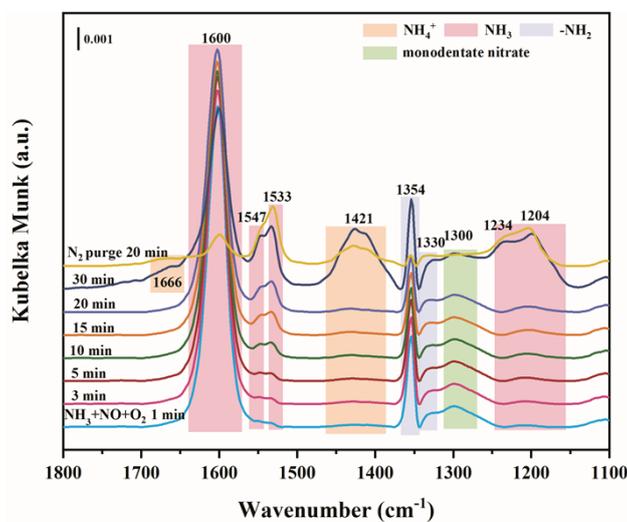


Fig. S12 *In situ* DRIFT spectra of 10%FeV/CeO₂-S obtained during exposure to 500 ppm NH₃ + 500 ppm NO + 5% O₂ for 30 min followed by 20 min N₂ purge at 250 °C.

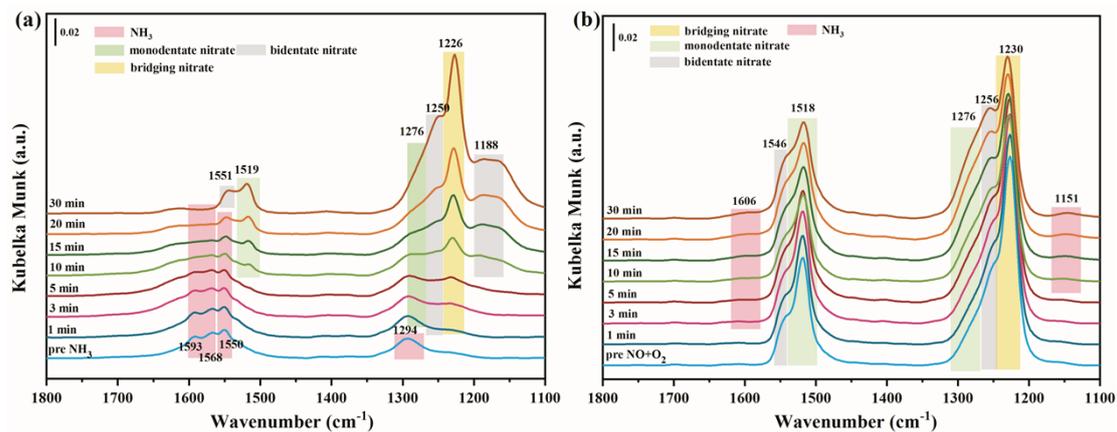


Fig. S13 *In situ* DRIFT spectra of CeO₂-S obtained during exposure to (a) 500 ppm NO + 5% O₂ after pre-adsorption of 500 ppm NH₃ for 30 min followed by 20 min N₂ purge, and (b) 500 ppm NH₃ after pre-adsorption of 500 ppm NO + 5% O₂ for 30 min followed by 20 min N₂ purge at 250 °C.

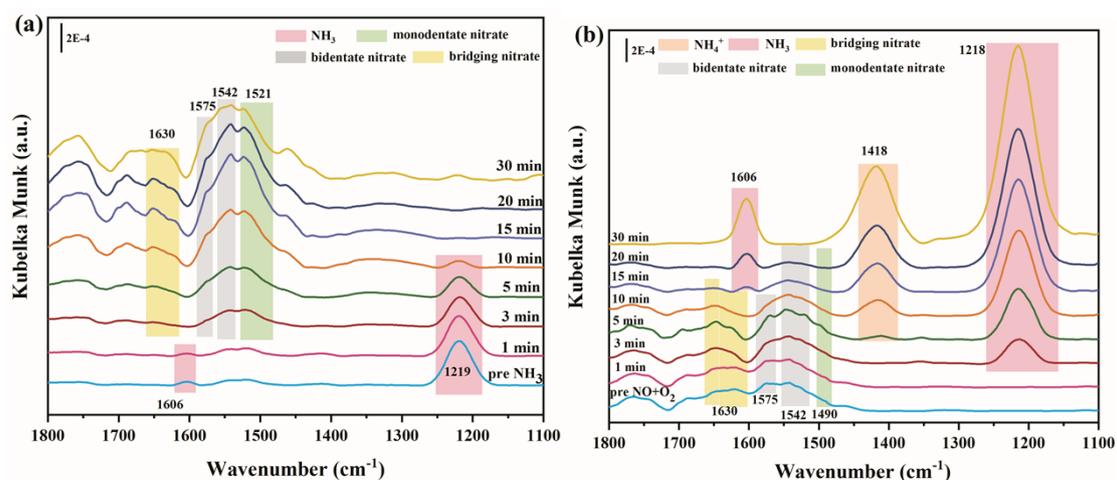


Fig. S14 *In situ* DRIFT spectra of FeVO₄ obtained during exposure to (a) 500 ppm NO + 5% O₂ after pre-adsorption of 500 ppm NH₃ for 30 min followed by 20 min N₂ purge, and (b) 500 ppm NH₃ after pre-adsorption of 500 ppm NO + 5% O₂ for 30 min followed by 20 min N₂ purge at 250 °C.

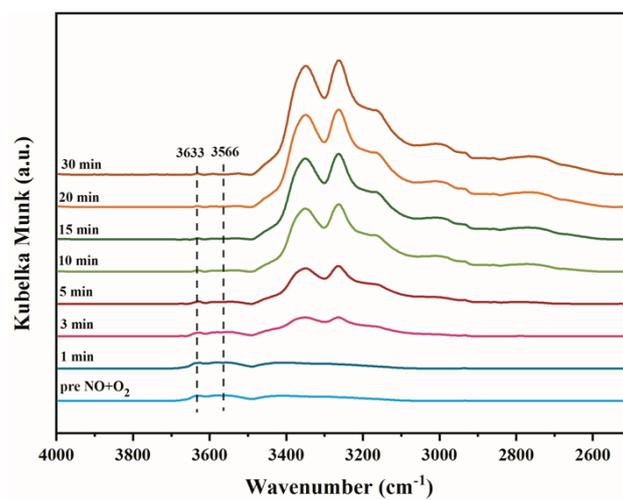


Fig. S15 *In situ* DRIFT spectra at 4000-2500 cm⁻¹ of reaction between NH₃ and pre-adsorbed NO + O₂ over 10%FeV/CeO₂-S at 250 °C.