

Electronic Supplementary Information

Novel FeVO₄ catalyst modified with NbTiO_x for efficient selective catalytic reduction of NO_x with NH₃

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Catalyst characterizations

The relative content of each element in the samples was analyzed using an X-ray fluorescence (XRF) analysis PANalytical Axios-MAX spectrometer. Powder X-ray diffraction (XRD) patterns were measured on a PANalytical X'Pert Pro diffractometer with Cu K α radiation operating at 40 kV and 40 mA. The data for 2θ ranging from 10° to 90° were collected with the step size of 0.02° .

The specific area of catalysts was measured by N₂ adsorption–desorption analysis using Quantachrome Autosorb iQ2 instrument cooled by liquid N₂ at -196°C . Prior to the N₂ physisorption, the samples were degassed under vacuum at 300°C for 1 h for analysis. The surface area was determined using the BET model, while the pore structure was determined using the Barrett-Joyner-Halenda (BJH) method.

The surface morphology of catalysts was measured by transmission electron microscopy (TEM, FEI Tecnai G2 F20).

Hydrogen temperature-programmed reduction (H₂-TPR) analysis was performed using the Auto Chem II instrument by Micromeritics. The samples (100 mg) underwent pretreatment at 300°C in a quartz reactor under 50% Ar/He (60 mL/min) for 0.5 h and cooled down to room temperature, followed by 10% H₂/Ar (50 mL/min) purging for 1 h. The H₂-TPR was performed from room temperature to 1000°C in 10% H₂/Ar gas flow at a rate of 50 mL/min and a heating rate of $10^\circ\text{C}\cdot\text{min}^{-1}$.

The X-ray Photoelectron Spectroscopy (XPS) was tested on an ESCALAB 250 XI (ThermoFisher Scientific) using Al K α radiation (1486.6 eV). To ensure accurate measurements, a calibration is performed using the C1s peak (BE=284.8 eV) as standard. The full spectrum pass energy is 100 eV, and the high-resolution spectrum pass energy is 20 eV.

The temperature programmed desorption of NH_3 (NH_3 -TPD) were carried out using a fixed-bed quartz flow reactor and a Fourier transform infrared gas analyzer. Prior to the TPD experiments, the samples weighing 300 mg were subjected to pretreatment at 400°C in a flow of 20% O_2/N_2 (300 mL/min) for 30 min, followed by cooling to room temperature. Then the catalysts were treated with 300 mL/min 20% NH_3/N_2 at 30°C for 1 h, and the physical adsorption was flushed by N_2 purge at room temperature. The temperature was then gradually raised from room temperature to 650°C at a rate of $2^\circ\text{C}\cdot\text{min}^{-1}$.

In situ Diffuse reflectance infrared Fourier transform spectroscopic (*in situ* DRIFTS) experiments were recorded on a Thermo Fisher FTIR spectrometer (Vertex 80V) equipped with an MCT detector. Before every measurement, all catalysts were pretreated in 20% O_2/N_2 with a total flow rate of 300 mL/min at 450°C for 30 min, and subsequently cooled down to 200°C . Then the background spectra were collected under a flowing N_2 atmosphere. DRIFTS experiments of NH_3 or $\text{NO} + \text{O}_2$ adsorption were conducted by exposing catalysts to NH_3 or $\text{NO} + \text{O}_2$ at 200°C until the absorbed bands became stable and then were purged under N_2 for 1 h at a flow rate of 300 mL/min. For the sample pre-adsorbed with NH_3 at 200°C , $\text{NO} + \text{O}_2$ was added. For the sample pre-adsorbed with $\text{NO} + \text{O}_2$ at 200°C , NH_3 was added. *In situ* DRIFTS spectra of the reaction were recorded respectively.

In order to collect DRIFTS spectra of NH_3 adsorption on different catalysts at different temperatures, the samples were cooled down to 150°C , 250°C and 350°C after pretreating, and the background spectra were collected under a flowing N_2 atmosphere respectively. Then the DRIFTS experiments of NH_3 adsorption were conducted by exposing catalysts to NH_3 at 150°C , 250°C and 350°C respectively until the absorbed bands became stable and then were purged under N_2 for 1 h at a flow rate of 300

mL/min. All spectra were recorded by accumulating 64 scans with a resolution of 4 cm^{-1} .

Results and discussion

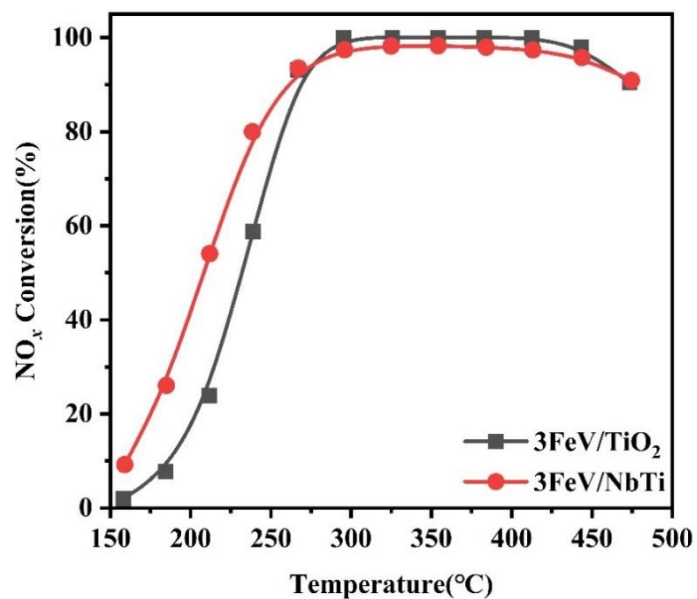


Fig. S1. NH₃-SCR activity of 3FeV/NbTi and 3FeV/TiO₂. Reaction conditions: [NH₃] = [NO] = 500 ppm, [H₂O] = 5 vol.%, [O₂] = 5 vol.%, N₂ balance, and GHSV=100,000 h⁻¹.

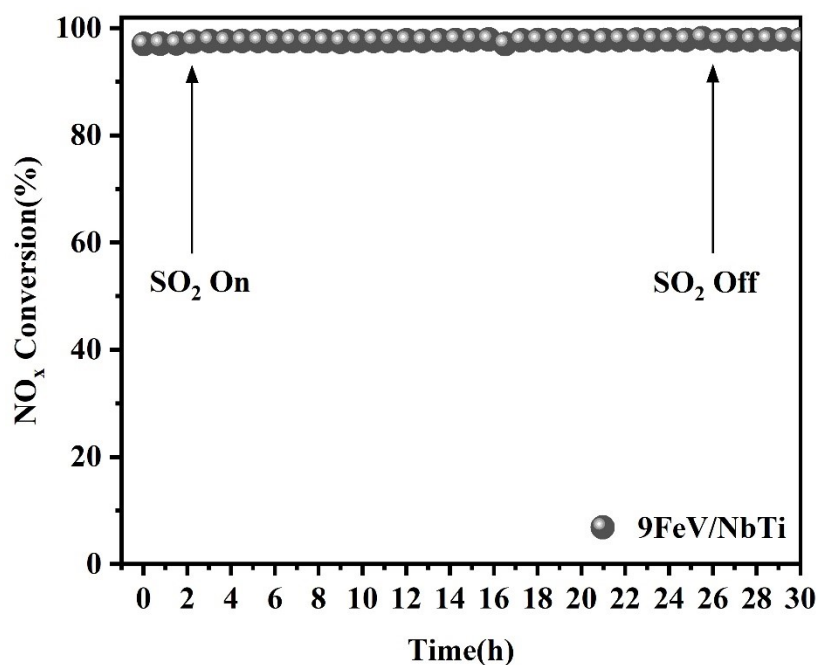


Fig. S2. Sulfur resistance of 9FeV/NbTi catalyst at 250°C. Reaction conditions: [NH₃] = [NO] = 500 ppm, [SO₂] = 300 ppm, [O₂] = 5 vol.%, N₂ balance, and GHSV=100,000 h⁻¹.

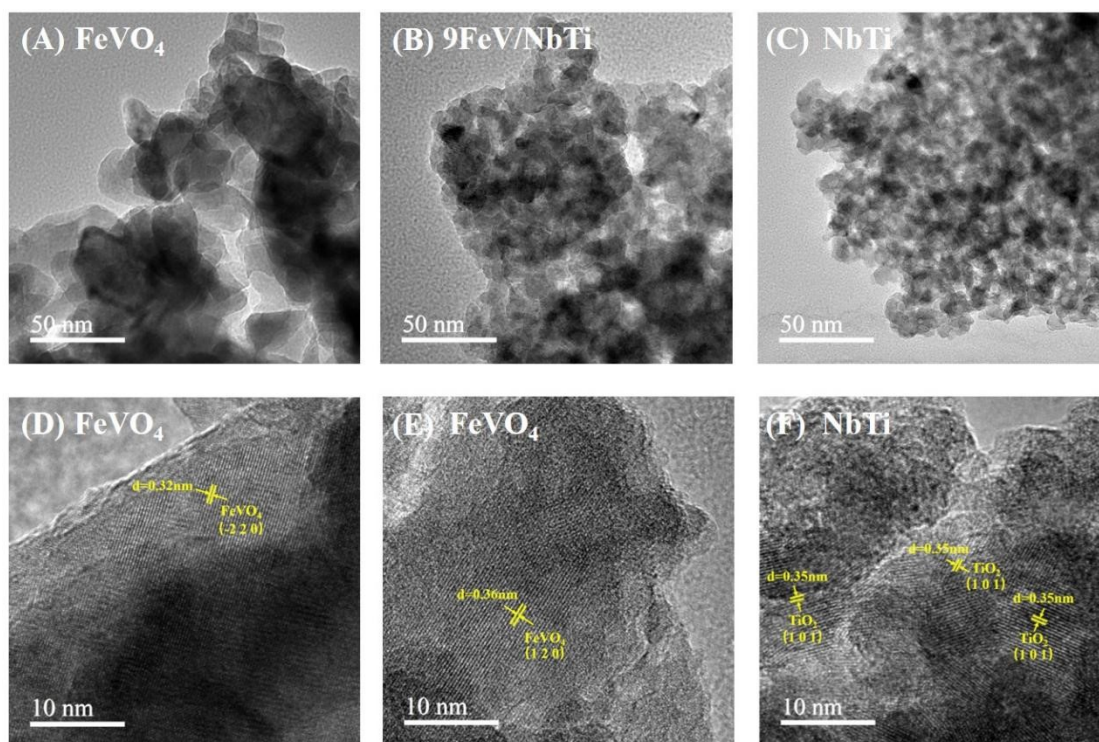


Fig. S3 The HR-TEM diagrams of FeVO_4 , NbTi composite oxide and 9FeV/NbTi catalysts

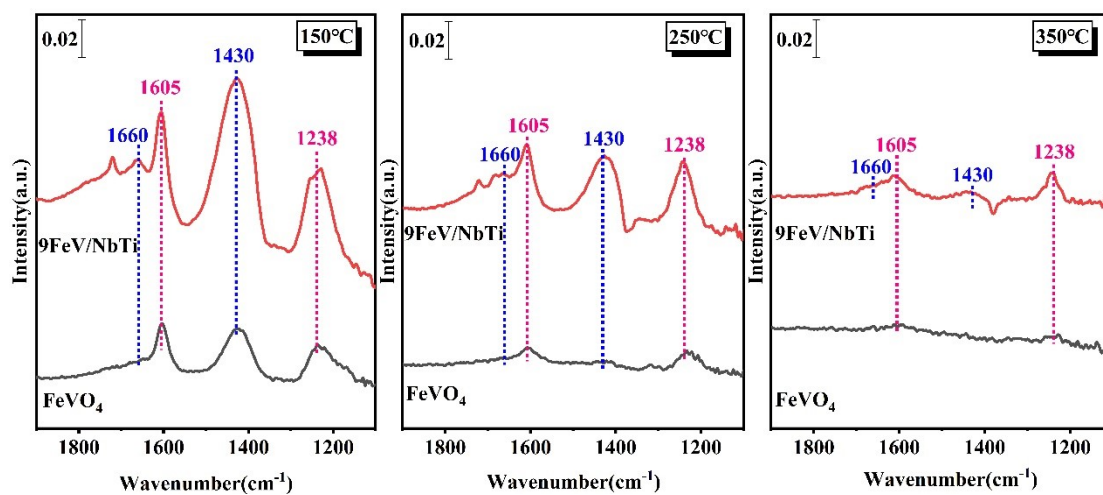


Fig. S4. DRIFT spectra of NH_3 adsorption on FeVO_4 , 9FeV/NbTi catalysts at 150°C, 250°C and 350°C.

Table S1. The proportion of different elements in the as-prepared catalysts ^a

| Samples | Fe/V ratio | Nb/Ti ratio | m(Fe ₂ O ₃ +V ₂ O ₅)/m(Nb ₂ O ₅ +TiO ₂) (%) |
|-------------------|------------|-------------|--|
| FeVO ₄ | 1.14 | — | — |
| 15FeV/NbTi | 1.17 | 0.29 | 14.93% |
| 9FeV/NbTi | 1.03 | 0.25 | 10.55% |
| 6FeV/NbTi | 0.97 | 0.22 | 7.04% |
| NbTi | — | 0.30 | — |

^a The ratio as calculated from powder X-ray fluorescence results.

Table S2. The H₂ consumption of NbTi composite oxide and xFeV/NbTi catalysts

| Samples | H ₂ consumption (μmol/g) | | |
|-------------------|-------------------------------------|--------|-------|
| | <602°C | >602°C | Total |
| FeVO ₄ | 1734 | — | 1734 |
| 15FeV/NbTi | 159 | 236 | 395 |
| 9FeV/NbTi | 136 | 203 | 339 |
| 6FeV/NbTi | 95 | 164 | 259 |
| NbTi | — | 229 | 229 |