

Water in ball-milling process affects the dispersion of vanadia species on V₂O₅/TiO₂ catalysts for NH₃-SCR

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Experimental

1 Catalyst preparation

The 1.0 wt.% V₂O₅/TiO₂ catalysts were synthesized by a ball-milling method adopting NH₄VO₃ as the vanadium precursor. NH₄VO₃, H₂O (when needed), and TiO₂ (DT-51, Millennium Chemicals) were mixed with several 5- and 10-mm diameter sintered alumina grinding balls in a grinding jar. A QM-3SP2 planetary ball mill was used to carry out the milling procedure at 30 Hz for 1 h. The resulting powders were dried at 100 °C overnight and then calcined at 500 °C for 4 h. The catalyst without H₂O participating in the milling process was denoted as VTi-1, and the one with H₂O (1 ml H₂O / 6 g TiO₂) was denoted as VTi-2.

2 Catalytic activity test

The activity tests were performed in a fixed-bed quartz flow reactor with 0.15 mL of the catalyst (40-60 mesh). The reaction gas consisted of 500 ppm NH₃ and NO, 5% O₂, balanced with N₂. The total flow rate was 500 mL min⁻¹, with a gas hourly space velocity (GHSV) of 100 000 h⁻¹. The concentrations of NO, NO₂, N₂O, and NH₃ were continuously analyzed by a Fourier transform infrared gas analyzer (Thermo Fisher IGS) equipped with a 2 m gas cell.

3 Catalyst characterization

NH₃ temperature-programmed desorption (NH₃-TPD) and H₂ temperature-programmed reduction (H₂-TPR) were conducted using the procedures reported in our previous works.¹ Nuclear magnetic resonance spectroscopy (NMR) and *in situ* diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) were carried out using the procedures reported in our previous works.²

Results

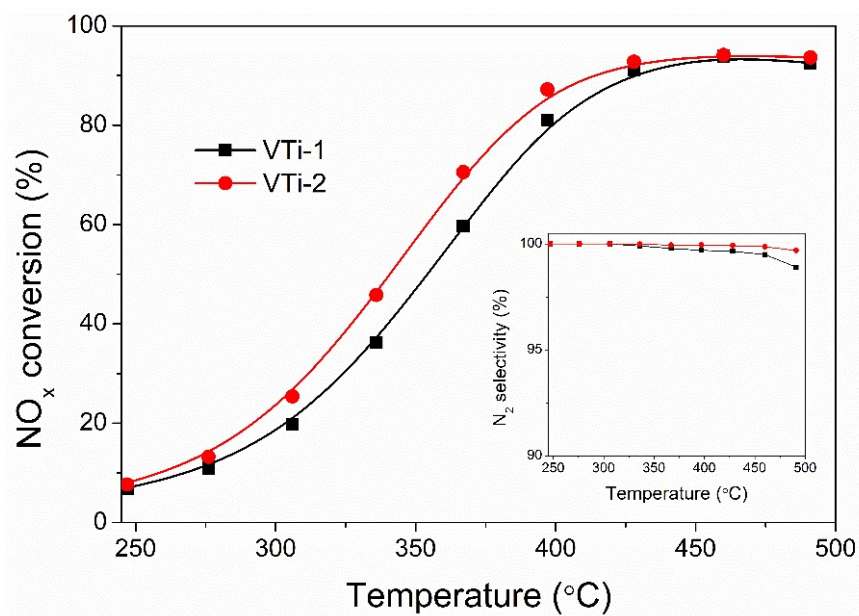


Figure S1. NH₃-SCR activity over vanadia-based catalysts in the presence of water. Reaction conditions: [NO]=500 ppm, [NH₃]=500 ppm, [H₂O]=5%, [O₂]=5%, balance N₂, GHSV=100 000 h⁻¹.

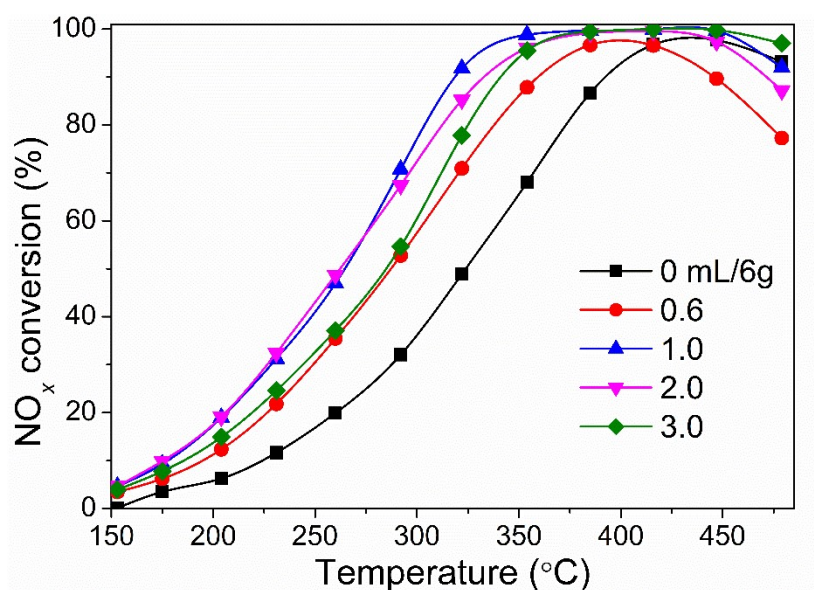


Figure S2 NO_x conversion over vanadia-based catalysts with different amount of water in ball-milling process.

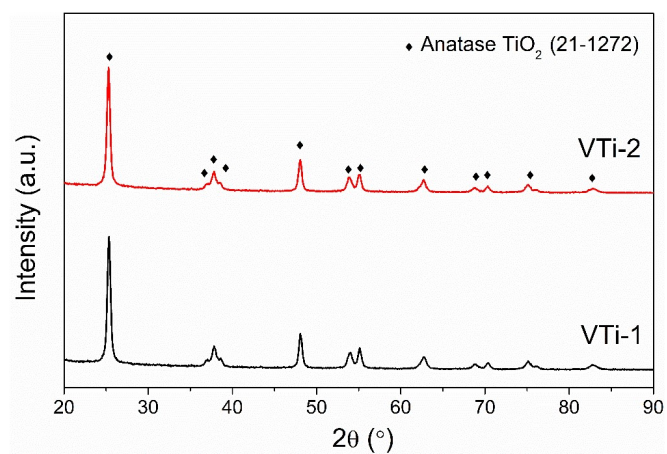


Figure S3. XRD results of vanadia-based catalysts.

Table S1. N₂ physisorption results of vanadia-based catalysts.

Catalysts	Specific surface area	Average pore diameter	Pore volume
VTi-1	66.40	15.78	0.293
VTi-2	67.74	13.52	0.259

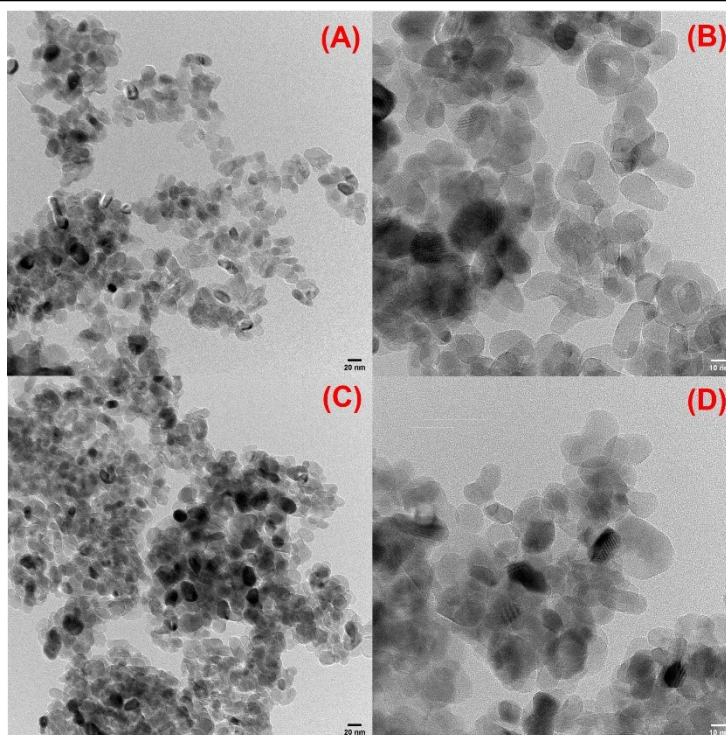


Figure S4 TEM images of VTi-1 (A, B) and VTi-2 (C, D).

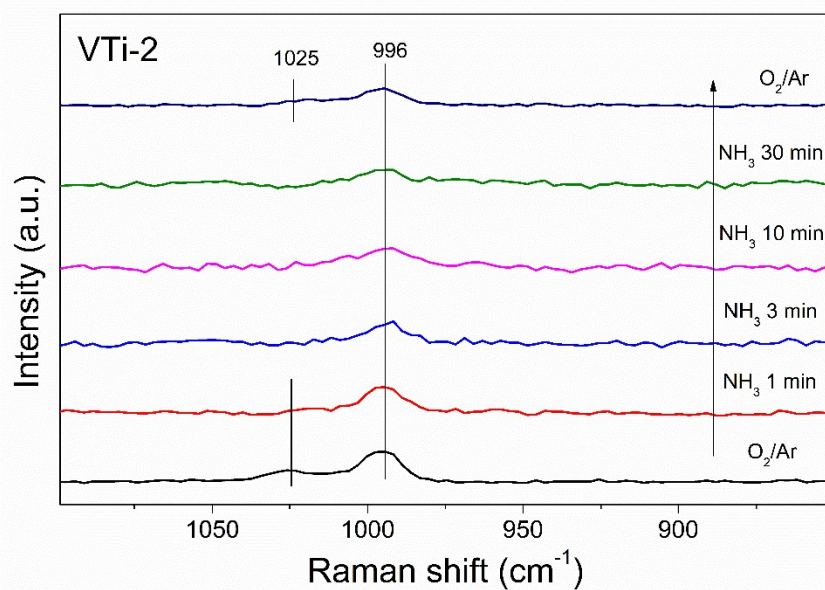


Figure S5. In situ Raman spectra of VTi-2 under different atmosphere at 200 °C.

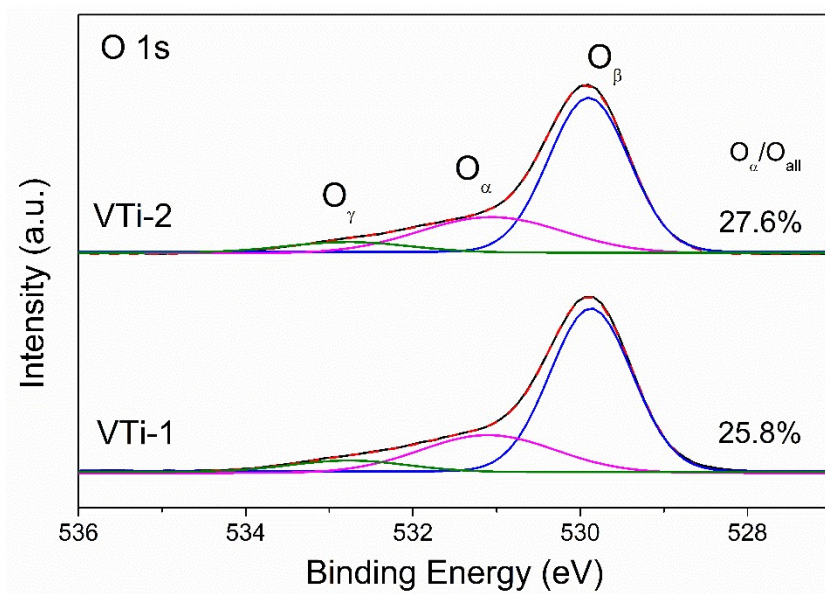


Figure S6. XPS results of O 1s on vanadia-based catalysts.

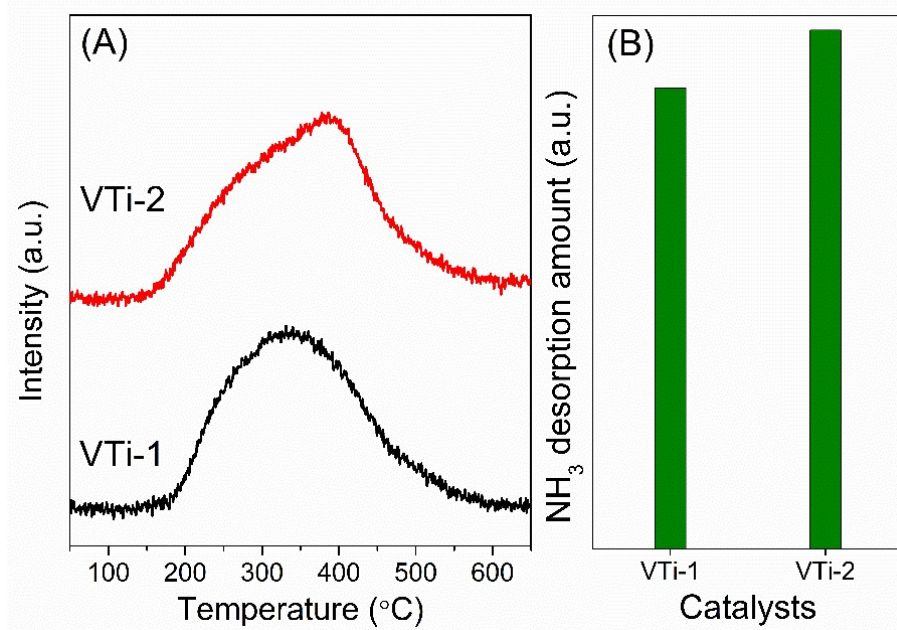


Figure S7. NH_3 -TPD results (A) and NH_3 desorption amount (B) of vanadia-based catalysts.

References

1. Z. Lian, J. Wei, W. Shan, Y. Yu, P. M. Radjenovic, H. Zhang, G. He, F. Liu, J. F. Li, Z. Q. Tian and H. He, *J. Am. Chem. Soc.*, 2021, **143**, 10454-10461.
2. G. He, Z. Lian, Y. Yu, Y. Yang, K. Liu, X. Shi, Z. Yan, W. Shan and H. He, *Sci. Adv.*, 2018, **4**, eaau4637.