Supporting

Vanadium-density-dependent thermal decomposition of NH₄HSO₄ on

V₂O₅/TiO₂ SCR catalysts

Tong Tong[a,b], Jianjun Chen[a,b*], Shangchao Xiong[a,b], Wenhao Yang[a,b], Qilei Yang[a,b], Lijun Yang[c], Yue

Peng[a,b], Zhiming Liu[c], Junhua Li[a,b]

a State Key Joint Laboratory of Environment Simulation and Pollution Control

School of Environment, Tsinghua University, Beijing, 100084, China

b.   *National Engineering Laboratory for Multi Flue Gas Pollution Control Technology and*

Equipment, School of Environment, Tsinghua University, Beijing, 100084, China

c. *State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical*

Technology, Beijing 100029, China

*Corresponding Author: Jianjun Chen

Phone: +86 10 62771093; fax: +86 10 62771093;

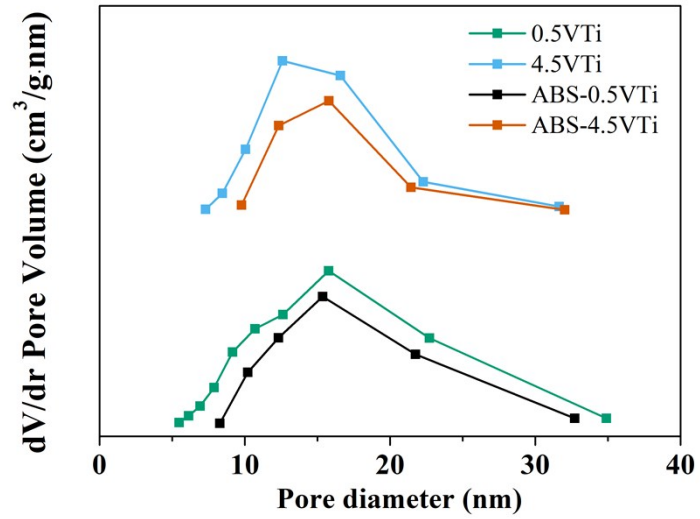*E-mail addresses: chenjianjun@tsinghua.edu.cn*

Fig.S1. BJH pore size distributions of the fresh catalysts and ABS-deposited catalysts.

Figure S1 shows the pore size distribution by BJH method of the catalysts. It can be seen that the pore volume corresponding to each pore size of the catalysts decreases, indicating that ABS was uniformly deposited in the catalysts pores.
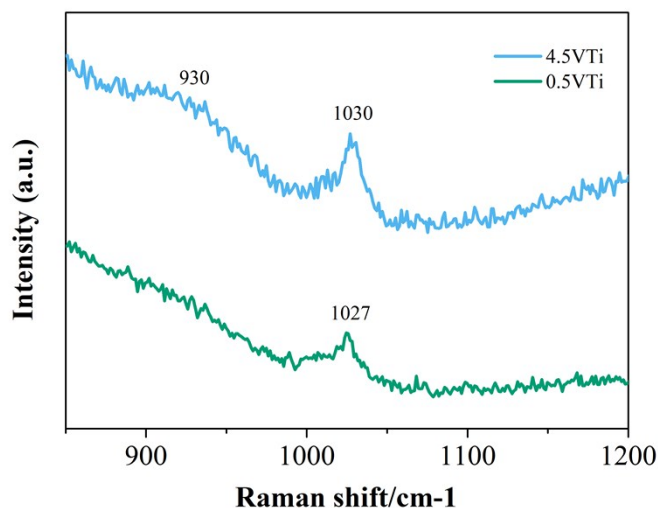
Fig.S2. Raman spectra of the fresh catalysts and ABS-deposited catalyst.

The Raman band at 1027 and 1030 cm^{-1} corresponds to the vibration of the terminal V=O bond. With the increase of oligomeric surface VOx sites, the shift from 1027 to 1030 cm^{-1} is attributed to the vibrational coupling of adjacent V=O bonds[1, 2]. The broad Raman band at 920−940 cm−1 on the 4.5V catalyst is arises from the vibrations of the bridging V−O−Ti bonds[3, 4].
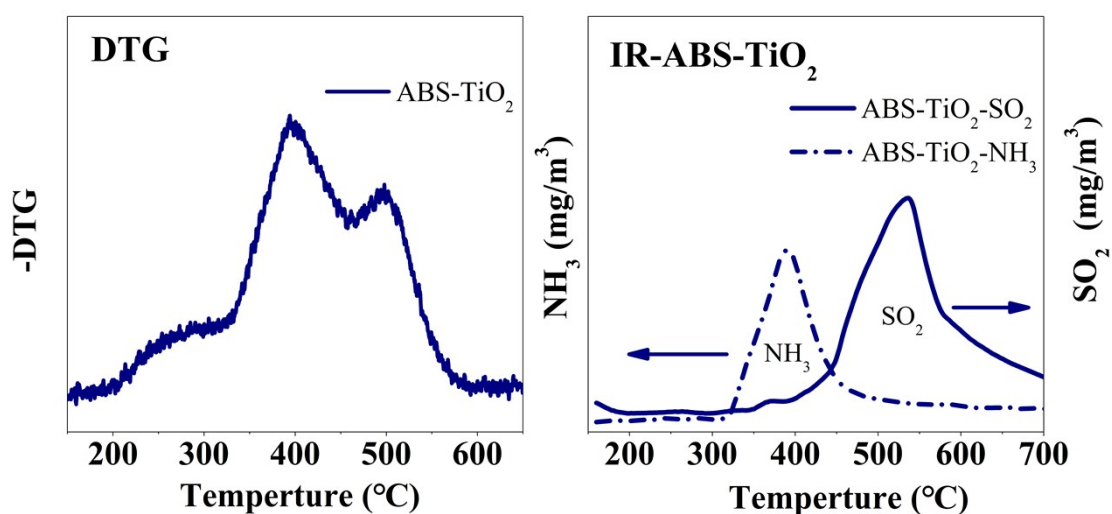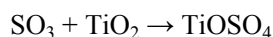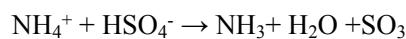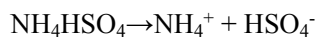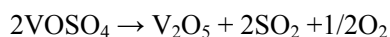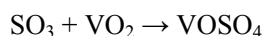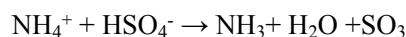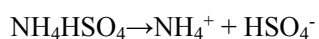

Fig.S3. DTG-IR of ABS-deposited TiO$_2$ catalysts.

The decomposition of ABS on V_2O_5/TiO_2 catalysts could be described by the following equations:

For the V_2O_5/TiO_2 catalyst with relatively a low vanadia loading:

$$NH_4HSO_4 \rightarrow NH_4^+ + HSO_4^-$$

$$NH_4^+ + HSO_4^- \rightarrow NH_3 + H_2O + SO_3$$

$$SO_3 + TiO_2 \rightarrow TiOSO_4$$

$$2TiOSO_4 \rightarrow 2TiO_2 + 2SO_2 + O_2$$

For the V_2O_5/TiO_2 catalyst with relatively a high vanadia loading:

$$NH_4HSO_4 \rightarrow NH_4^+ + HSO_4^-$$

$$NH_4^+ + HSO_4^- \rightarrow NH_3 + H_2O + SO_3$$

$$SO_3 + VO_2 \rightarrow VOSO_4$$

$$2VOSO_4 \rightarrow V_2O_5 + 2SO_2 + 1/2O_2$$

References

[s1] Vuurman, W. M.A, Structural determination of supported V_2O_5-WO_3/TiO_2 catalysts by in situ Raman spectroscopy and x-ray photoelectron spectroscopy J. Phy. Chem. (1991).

[s2] S.K. Du, Surface structures of supported tungsten oxide catalysts under dehydrated conditions, J. Mol. Catal. A: Chem. 106 (1996) 93-102.

[s3] S.F. Vyboishchikov, J. Sauer, (V_2O_5)n Gas-Phase Clusters (n =1−12) Compared to V_2O_5 Crystal: DFT Calculations, J. Phys. Chem. A 105 (2001) 8588-8598.

[s4] S. Guimond, M.A. Haija, S. Kaya, J. Lu, J. Weissenrieder, S. Shaikhutdinov, H. Kuhlenbeck, H.J. Freund, J. Döbler, J.J.T.i.C. Sauer, Vanadium oxide surfaces and supported vanadium oxide nanoparticles, Top. Catal. 38 (2006) 117-125.