Supporting Information

New insight into the promotion effect of Cu doped V_2O_5/WO_3-TiO_2 for low temperature NH_3-SCR performance

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NH_3-SCR performance without H_2O

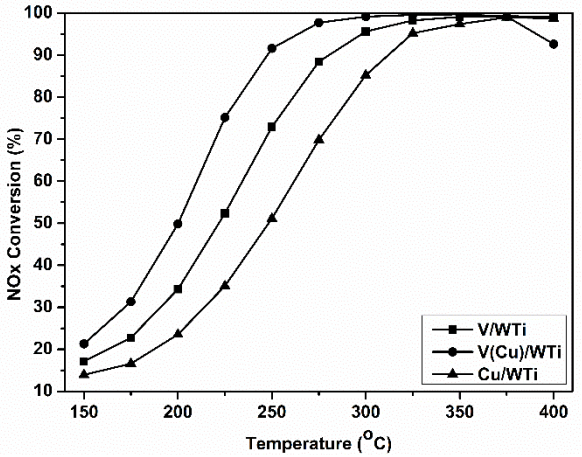

Fig.S1 NH_3-SCR performance on V/WTi, V(Cu)/WTi and Cu/WTi catalysts without H_2O. 500 ppm NH_3, 500 ppm NO, 5 % O_2 and N_2 balance, GHSV=10,000 h^{-1}.

Table S1 surface coverages of Vanadium species on catalysts

Samples	S_{BET} （m^2/g）	V ($\mu mol/m^2$)
V/WTi	41	2.7
V(Cu)/WTi	37	2.9

Raman

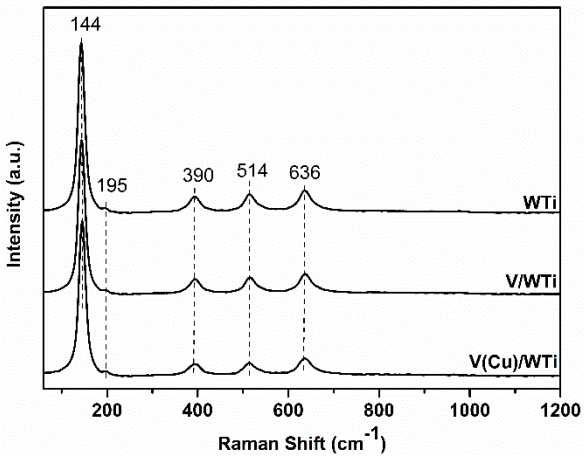

Fig.S2 Raman spectra of the catalysts

XPS

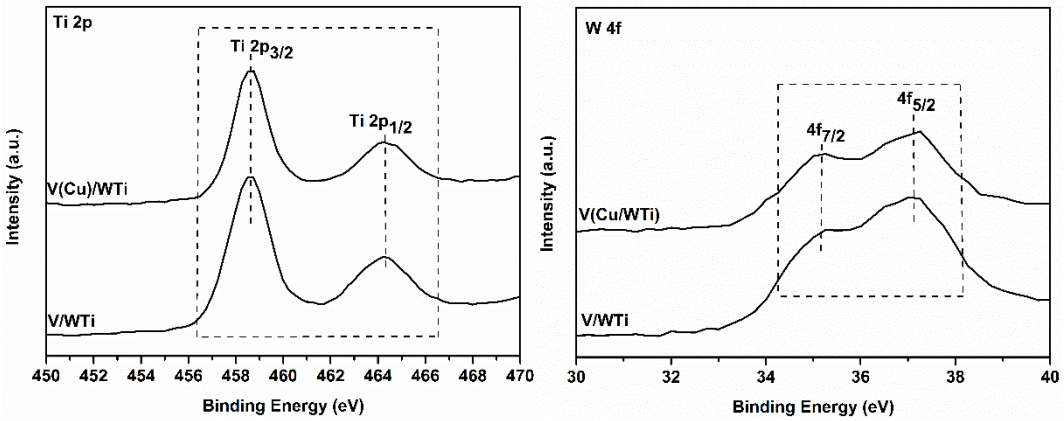

Fig.S3 XPS spectra of the obtained samples: Ti 2p, W 4f.

Reaction between $NO+O_2$ and adsorbed NH_3 species

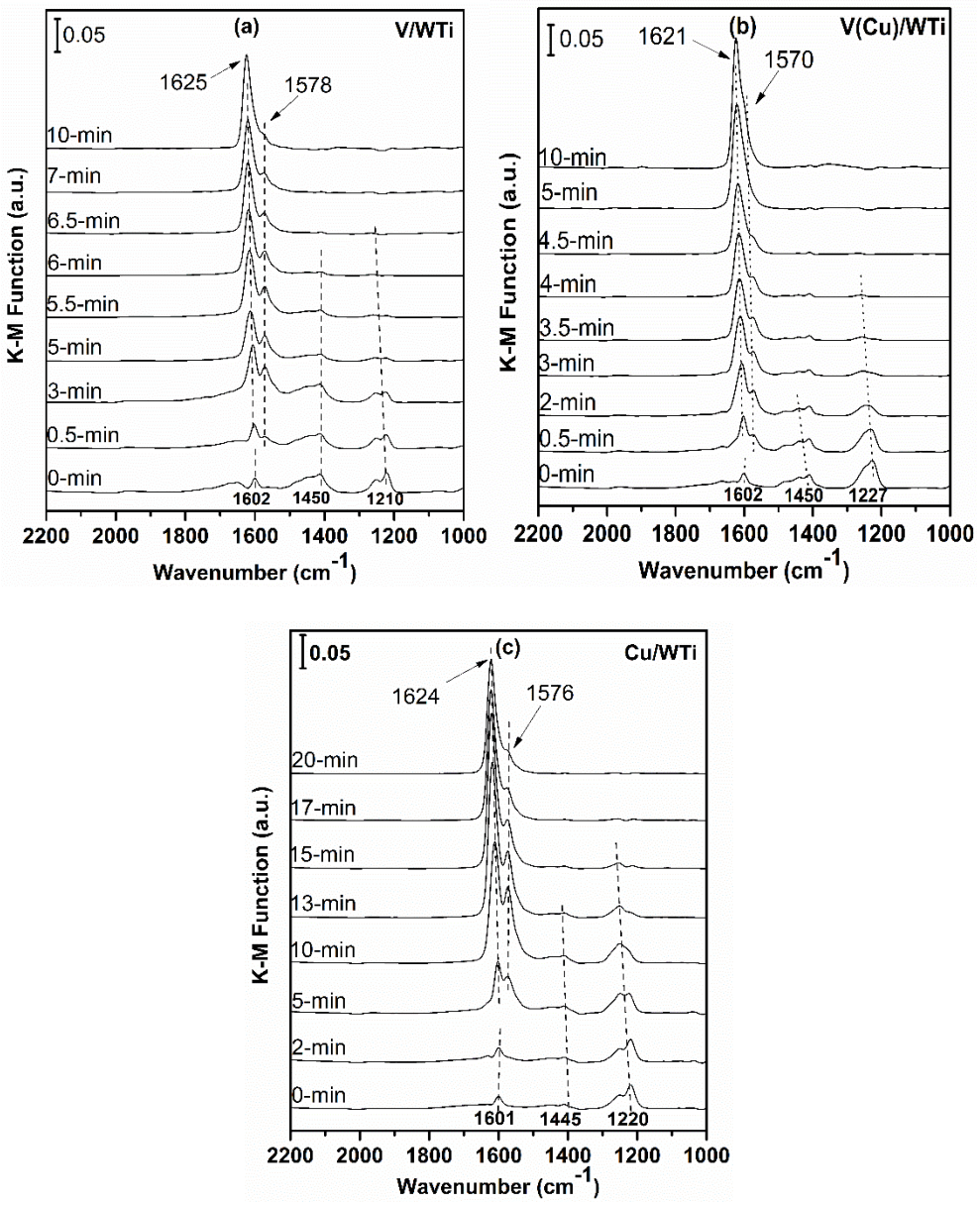

Fig.S4 DRIFTS spectra of catalysts pretreated with 3000 ppm NH_3, followed by exposed to 3000 ppm NO+4 % O_2 as a function of time at 200˚C.

For V/WTi sample, after NH_3 were pre-adsorbed and N_2 purging for 30 min, the coordinate NH_3 lined to Lewis acid sites (1602 and 1210 cm^{-1}) and Brønsted (1672 and 1450 cm^{-1}) acid sites form on the surface. After $NO+O_2$ introduced, the intensities of

all bands assigned to NH_3 species decrease. Meanwhile, some new bands attributed to adsorbed nitrate species (1625 and 1578 cm^{-1}) appear. The result indicates the adsorbed NH_3 species are reactive in the NH_3-SCR process. For Cu/WTi sample, similar bands due to NH_3 adsorption species are observed, introducing $NO+O_2$ results in the NH_3 adsorption species decreasing slowly, accompanying the appearance of nitrates species (1624 and 1576 cm^{-1}). For V(Cu)/WTi sample, the similar phenomenon can be observed during the process. But the consumption rate of the NH_3 adsorption species linked to the Lewis sites distinguishes from other catalysts.

NH_3+NO+O_2 reaction

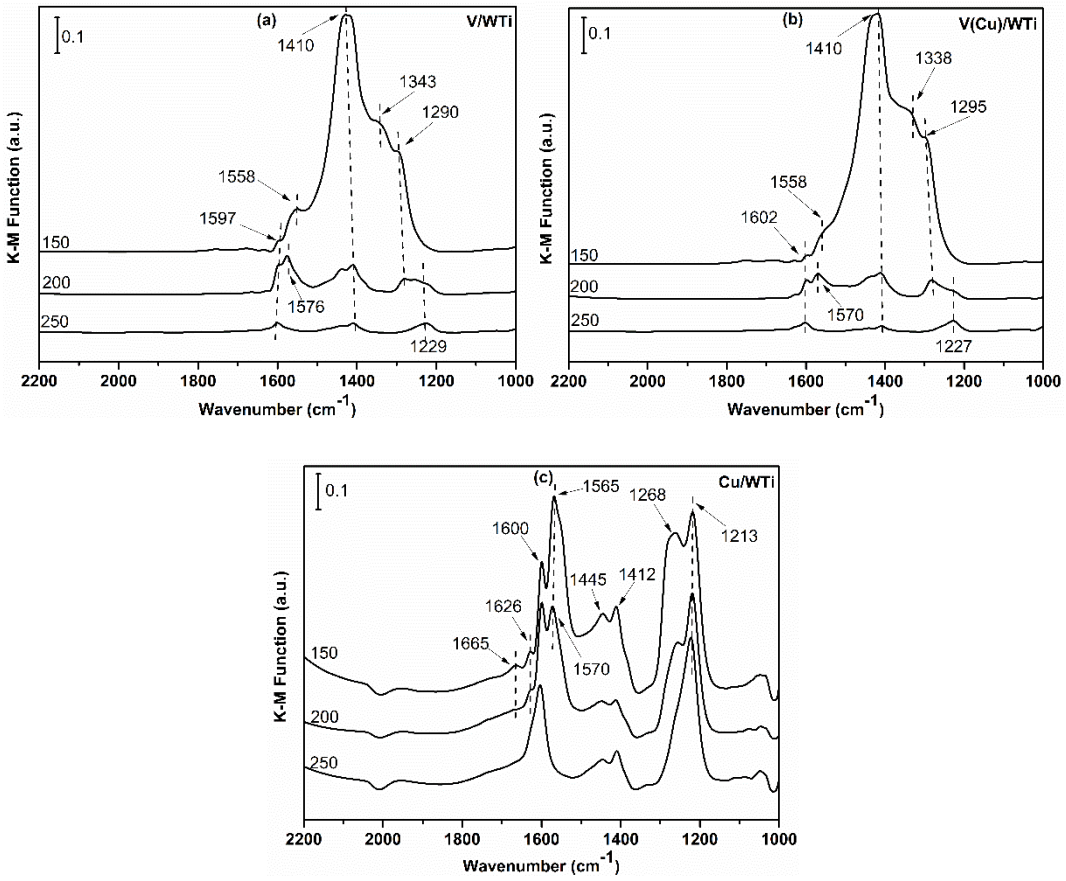

Fig.S5 DRIFTS spectra of catalysts in a flowing of NH_3+ NO+ O_2 at 150, 200 and 250˚C.

To investigate the surface species on the catalyst under the steady-state condition, DRIFTS spectra were recorded in a flow of $NO+NH_3+O_2$ from 150 to 250 ˚C. On the V/WTi sample, bands due to nitrates (1290 cm^{-1}), coordinated NH_4^+ (1434 cm^{-1}), -NH_2 species (1558 cm^{-1}) and NH_3 (1597 cm^{-1}) are observed at 150 ˚C. In addition, a new band appears at 1343 cm^{-1}, which is significantly different from the adsorbed nitrates and NH_3 species mentioned above, which can be attributed to the intermediates species converted by surface adsorbed NH_3 and NO_x species [1, 2]. With the increasing of temperature to 250 ˚C, the intermediates species (1343 cm^{-1}) and the nitrates (1290cm^{-1}) vanished completely with the NH_4^+ (1434 cm^{-1}) diminishing quickly. During the process, -NH_2 species (1558 cm^{-1}) disappear with nitrates (1576 cm^{-1}) appearing, and then only adsorbed NH_3 species (1597 and 1229 cm^{-1}) still exist at 250 ˚C. In regard with the V(Cu)/WTi sample, the similar process can be observed. While the intensities of -NH_2 species (1558 cm^{-1}) are obviously weaker than those of V/WTi sample, which indicates that -NH_2 species (1558 cm^{-1}) adsorbed on the V(Cu)/WTi are higher active than those of V/WTi sample. The intensities of -NH_2 species almost vanished at 200 ˚C due to the rapid consumption by the NO_x reagent, which is in agreement with the results of reaction between $NO+O_2$ and adsorbed NH_3 species. Meanwhile, the band of nitrates species at 1570 cm^{-1} appears and the intensities of them are obviously weaker than those of V/WTi sample, which may be caused by the competitive adsorption between NH_3 and $NO+O_2$ or the weaker adsorbed nitrates on the catalyst surface. Therefore it is beneficial for the reaction between adsorbed NH_3 species and the gas NO or weak

adsorbed NO according to the E-R mechanism imposed by Topsøe [3]. In view of Cu/WTi sample, it is clear that no intermediates species (1335 cm^{-1}) can be observed and large amounts of $–NH_2$ species (1565 cm^{-1}) exist on the catalyst surface at 150˚C, which strongly indicates the weakest NH_3-SCR performance among the threes catalysts at low temperature.

Notes and references

1. L. Chen, J. Li and M. Ge, *Environ. Sci. Technol.*, 2010, **44**, 9590-9596.
2. X. Yao, L. Zhang, L. Li, L. Liu, Y. Cao, X. Dong, F. Gao, Y. Deng, C. Tang, Z. Chen, L. Dong and Y. Chen, *Appl. Catal., B*, 2014, **150–151**, 315-329.
3. J. A. Dumesic, N. Y. Topsøe, H. Topsøe, Y. Chen and T. Slabiak, *J. Catal.*, 1996, **163**, 409-417.