

A novel mechanism for poisoning of metal oxides SCR catalyst: base-acid explanation correlated with redox property

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Electronic Supplementary Information

Catalyst preparation

The CeMo/Ti and VW/Ti catalysts were prepared by impregnation method. Degussa AEROSIL TiO₂ P25 was used as support. 10 wt.% CeO₂-MoO₃/TiO₂ catalyst (the molar ratio of Ce:Mo=2:1, loading 10 wt.% totally) was prepared by impregnating TiO₂ powder with an aqueous solution of cerium nitrate (Ce(NO₃)₃·6H₂O), ammonium molybdate ((NH₄)₆Mo₇O₂₄·4H₂O) and oxalic acid (H₂C₂O₄·2H₂O), stirred for 4 h, then dried at 120 °C and calcined at 500 °C for 4 h in air. For comparison, the V₂O₅-WO₃/TiO₂ catalyst with 1 wt.% V₂O₅ and 5 wt.% WO₃ was also prepared by the same impregnation method using NH₄VO₃, (NH₄)₁₀W₁₂O₄₁, and H₂C₂O₄·2H₂O as precursors.

The Mn-Ce-O catalyst was prepared by co-precipitation method. Manganese nitrate and cerium nitrate were employed as precursors for catalyst components; ammonium carbonate was utilized as a precipitator. The mash obtained from co-precipitation underwent ultrasonication, filtration, thorough washing with DI water, desiccation, and final calcination at 500 °C for 6 h in static air. MnO₂ were synthesized by hydrothermal methods. KMnO₄ and MnSO₄·H₂O were mixed in distilled water and then hydrothermal treated in a Teflon-lined autoclave at 160 °C for 12h.

Characterization of NH⁴⁺ and Cl⁻ after SCR reaction with HCl

After SCR activity test with HCl, the CeMo/Ti and VW/Ti samples were characterized by ICP. 0.45 wt.% of Cl⁻ and 0.15 wt.% of NH⁴⁺ were found in CeMo/Ti sample; meanwhile, 0.10 wt.% of Cl⁻ and 0.91 wt.% of NH⁴⁺ were found in VW/Ti sample.

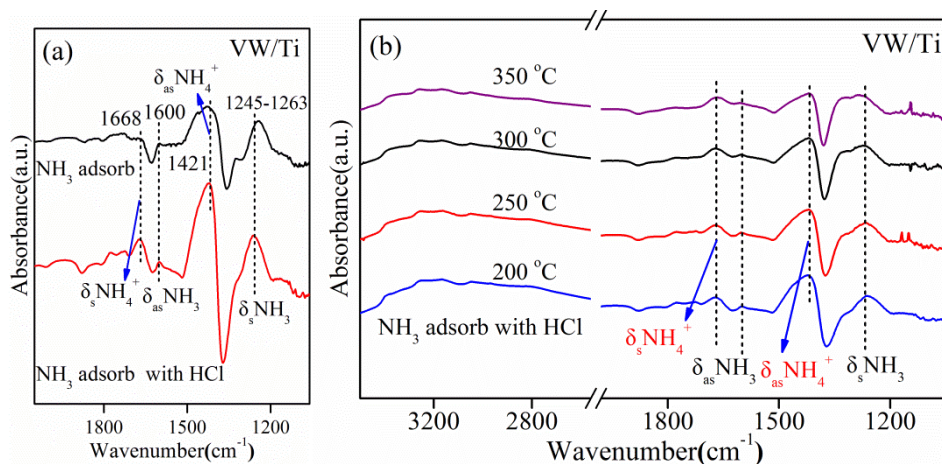


Fig. S1 DRIFT spectra of the effect of HCl on NH₃ adsorption over VW/Ti catalyst at different temperatures.

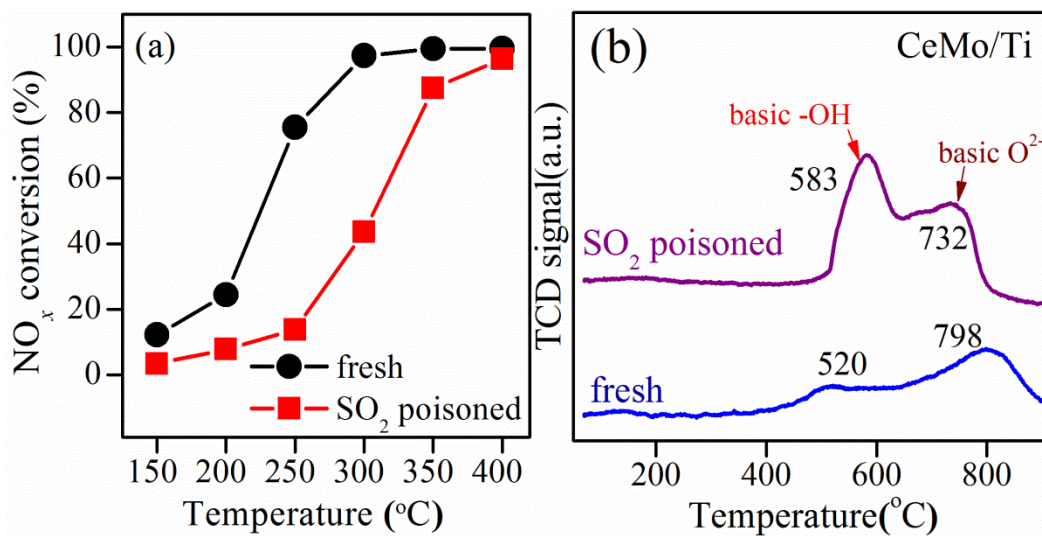


Fig. S2 The effect of SO₂ poisoning on the SCR activity over CeMo/Ti catalyst (a); and CO₂-TPD curves of fresh and SO₂ poisoned CeMo/Ti catalysts.

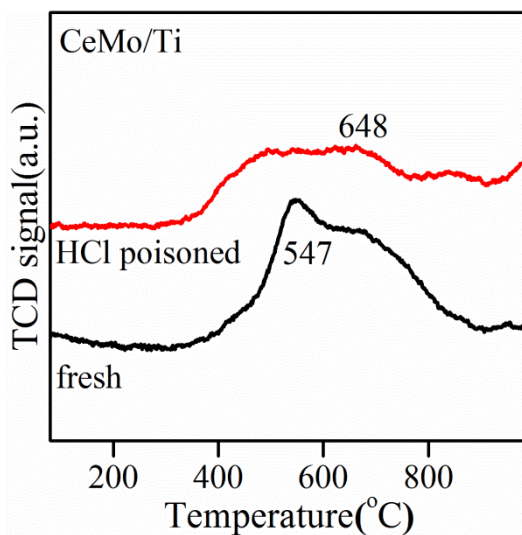


Fig. S3 The H₂-TPR spectra of CeMo/Ti catalyst before and after HCl poisoning.

The H₂ temperature programmed reduction (H₂-TPR) was carried out with a Micromeritics AutoChem II 2920 instrument. Prior to H₂-TPR experiment, the sample was preheated in a He flow at 450 °C for 1 h. The consumed amount of H₂ as a function of temperature was evaluated by the signal of Thermal Conductivity Detector (TCD). The fresh CeMo/Ti sample showed a broad band at 400-800 °C, with a sharp peak at 547 °C. After HCl poisoning, the broad band could also be seen, but the peak disappeared.

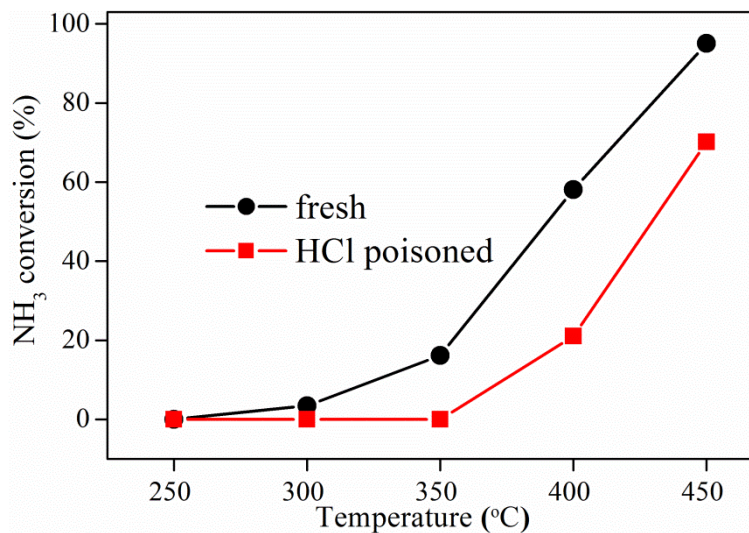


Fig. S4 The effect of HCl poisoning on NH₃ conversion in NH₃ oxidation over CeMo/Ti catalyst.

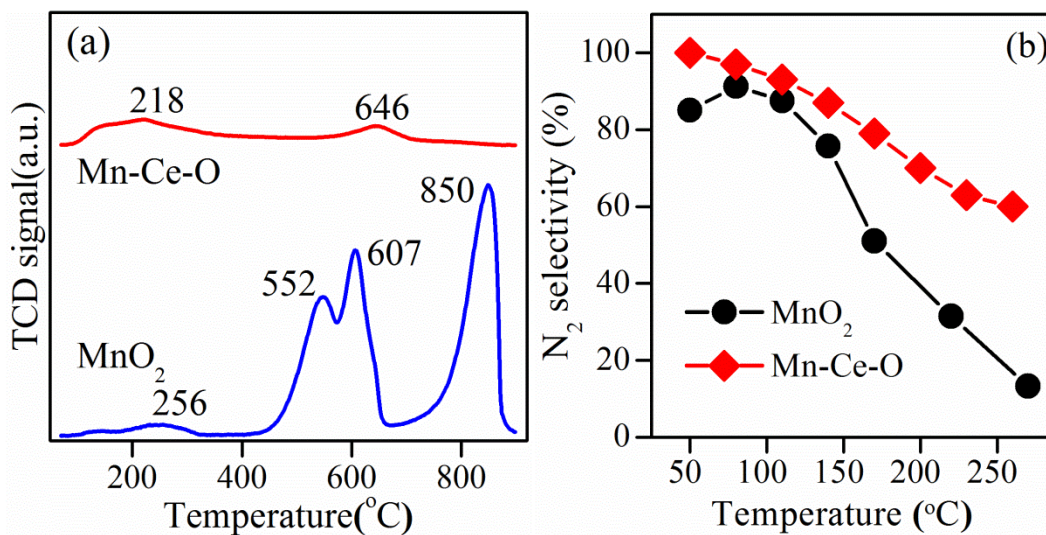


Fig. S5 (a) CO₂-TPD curves of MnO₂ and Mn-Ce-O catalysts; (b) N₂ selectivity vs temperature in SCR reaction over two catalysts.

Table. S1 BET specific surface area of HCl and NH₄Cl poisoned catalysts.

Samples		BET surface area (m ² g ⁻¹)
VW/Ti	fresh	95.00
	HCl poisoned	91.45
	NH ₄ Cl poisoned	94.01
CeMo/Ti	fresh	53.24
	HCl poisoned	51.39
	NH ₄ Cl poisoned	54.99