

Supporting Information

TiO₂-modified CeVO₄ catalyst for the selective catalytic reduction of NO_x with NH₃

Yingjie Li ^{a,b,c}, Zhihua Lian ^{a*}, Jinhan Lin ^{a,b}, Meng Wang ^{a,b}, Wenpo Shan ^{a,b *}

^a Center for Excellence in Regional Atmospheric Environment and Key Laboratory of Urban Pollutant Conversion, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China;

^b Zhejiang Key Laboratory of Urban Environmental Processes and Pollution Control, Ningbo Urban Environment Observation and Research Station, Institute of Urban Environment, Chinese Academy of Sciences, Ningbo 315800, China;

^c University of Chinese Academy of Sciences, Beijing 100049, China

Table S1 Physical properties of the catalysts.

Sample	S _{BET} (m ² /g) ^a	V _p (cm ³ /g) ^b	D _p (nm) ^c	Crystallite size (nm) ^d
CeVO ₄	20.3	0.14	28.4	25.0
CeVTi _{2.5}	33.6	0.12	14.4	16.8
CeVTi ₅	50.6	0.14	10.2	4.9
CeVTi ₁₀	88.9	0.23	8.6	6.3
CeVTi ₂₀	105.3	0.27	8.7	6.5
TiO ₂	106.8	0.19	5.0	9.1

^a BET surface area^b BJH desorption pore volume^c BJH adsorption pore size^d Scherrer equation from XRD data

Table S2 The results of H₂ consumption.

Sample	H ₂ consumption (μmol/g) ^a		
	Below 600 °C	Above 600 °C	Total
CeVO ₄	102	3763	3866
CeVTi _{2.5}	2375	1206	3581
CeVTi ₅	2463	186	2620
CeVTi ₁₀	1835	160	1995
CeVTi ₂₀	1079	79	1158
TiO ₂	28	-	28
V ₂ O ₅	-	11878	11878
CeO ₂	1008	937	1945

^a quantified by the H₂-TPR

Table S3 The surface atomic concentration of CeVTi_x catalysts obtained from XPS.

Sample	Surface atomic concentration (%)				
	Ce	V	Ti	O	Surface V/Ce molar ratio
CeVO ₄	15.08	15.25	-	69.67	1.01
CeVTi _{2.5}	5.82	7.80	18.06	68.32	1.34
CeVTi ₅	4.01	5.57	22.43	67.99	1.39
CeVTi ₁₀	2.50	4.22	26.81	66.47	1.69
CeVTi ₂₀	1.44	2.77	29.47	66.32	1.92
TiO ₂	-	-	25.70	74.30	-

Table S4 The XPS results on Ce-V-Ti catalysts.

Sample	O _α /(O _α + O _β + O _γ) (%)	Ce ⁴⁺ /(Ce ³⁺ + Ce ⁴⁺) (%)	V ⁴⁺ /(V ⁴⁺ + V ⁵⁺) (%)
CeVO ₄	9.4	35.2	4.6
CeVTi _{2.5}	15.3	53.9	22.6
CeVTi ₅	19.5	54.9	26.0
CeVTi ₁₀	15.9	46.1	20.5
CeVTi ₂₀	15.0	43.9	16.7
TiO ₂	12.5	-	-

Table S5 Amounts of NH₃ adsorption over Ce-V-Ti catalysts.

Samples	NH ₃ adsorption (μmol/g)
CeVO ₄	41.3
CeVTi _{2.5}	68.1
CeVTi ₅	124.5
CeVTi ₁₀	221.9
CeVTi ₁₀	252.2
TiO ₂	313.4

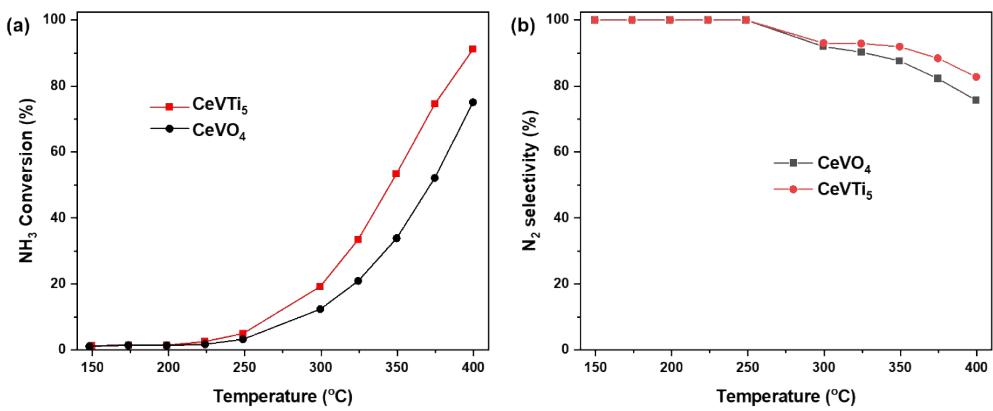


Fig. S1 NH₃ conversion in NH₃ oxidation reactions over CeVO₄ and CeVTi₅ catalysts. NH₃ oxidation efficiency (a), selectivity for N₂ (b). Reaction conditions: 500 ppm NH₃, 5% O₂ and N₂ balance, under a GHSV of 200,000 h⁻¹.

In the oxidation of NH₃ reaction, the NH₃ conversion and the selectivity for the formation of N₂ were defined by the following equations:

$$\text{NH}_3 \text{ conversion} = \left(\frac{[\text{NH}_3]_{\text{in}} - [\text{NH}_3]_{\text{out}}}{[\text{NH}_3]_{\text{in}}} \right) \times 100\% \quad (1)$$

$$\text{N}_2 \text{ selectivity} = \left(1 - \frac{[\text{NO}]_{\text{out}} + [\text{NO}_2]_{\text{out}} + 2[\text{N}_2\text{O}]_{\text{out}}}{[\text{NH}_3]_{\text{in}} - [\text{NH}_3]_{\text{out}}} \right) \times 100\% \quad (2)$$

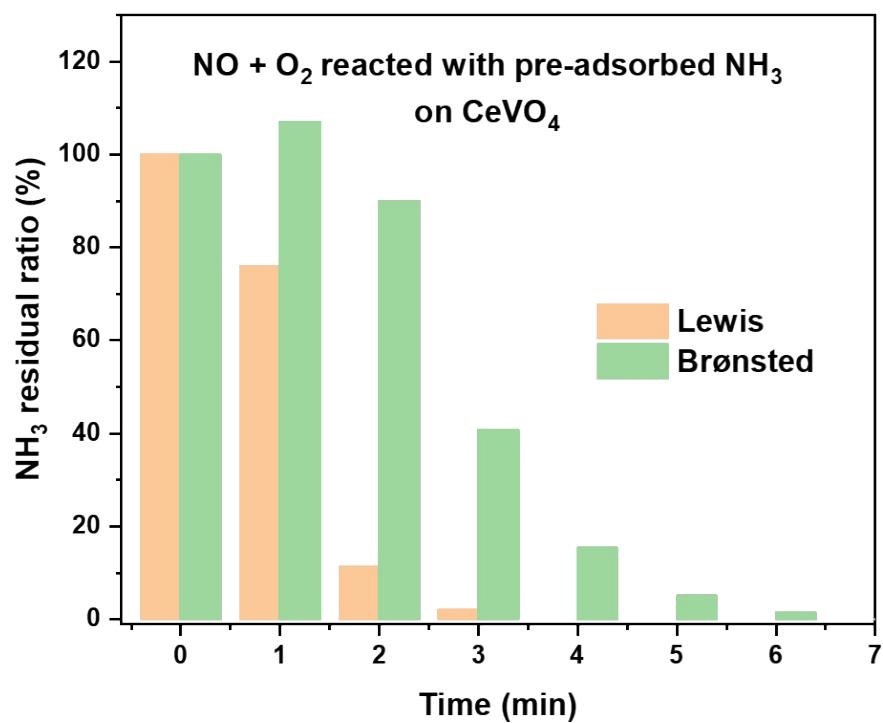


Fig. S2 The NH₃ residual ratio by calculating integral area at Lewis acid site (1187 cm⁻¹) and Brønsted acid site (1423 cm⁻¹) with the reaction time under the reaction between NO + O₂ and pre-adsorbed NH₃ on CeVO₄ catalyst.

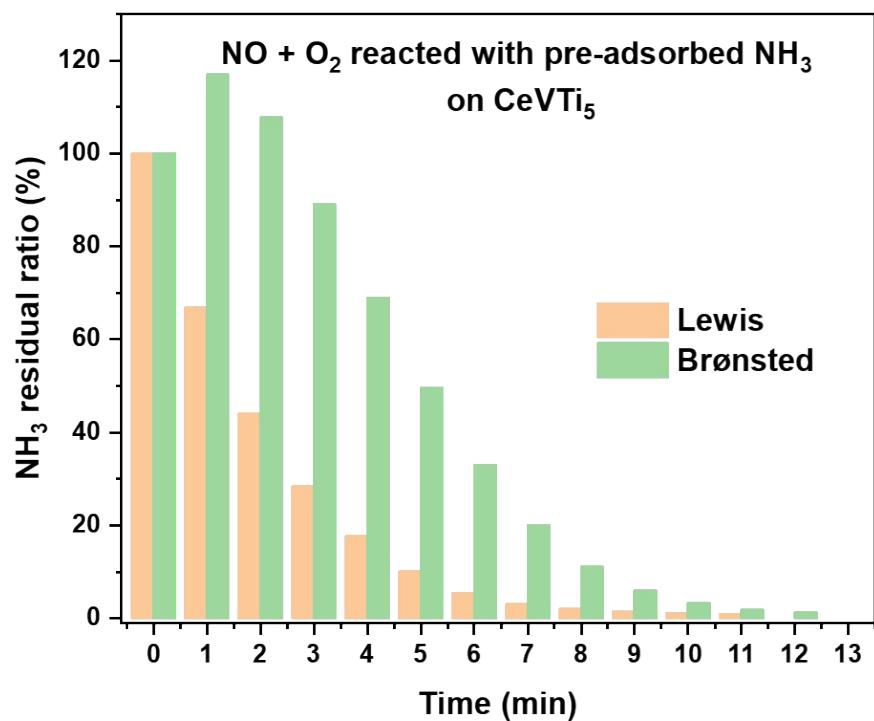


Fig. S3 The NH₃ residual ratio by calculating integral area at Lewis acid site (1228 cm⁻¹) and Brønsted acid site (1423 cm⁻¹) with the reaction time under the reaction between NO + O₂ and pre-adsorbed NH₃ on CeVTi₅ catalyst.