

1 **Characterization of WMnCeTiO_x Catalysts Prepared by Different Methods for**
2 **Selective Reduction of NO with NH₃**

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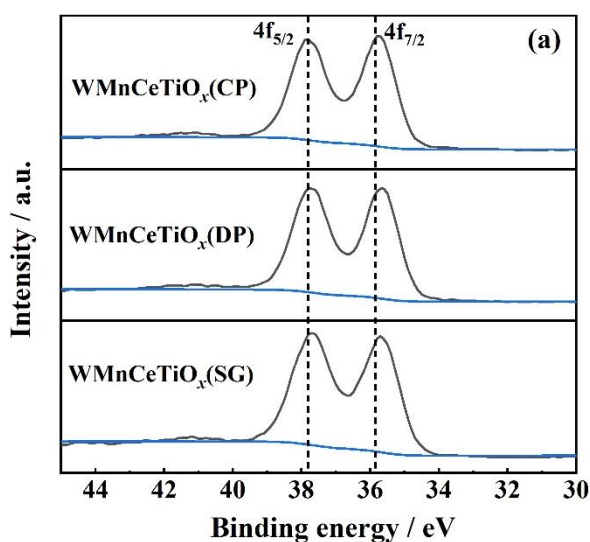
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12 **1. XPS**



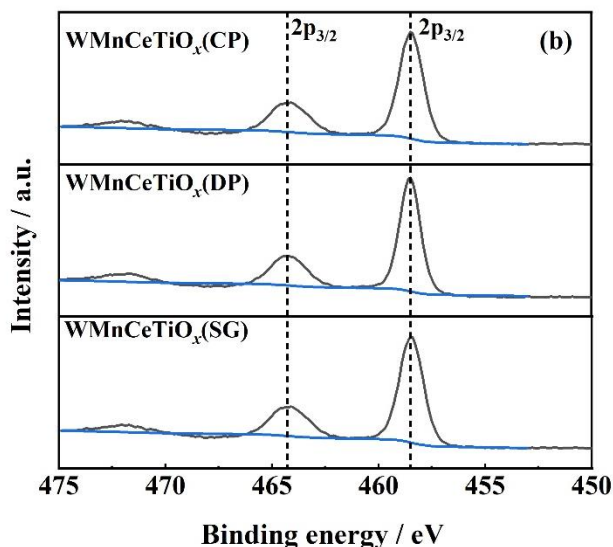


Fig. S1 XPS spectra of W 2*f*(a) and Ti 2*p* (b) of prepared catalysts

The spectra of W 2*f* and Ti 2*p* were shown in Fig. S1. The XPS spectra of W 2*f* over the prepared catalysts were presented in Fig. S1(a). The XPS spectra were divided into two sub-peaks of WO₃, indicating that the main existing form of W on the prepared catalysts is WO₃. It suggested that chemical valence may not be the main reason for SCR performance of the prepared for WMnCeTiO_x catalysts. The XPS spectra of Ti 2*p* over prepared catalysts were presented in Fig. S1(b), which can be fitted into two peaks. However, the spectrogram of Ti 2*P* in each catalyst is similar, indicating that the chemical valence state of Ti may not the main reason for the difference of catalyst activity.

2. In-situ DRIFTS

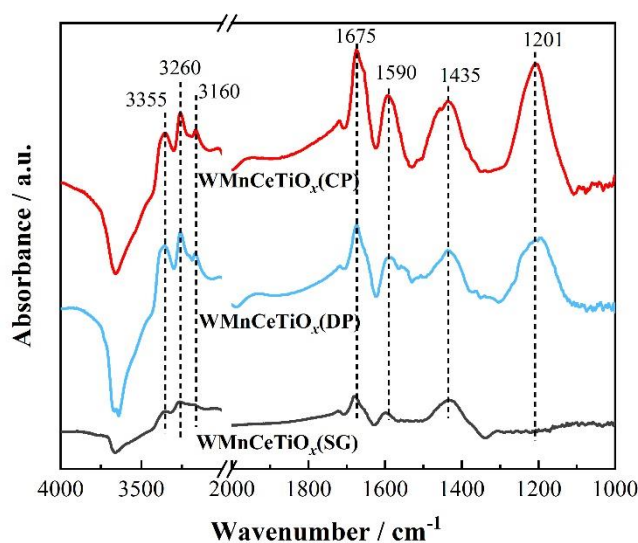
2.1 Adsorption of NH₃

Fig. S2 displayed the in-situ DRIFTS spectra of NH₃ adsorption over prepared catalysts. After pretreatment of the catalyst sample, 500 ppm of NH₃ was introduced into the feed gas for 30 min, and then IR spectra were recorded. Several bands were observed in the ranges of 1000–1700 and 3000–4000 cm⁻¹. the band at 1201, 1590 cm⁻¹ could be

33 assigned to symmetric and asymmetric bending vibrations of the N–H bonds in NH₃
34 coordinately linked to Lewis acid sites while the bands at 1675 and 1435 cm⁻¹ could be
35 attributed to asymmetric and symmetric bending vibrations of NH₄⁺ species on
36 Brønsted acid sites. In the NH stretching region, bands were found at 3355, 3260 and
37 3160 cm⁻¹.

38 The DRIFTS spectra of NH₃ adsorption on WMnCeTiO_x(CP) catalyst were very similar
39 to that of WMnCeTiO_x(DP) and WMnCeTiO_x(SG) catalyst. However, the band at 1201,
40 1435, 1790 and 1675 cm⁻¹ were much stronger than WMnCeTiO_x(DP) and
41 WMnCeTiO_x(SG) catalysts, which indicated that the surface acidity (Lewis and
42 Brønsted acid sites) of WMnCeTiO_x(CP) catalyst is stronger than WMnCeTiO_x(DP)
43 and WMnCeTiO_x(SG) catalyst, and WMnCeTiO_x(CP) catalyst has the higher NO_x
44 conversion efficiency than WMnCeTiO_x(DP) and WMnCeTiO_x(SG) catalysts at low
45 temperature (below 225 °C).

46 In brief, the results of both NH₃-TPD and DRIFTS characterizations indicated that the
47 adsorption capacity for NH₃ of the different WMnCeTiO_x catalysts decreases in the
48 order of WMnCeTiO_x(CP) > WMnCeTiO_x(DP) > WMnCeTiO_x(SG), which was
49 consistent with the change of catalytic activities for the corresponding catalysts. Thus,
50 it can be concluded that the difference between the activities of the three WMnCeTiO_x
51 catalysts is related to their NH₃ adsorption abilities.



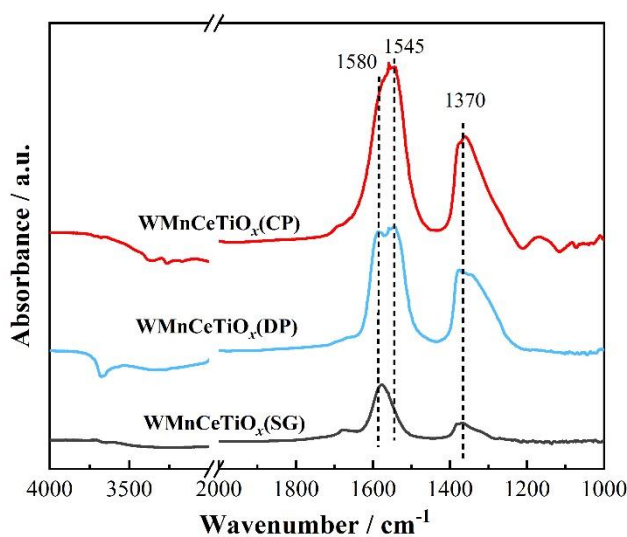
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53 Fig. S2 DRIFTS spectra of NH_3 adsorption on $\text{WMnCeTiO}_x(\text{CP})$, $\text{WMnCeTiO}_x(\text{DP})$

54 and $\text{WMnCeTiO}_x(\text{SG})$ catalysts at 250 °C

55 2.2. Adsorption of $\text{NO} + \text{O}_2$

56 Fig. S3. showed in-situ DRIFTS spectra of $\text{NO} + \text{O}_2$ adsorption over the prepared
 57 catalysts. After pretreatment of each catalyst sample, the catalysts were exposed to a
 58 flow of 500 ppm NO and 5 % O_2 at 250 °C for 30 min, and then IR spectra were recorded.
 59 Several distinct peaks were observed in the ranges of 1000-2000 cm^{-1} on WMnCeTiO_x
 60 catalyst. The bands appeared at 1358, 1370, 1545 and 1580 cm^{-1} , which were ascribed
 61 to bidentate nitrate (1545, 1580 cm^{-1}), monodentate nitrate(1370 cm^{-1}) .All of the bands
 62 over $\text{WMnCeTiO}_x(\text{CP})$ catalyst were higher than $\text{WMnCeTiO}_x(\text{DP})$ and
 63 $\text{WMnCeTiO}_x(\text{SG})$ catalysts. It demonstrated that more nitrate species had been
 64 adsorbed on the surface of $\text{WMnCeTiO}_x(\text{CP})$ catalyst. It has been reported that the
 65 adsorbed nitrate species can rapidly react with adjacent adsorbed NH_4^+ or NH_3 to
 66 produce more reactive intermediates, which can further react with gaseous NO to form
 67 N_2 and H_2O and promote the “fast SCR” reaction. This is consistent with the results of
 68 the activity measurements.



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70 Fig. S3 In-situ DRIFTS spectra of NO + O₂ adsorption on WMnCeTiO_x(CP), WMnCeTiO_x(DP)
71 and WMnCeTiO_x(SG) catalysts

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73 **Table S1** Comparison of NO_x conversion and SO₂ resistance with the literatures related with
74 WMnCeTiO_x catalysts

Catalysts	Reaction condition	NO _x conversion	SO ₂ resistance	Reference
WMnCeTiO _x (CP)	NO = NH ₃ = 500 ppm, O ₂ = 5 %, GHSV = 30000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 200 ppm (when used)	90 % (@200 °C)	89 % (@250 °C, 5 h)	This work
WMnCeTiO _x (DP)	NO = NH ₃ = 500 ppm, O ₂ = 5 %, GHSV = 30000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 200 ppm (when used)	90 % (@200 °C)	76 % (@250 °C, 5 h)	This work
WMnCeTiO _x (SG)	NO = NH ₃ = 500 ppm, O ₂ = 5%, GHSV = 30000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 200 ppm (when used)	90 % (@270 °C)	16 % (@250 °C, 5 h)	This work
CeO ₂ -WO ₃ (SP)	NO = NH ₃ = 500 ppm, O ₂ = 3 %, GHSV = 47000 h ⁻¹ ,	85 %	-	[1]

Catalysts	Reaction condition	NO _x conversion	SO ₂ resistance	Reference
	flow rate 300 mL/min,	(@200 °C)		
CeO ₂ -WO ₃ (IM)	NO = NH ₃ = 500 ppm, O ₂ = 3%, GHSV = 47000 h ⁻¹ , flow rate 300 mL/min,	79 % (@200 °C)	-	[1]
CeO ₂ -WO ₃ (SG)	NO = NH ₃ = 500 ppm, O ₂ = 3 %, GHSV = 47000 h ⁻¹ , flow rate 300 mL/min,	20 % (@ 200 °C)	-	[1]
Ce/TiO ₂ (IM)	NO = NH ₃ = 500 ppm, O ₂ = 5 %, GHSV = 30000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 100 ppm (when used)	92 % (@ 275 °C)	85 % (@ 300 °C, 10 h)	[2]
Ce-Nb-Ti(CP)	NO = NH ₃ = 1000 ppm, O ₂ = 3 %, GHSV = 90000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 500 ppm (when used)	80 % (@ 250 °C)	50 % (@ 250 °C, 10 h)	[3]
Ce-Nb-Ti(IM)	NO = NH ₃ = 1000 ppm, O ₂ = 3 %, GHSV = 90000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 500 ppm (when used)	80 % (@ 250 °C)	48 % (@ 250 °C, 10 h)	[3]
Ce-Nb-Ti(SP)	NO = NH ₃ = 1000 ppm, O ₂ = 3 %, GHSV = 90000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 500 ppm (when used)	55 % (@ 250 °C)	42 % (@ 250 °C, 10 h)	[3]
CeWTiO _x (IM)	NO = NH ₃ = 1000 ppm, O ₂ = 5 %, GHSV = 30000 h ⁻¹ , flow rate 500 mL/min, SO ₂ = 100 ppm (when used)	88 % (@ 250 °C)	72 % (@ 250 °C, 7 h)	[4]
CeO ₂ -ZrO ₂ - WO ₃ (IM)	NO = NH ₃ = 600 ppm, O ₂ = 5 %, GHSV = 50000 h ⁻¹ , flow rate 833 mL/min,	20 % (@ 200 °C)		[5]
CeO ₂ -ZrO ₂ -	NO = NH ₃ = 600 ppm,	39 %	-	[5]

Catalysts	Reaction condition	NO _x conversion (@ 200°C)	SO ₂ resistance	Reference
WO ₃ (SG)	O ₂ = 5 %, GHSV = 50000 h ⁻¹ , flow rate 833 mL/min,	(@ 200°C)		
CeO ₂ -ZrO ₂ - WO ₃ (HT)	NO = NH ₃ = 600 ppm, O ₂ = 5 %, GHSV = 50000 h ⁻¹ , flow rate 833 mL/min,	89 % (@ 200 °C)	-	[5]
CeO ₂ -ZrO ₂ - WO ₃ (SP)	NO = NH ₃ = 600 ppm, O ₂ = 5 %, GHSV = 50000 h ⁻¹ , flow rate 833 mL/min,	89 % (@ 200 °C)	-	[5]
Mn/CeO ₂ (HT)	NO = NH ₃ = 500 ppm, O ₂ = 5 %, GHSV = 30000 h ⁻¹ , flow rate 600 mL/min	89 % (@ 210 °C)	-	[6]

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