**Supplementary Information**

**Effect of** **samarium on** **the N2 selectivity of Sm*x*Mn0.3–*x*Ti catalysts** **during selective catalytic reduction of NO*x* with NH3**

*Shengyang Zhang*1), *Bolin Zhang*1,2),🖂, *Boyu Wu*1), *Bo Liu*1), and *Shengen Zhang*1),🖂

1) Institute for Advanced Materials and Technology, University of Science and Technology Beijing, Beijing 100083, China

2) Shunde Innovation School, University of Science and Technology Beijing, Foshan 528399, China

🖂 Corresponding authors: Bolin Zhang E-mail: zhangbolin@ustb.edu.cn;

Shengen Zhang E-mail: zhangshengen@mater.ustb.edu.cn

Fig. S1 and Fig. S2 showed the Nitrogen adsorption–desorption isotherms and pore size distribution curves for different catalysts. The physical adsorption isotherm classification was given by the International Union of Pure and Applied Chemistry (IUPAC). The adsorption–desorption isotherm was inconsistent with capillary condensation, resulting in adsorption hysteresis loop [1–2]. As shown in Fig. S1, Sm*x*Mn0.3–*x*Ti catalysts (*x* = 0, 0.1, 0.15, 0.2, 0.3) all belonged to type IV isotherm with H1 hysteresis loops. This indicated the presence of mesoporous in the catalysts. The pore size distributions of different catalysts were obtained by Barrett–Joyner–Halenda (BJH) method and measured from N2 desorption isotherm using the cylindrical pore model[3].

Fig. S2 showed that the pore sizes of mesopores were in range of 2–50 nm. The most probable pore-size distribution was ~25 nm for Mn0.3Ti catalyst. When the most probable pore‒size distribution decreased to ~4 nm for the other catalysts doping Sm, it might prolong the reaction time of the NH3-SCR reaction in pore size.



**Fig. S1.** **Nitrogen adsorption–desorption isotherms of different catalysts.**

 

**Fig. S2. BJH** **pore-size distribution curves of (a) Mn0.3Ti, (b) Sm0.1Mn0.2Ti, (c) Sm0.15Mn0.15Ti, (d) Sm0.2Mn0.1Ti, and (e) Sm0.3Ti.**

Fig. S3 shows the deconvoluted results of different elements in total XPS spectrum. The XPS spectrum of Mn2p, Sm 3d, and O 1s was obtained from total XPS spectrum (Fig. 5).

Fig. S4 indicated the relationship between the N2 selectivity and the surface atomic ratio of M (M = Mn4+ or Sm3+) at 200°C. As *x* of Sm*x*Mn0.3–*x*Ti catalyst (*x* ≤ 0.2) increased, the proportion of Mn4+ species and N2O concentration decreased, which showed the increased N2 selectivity. As *x* of Sm*x*Mn0.3–*x*Ti catalyst (with *x* ≤ 0.2) increased, the proportion of Sm3+ species increased and N2 selectivity increased from 66% to 87% above. This indicated that the high N2 selectivity of all the prepared catalysts was indeed correlated with the surface ratio of Sm3+ and Mn4+.



**Fig. S3. XPS spectra of survey spectra for different catalysts.**



**Fig. S4. Relationship between the N2 selectivity, N2O concentration, the surface atomic ratio of M (M = Mn4+ or Sm3+), and the molar ratio of Sm in Sm*x*Mn0.3–*x*Ti catalysts (*x* = 0, 0.1, 0.15, 0.2, 0.3).** **Inlet reaction condition: 600 ppm NH3, 600 ppm NO, 5vol% O2, and N2 balance, GHSV = 36000 h−1.**

##### References

[1] D.W. Kwon, K.B. Nam, and S.C. Hong, Influence of tungsten on the activity of a Mn/Ce/W/Ti catalyst for the selective catalytic reduction of NO with NH3 at low temperatures, *Appl*. *Catal*. *A*: *Gen*., 497(2015), p. 160.

[2] Z. Amirsardari, A. Dourani, M.A. Amirifar, and N.G. Massoom, Comparative characterization of iridium loading on catalyst assessment under different conditions. *Int*. *J*. *Miner*. *Metall*. *Mater*., 2021. 28(7): p. 1233-1239.

[3] S.B. Ma, X.Y. Zhao, Y.S. Li, T.R. Zhang, F.L. Yuan, X.Y. Niu, and Y.J. Zhu, Effect of W on the acidity and redox performance of the Cu0.02Fe0.2W*a*TiO*x*(*a* = 0.01, 0.02, 0.03) catalysts for NH3-SCR of NO, *Appl*. *Catal*. *B*: *Environ*., 248(2019), p. 226.