Supporting Information

Mechanistic insight into Mn-Ce synergy drives efficient low-temperature SCR over fly ash

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Caption

Fig. S1. NO_x conversion of catalysts in NH_3-SCR reaction.

Fig. S2. N_2 selectivity of catalysts in NH_3-SCR reaction.

Fig. S3. SEM images of (a) FA, (b) AFA, (c) Mn-Ce/AFA.

Fig. S4. The amount of strong acid, medium strong acid and weak acid of catalysts.

Fig. S5. *In situ* DRIFTS spectra of the transient reactions at 125℃ for (a, b) Mn-Ce/AFA; (c, d) Mn-Fe/AFA catalysts of NH_3 adsorption.

Fig. S6. *In situ* DRIFTS spectra of the transient reactions at 125℃ for (a, b) Mn-Ce/AFA; (c, d) Mn-Fe/AFA catalysts of $NO+O_2$ adsorption.

Table S1 Comparison with catalytic reactions by catalysts used in other published work-related studies.

Table S2 Chemical composition of original and acid-modified fly ash (mass fraction).

Material characterization

The atomic surface concentration of catalyst was determined by XPS method. The binding energies of C 1s, O 1s, Mn 2p, Ce 3d and O1s were determined. The concentration of ions on the catalyst surface was calculated according to the peak area ratio of the sample. The overlapping peaks were deconvolved and fitted by finding the optimal combination of Gaussian curve and Lorentz curve. For the NH_3-TPD experiment, the sample was initially pretreated in a high purity helium environment (30 mL/min) at 300℃. Then, 10% NH_3/He mixture (30 mL/min) was introduced for 1 hour to saturation, He purge was switched for 1 hour to remove the weak physical adsorption NH_3 on the surface, and finally, the desorption data was collected by heating from 100℃ to 800℃ at a rate of 10℃/min. H_2-TPR test, purge at 300℃ with high purity He gas for 1 hour, when the temperature dropped to 50℃, add 10% H_2/He mixture (30 mL/min) for 1 hour to saturation. The H_2-TPR analysis was carried out at the catalyst temperature of 700℃ and the rate of 10℃/min. In situ infrared spectroscopy was recorded using the VERTEX 70 (Bruker, Germany) spectrometer with the CaF_2 window. In the experiment, wafers containing 50 mg of catalyst were placed in a gas flow pool, purged with high-purity nitrogen at 350℃ for 30 minutes, and then cooled to 125℃. The background spectrum was recorded at the same time and then subtracted from the sample spectrum.

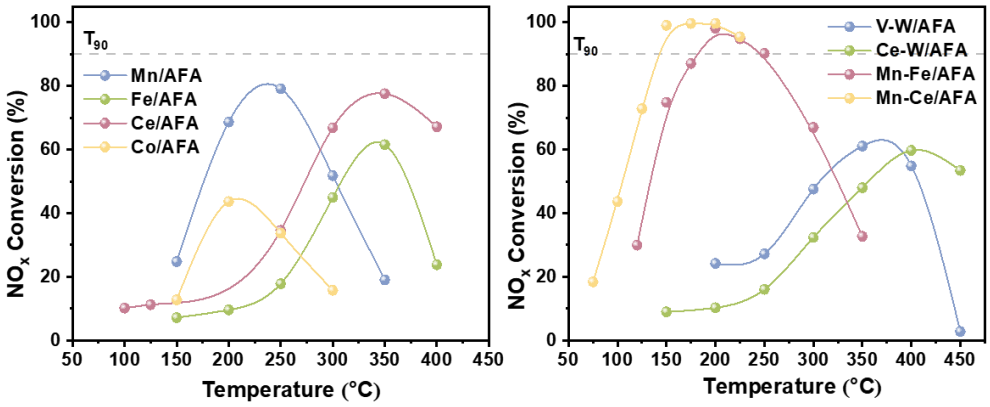

Fig. S1. NO_x conversion of catalysts in NH_3-SCR reaction.

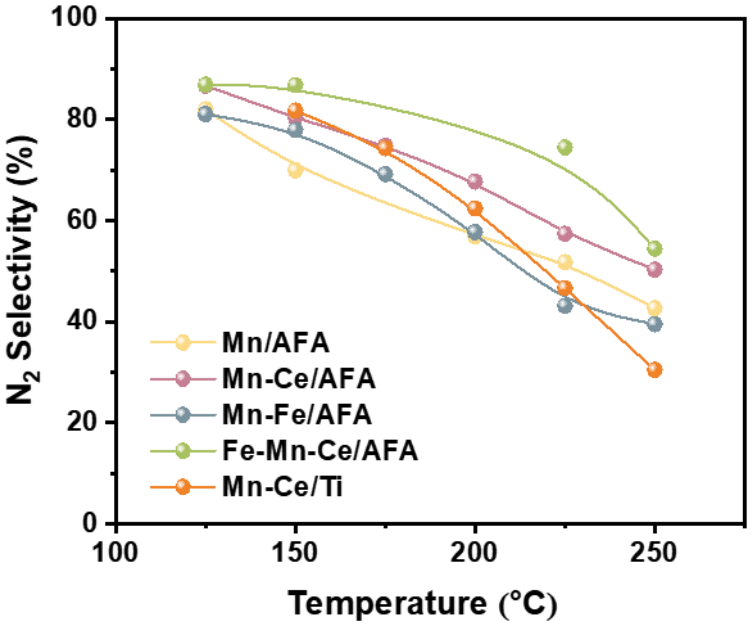

Fig. S2. N_2 selectivity of catalysts in NH_3-SCR reaction.

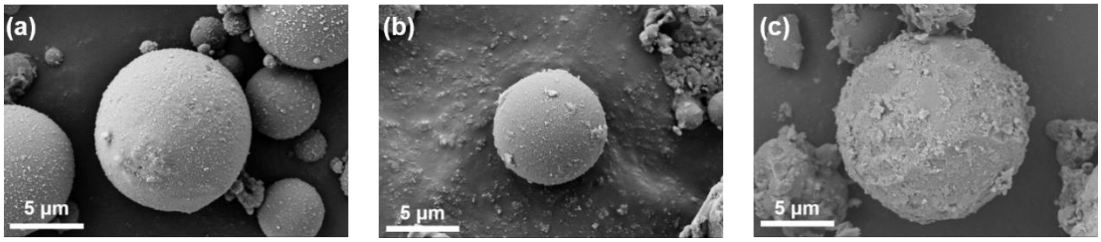

Fig. S3. SEM images of (a) FA, (b) AFA, (c) Mn-Ce/AFA.

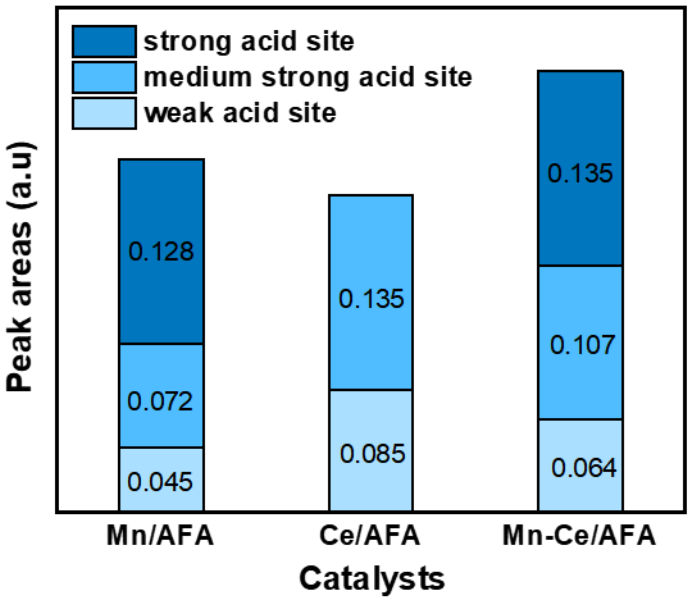

Fig. S4. The amount of strong acid, medium strong acid and weak acid of catalysts.

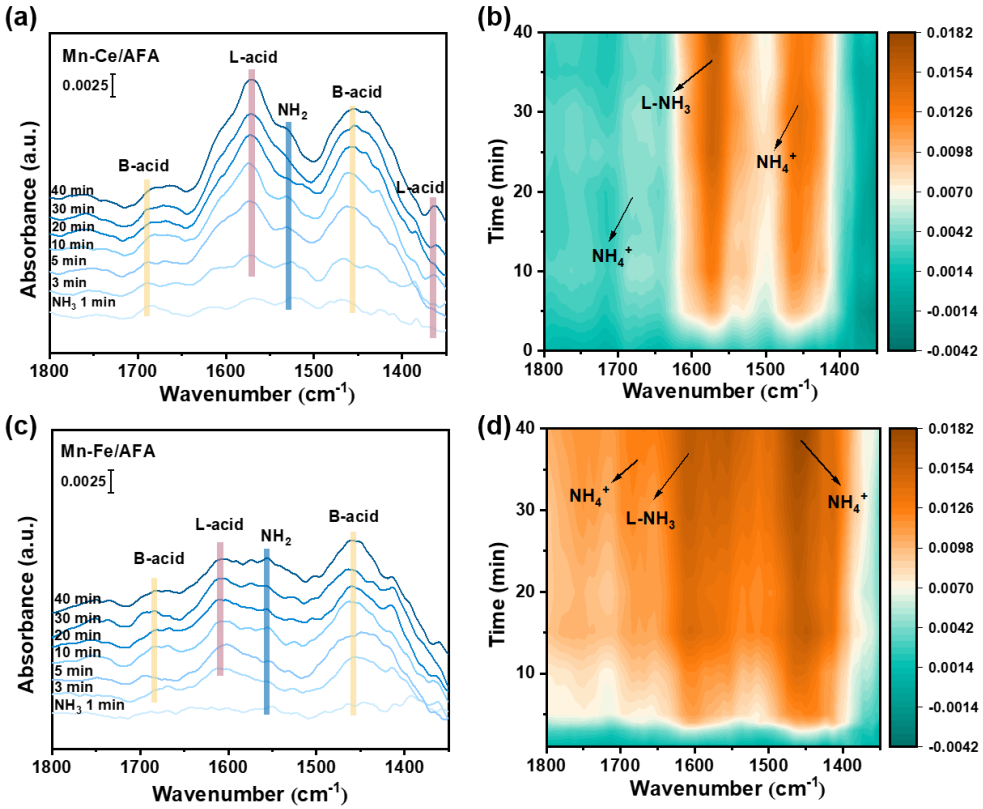

Fig. S5. *In situ* DRIFTS spectra of the transient reactions at 125℃ for (a, b) Mn-Ce/AFA; (c, d) Mn-Fe/AFA catalysts of NH_3 adsorption.

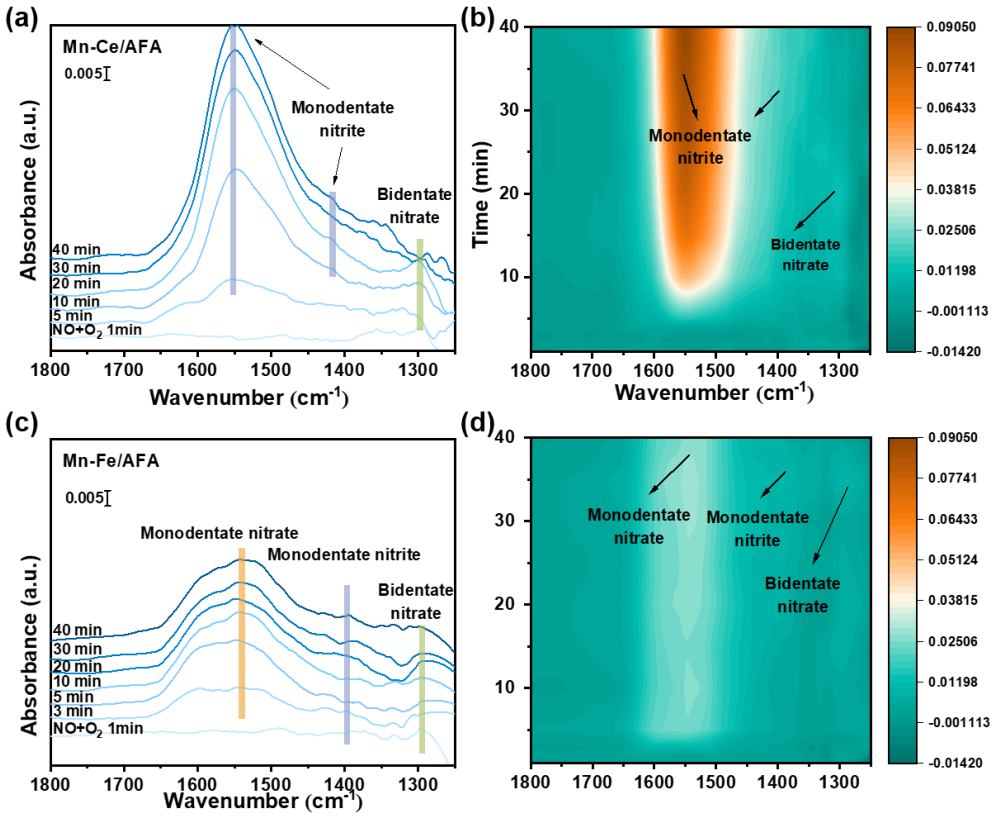

Fig. S6. *In situ* DRIFTS spectra of the transient reactions at 125℃ for (a, b) Mn-Ce/AFA; (c, d) Mn-Fe/AFA catalysts of $NO+O_2$ adsorption.

Table S1 Comparison with catalytic reactions by catalysts used in other published work-related studies

Catalyst	Reaction conditions				Content (%)		T_{90} (℃)	Reference
	NO (ppm)	H_2O (%)	SO_2 (ppm)	GHSV (mL/g/h)	Mn	Ce		
Mn-Ce/AFA	500	5	\	60,000	4.1	4.2	150	This Work
Mn-Ce/TiO_2	800	2.5	200	60,000	\	\	160	Li et al., 2024
Ce-Mn-Cu-Beta-1	500	5	\	200,000	1.9	1	200	Guo et al., 2025
$CeMnTiO_2$	500	5	\	60,000	5	5	185	Li et al., 2024
CeMnOx/Cu-SSZ-39	500	\	\	100,000	1.5	3.5	180	Tang et al., 2024
FZ@CM/Sil-1-H	500	10	\	70,000	3.5	4	240	Tian et al., 2024

Table S2 Chemical composition of original and acid-modified fly ash (mass fraction)

Chemical composition	Mass fraction (%)	
	FA	AFA
SiO_2	46.954	56.206
Al_2O_3	31.91	30.769
Fe_2O_3	8.232	6.476
CaO	6.259	1.665
TiO_2	1.827	1.73
K_2O	1.249	1.279
MgO	0.912	0.717
Other composition	2.657	3.54

We can observe that pickling can significantly reduce the content of alkaline earth metals and iron oxides in fly ash, which may account for the increased catalytic activity.

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