Supporting Information

Dual kinetic effect from confined iron nanoparticles in zeolite modulates high-temperatures catalytic NO reduction and NH_3 oxidation

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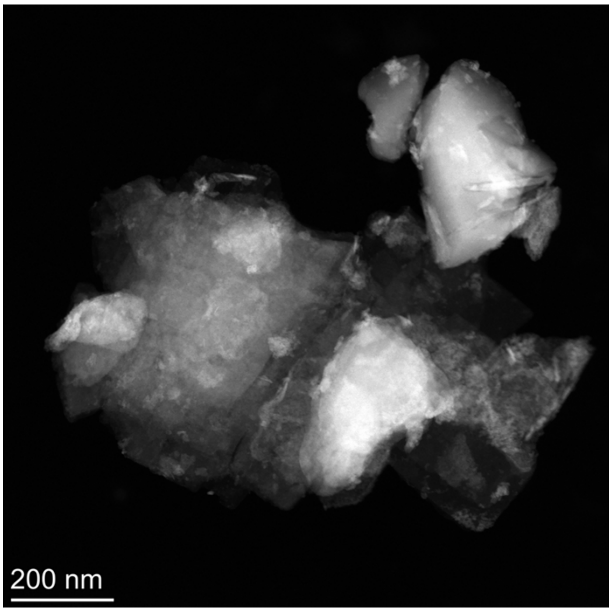

Fig. S1 Morphological TEM images of 0.5Fe@ZSM-5.

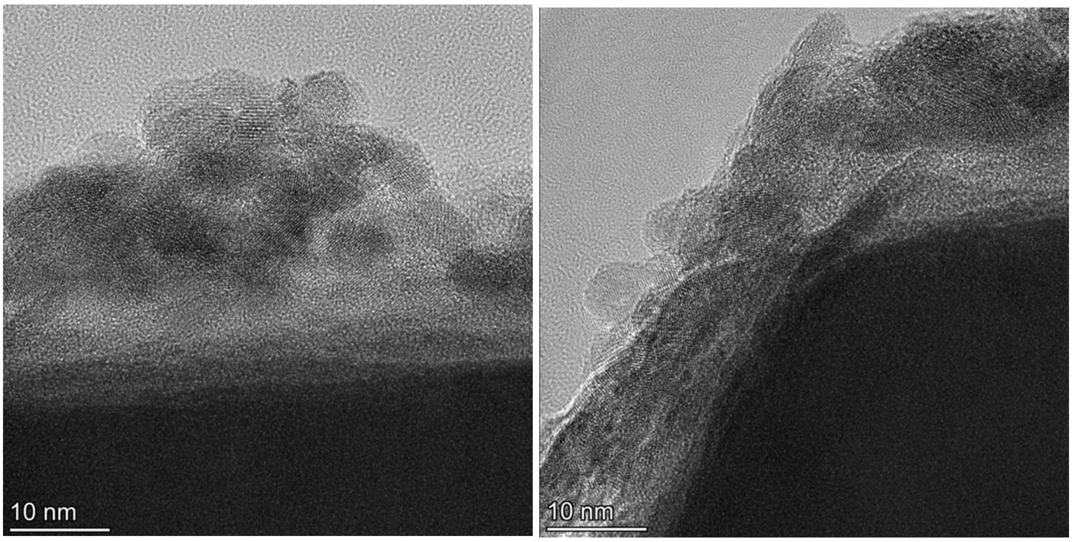

Fig. S2 Morphological nanoparticles on 0.5Fe@ZSM-5.

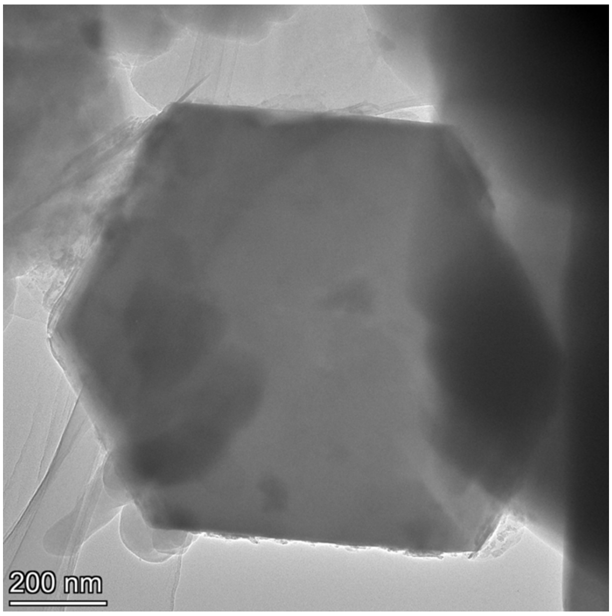

Fig. S3 Morphological TEM images of 0.1Fe@ZSM-5.

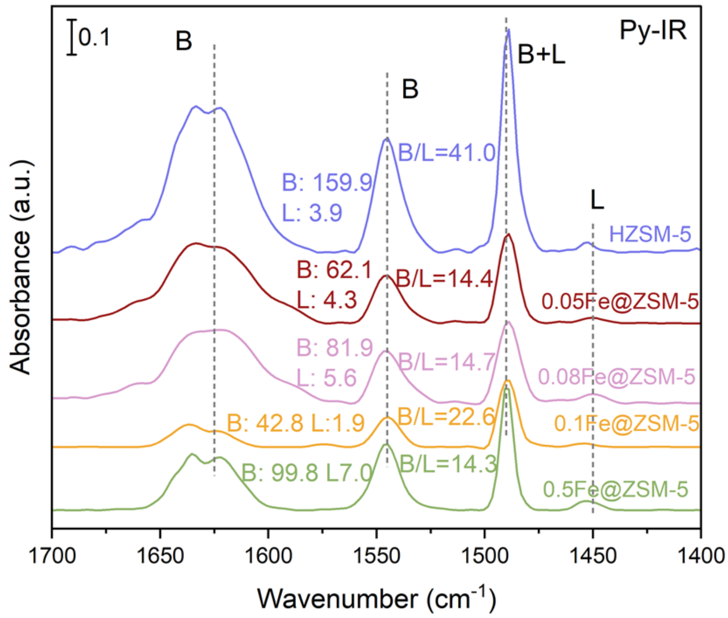

Fig. S4 Py-IR spectra of fresh HZSM-5 and Fe@ZSM-5.

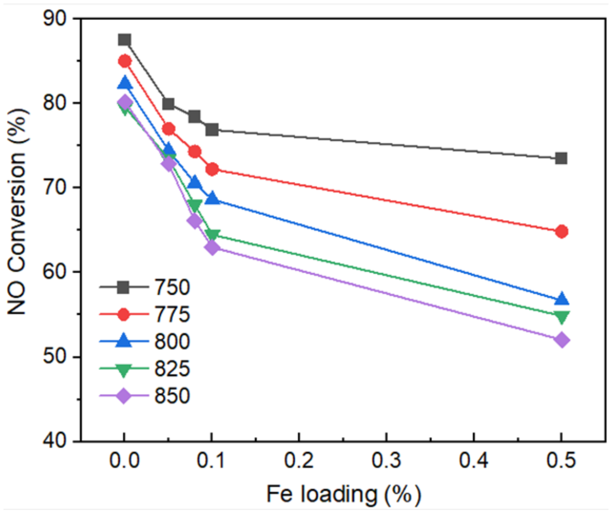

Fig. S5 Fe loadings on NO conversion of NH_3-SCR.

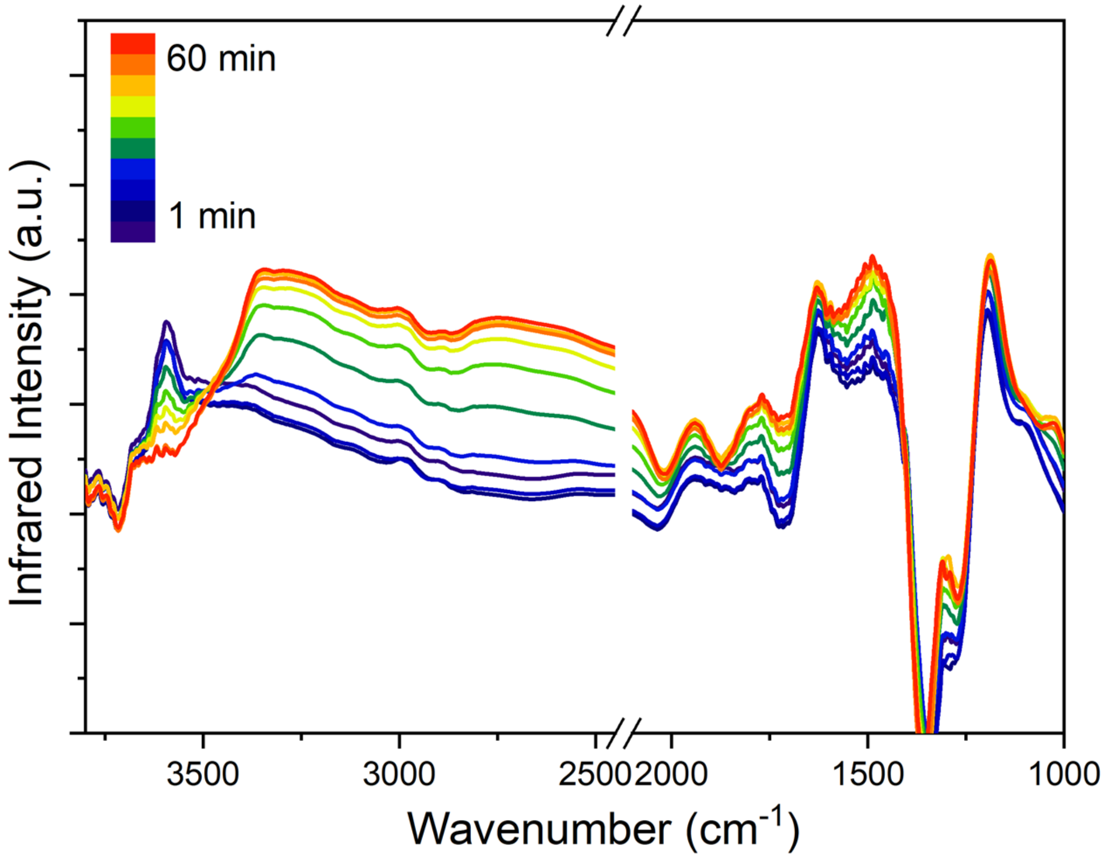

Fig. S6 Evolution of DRIFTS over 0.1Fe@ZSM-5 during NH_3 adsorption at 800 °C. Gas feed refers to 1000 ppm NH_3, balance He.

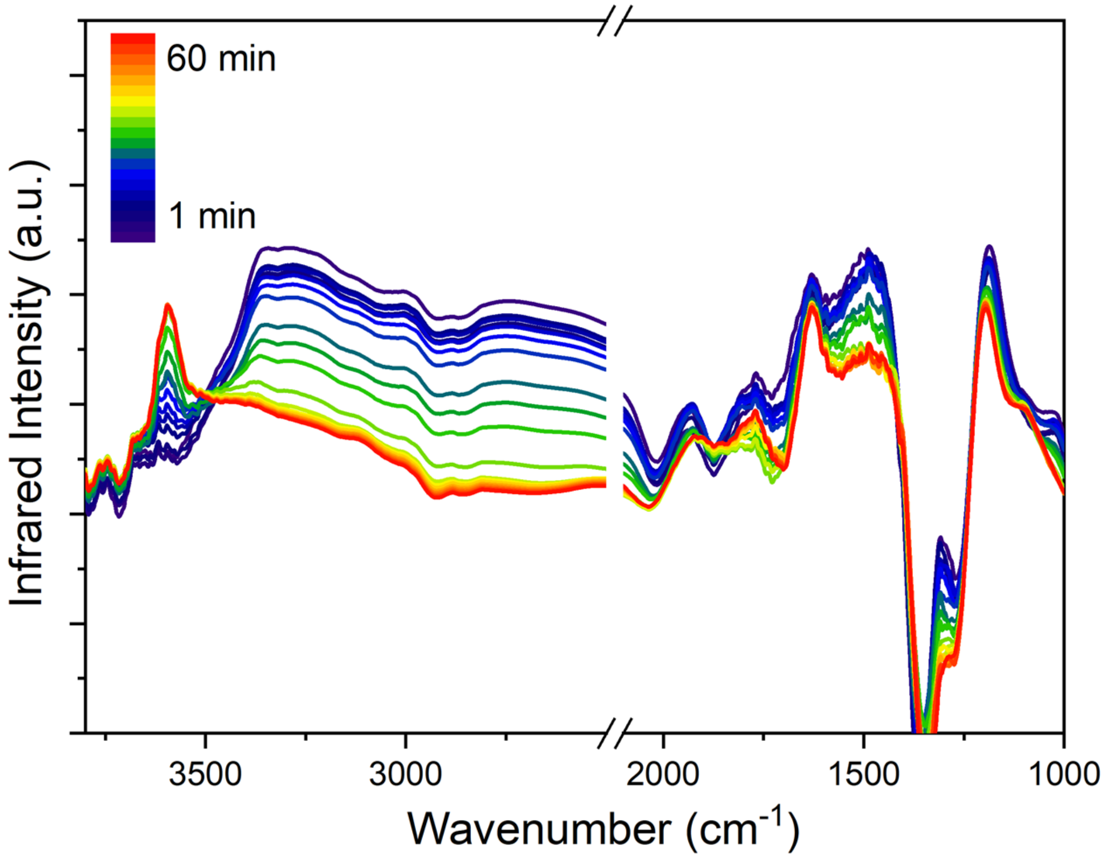

Fig. S7 Evolution of DRIFTS over 0.1Fe@ZSM-5 during O_2 oxidation at 800 °C. Gas feed refers to 1000 ppm NH_3, balance He.

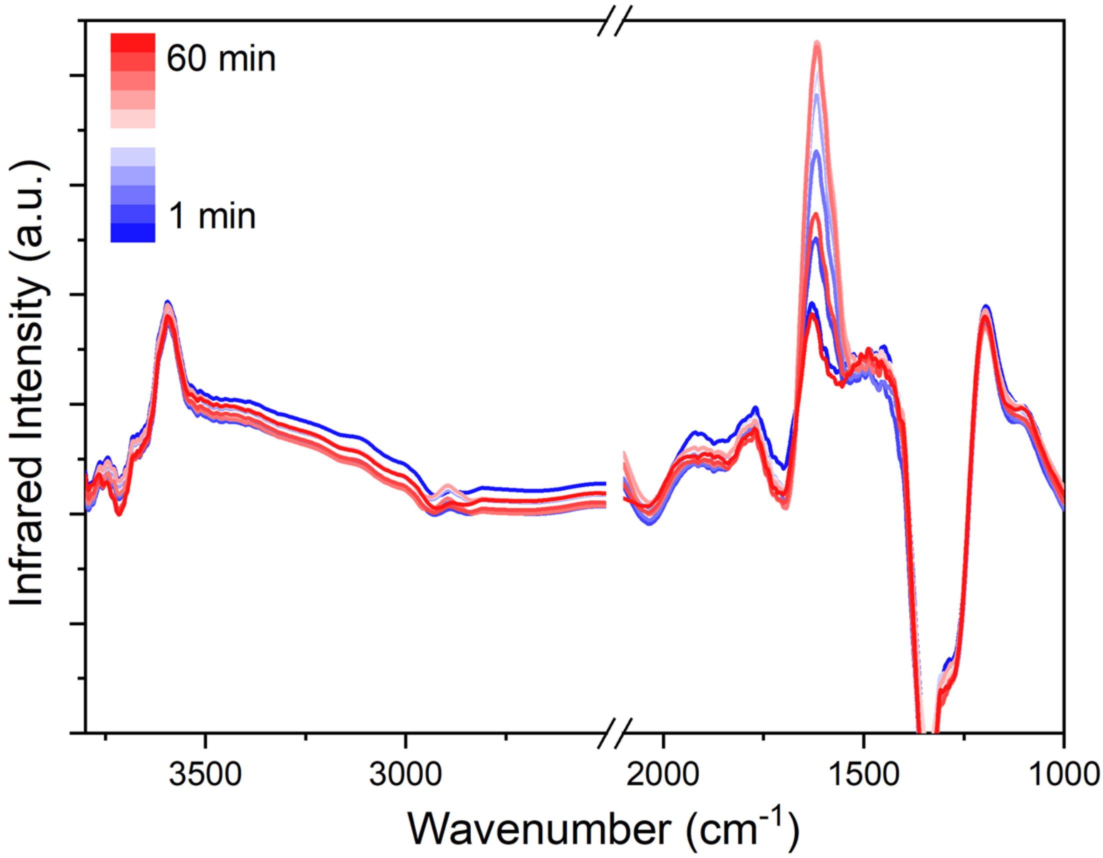

Fig. S8 Evolution of DRIFTS over 0.1Fe@ZSM-5 during NO reduction at 800 °C. Gas feed refers to 1000 ppm NH_3, balance He.

Table S1 Fe concentration of Fe@ZSM-5 (determined by ICP-OES).

Samples	Fe loading (%)
0.05Fe@ZSM-5	0.122
0.08Fe@ZSM-5	0.170
0.1Fe@ZSM-5	0.361
0.5Fe@ZSM-5	0.670

Table S2 Semi-quantitative analysis of acidity amount on zeolites from Py-IR.

Catalyst	B_{NH4} amounts (umol g^{-1})	L_{NH3} amounts (umol g^{-1})	Total acidity (umol g^{-1})	B_{NH4}/L_{NH3} Ratio
HZSM-5	159.9	3.9	163.8	41.0
0.05@ZSM-5	62.1	4.3	66.4	18.4
0.08@ZSM-5	81.9	5.6	87.5	14.7
0.1@ZSM-5	42.8	1.9	44.7	22.6
0.5@ZSM-5	99.8	7.0	106.8	14.3

Table S3 Fe K-edge EXAFS fitting parameters of Fe foil and Fe@ZSM-5.

Samples	Scattering path	$\bar{CN}$	Bond Length (Å)	ΔE_0 (eV)	σ^2 (Å^2)	R factor
Fe foil	Fe-Fe1	7.0	2.47	4.58	0.005	0.0036
	Fe-Fe2	8.2	2.84		0.009	
0.05Fe@ZSM-5	Fe-Fe1	0.9	2.49	9.90	0.004	0.0080
	Fe-Fe2	2.0	2.92		0.019	
	Fe-O	4.1	1.96		0.008	
0.1Fe@ZSM-5	Fe-Fe1	1.7	2.49	9.80	0.003	0.0139
	Fe-Fe2	2.8	2.90		0.014	
	Fe-O	2.5	1.91		0.005	
0.5Fe@ZSM-5	Fe-Fe1	5.4	2.46	1.89	0.006	0.0089
	Fe-Fe2	7.5	1.91		0.011	
	Fe-O	1.8	2.82		0.014	

Note: Amplitude reduction term S_0^2 =0.90. The distances for Fe-Fe and Fe-O paths were calculated by FEFF6 of Artemis codes.

Table S4 Reaction kinetic parameters under NH_3+NO+O_2 conditions and comparison to previous work.

Sample	Rate constant	Ea	A	Reference
0.1Fe@ZSM-5	k_{NH_3}	98.3 kJ mol^{-1}	9.5×10^{8}	This work
0.1Fe@ZSM-5	k_{re}	52.12 kJ mol^{-1}	3.56×10^{8}	This work
$FeNb_{0.4}O_x$-C	k	45.9 kJ mol^{-1}	3.2×10^{17}	[1]
1.20% Fe/SSZ-13	k	52.9 kJ mol^{-1}	1500	[2]
Fe0.17-AEI-fresh	k	66.3 kJ mol^{-1}	4.7×10^{5}	[3]

Table S5 Model-related parameter values.

Parameter	Definition	Value (Unit)
R	Catalyst particle diameter	0.15 (mm)
U	Gas flow velocity	0.11 (m s^{-1})
ρ	Gas density (air)	1.29 (kg m^{-3})
ρ_{catal}	Catalyst particle density	800 (kg m^{-3})
ε	Porosity	0.58
$D_{x,KA}$	Knudsen diffusion coefficient	0.039 (cm^2 s^{-1})
S_{catal}	Specific surface area	280 (m^2 g^{-1})
C_{NH3}、C_{NO}、C_{O2}	Initial NH_3, NO, and O_2 concentrations	1000 ppm、1000 ppm、6 vol.%
n_{NH3}、n_{NO}、n_{O2}	Standard reaction orders	0, 1, and 0.5

References

1. W. Zhang, X. Shi, Z. Yan, Y. Shan, Y. Zhu, Y. Yu and H. He, Design of high-performance iron-niobium composite oxide catalysts for NH_3-SCR: Insights into the interaction between Fe and Nb, *ACS Catal.*, 2021, **11**, 9825-9836.
2. L. Kovarik, N. M. Washton, R. Kukkadapu, A. Devaraj, A. Wang, Y. Wang, J. Szanyi, C. H. F. Peden and F. Gao, Transformation of active sites in Fe/SSZ-13 SCR catalysts during hydrothermal aging: A spectroscopic, microscopic, and kinetics study, *ACS Catal.*, 2017, **7**, 2458-2470.
3. G. Sun, R. Yu, L. Xu, B. Wang and W. Zhang, Enhanced hydrothermal stability and SO_2-tolerance of Cu-Fe modified AEI zeolite catalysts in NH_3-SCR of NO_x, *Catal. Sci. Technol.*, 2022, **12**, 3898-3911.