Electronic Supplementary Material (ESI) for Catalysis Science .

Supplementary Information:

The role of various iron species in Fe-Beta catalysts with low iron loadings for NH_3-SCR

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Mass Diffusion Effect

1. NH_3-SCR reaction

We carried out a series of experiments on Fe-0.52 sample to rule out the mass transfer limitation. Fig.S1 and Fig.S2 present the NO_x conversion rate as a function of GHSV (140,000-700,000 h^{-1}) and particle size (20-120 mesh) at 280 ^oC. It is found that the rate of NO_x conversion is constant at GHSV ≥ 420,000 h^{-1} and diameter ≥ 60-80 mesh. So, the GHSV= 420,000 h^{-1} and diameter= 60-80 mesh was elected to rule out the mass transfer limitation. And we confirm that the internal and external mass transfer effects could be neglected during the kinetic experiments.

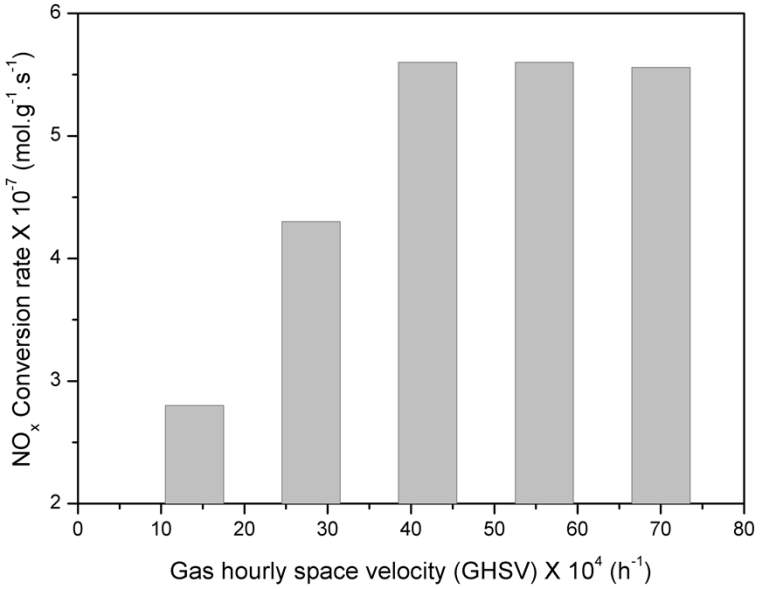

Fig.S1. NO_x conversion rate of Fe-0.52 catalyst (60 ~ 80 mesh) for SCR reaction as a function of GHSV at 280 ^oC.

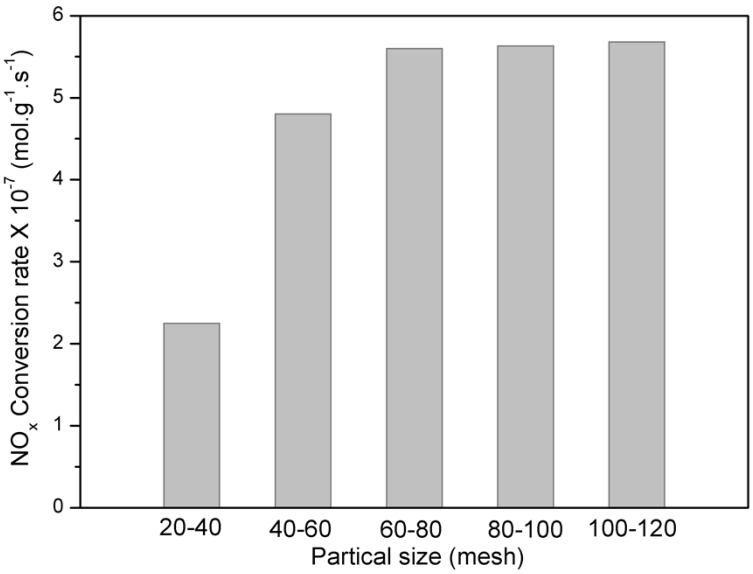

Fig.S2. NO_x conversion rate of Fe-0.52 catalyst for SCR reaction as a function of particle size at 280 ^{o}C (GHSV=420,000 h^{-1}).

2. NH_3 oxidation

Fig.S3 and Fig.S4 are the NH_3 conversion rate as a function of GHSV (140,000-700,000 h^{-1}) and particle size (20-120 mesh) at 520 ^{o}C, respectively. The results indicate the rate of NH_3 conversion is constant at GHSV ≥ 420,000 h^{-1} and diameter ≥ 60-80 mesh. Thus, the GHSV= 420,000 h^{-1} and diameter= 60-80 mesh was elected to rule out the mass transfer limitation.

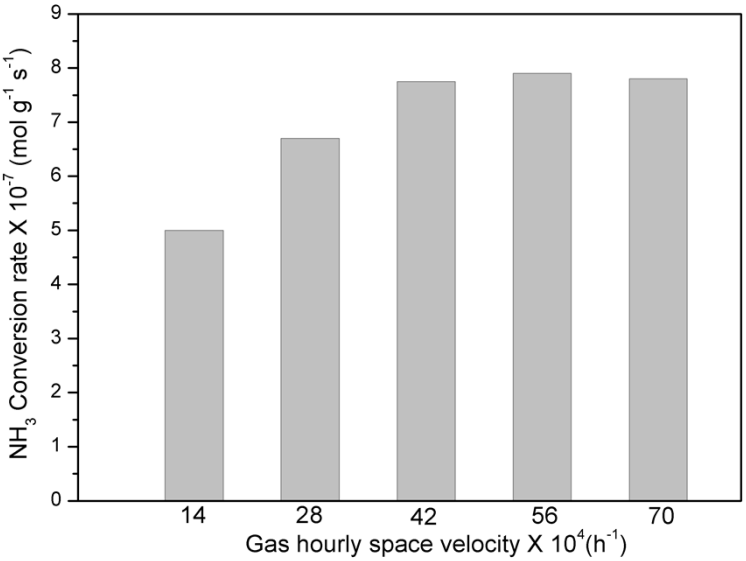

Fig.S3. NH_3 conversion rate of Fe-0.52 catalyst (60 ~ 80 mesh) for NH_3 oxidation as a function of GHSV at 520 ^{o}C.

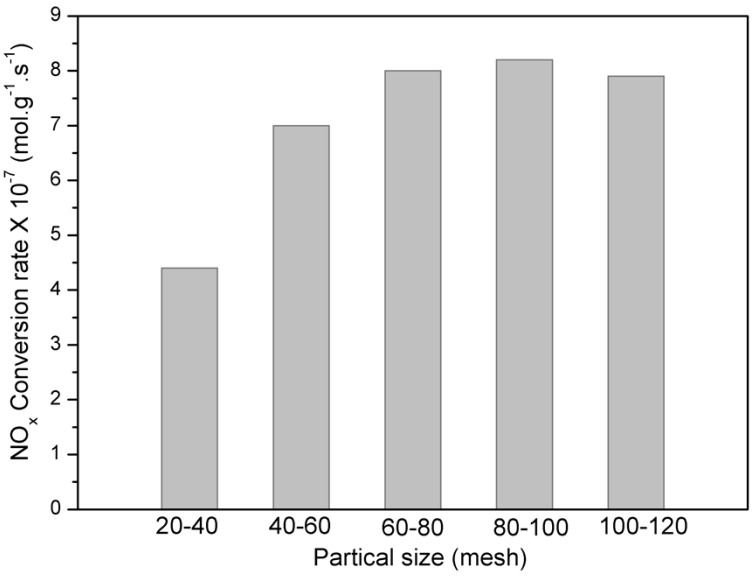

Fig.S4. NH_3 conversion rate of Fe-0.52 catalyst for NH_3 oxidation as a function of particle size at 520 ^oC (GHSV=420,000 h^{-1}).

The activation energy of NH_3-SCR reaction on different catalyst derived from literatures

. Table S1 the list of literature finding for activation energy of NH_3-SCR reaction on different catalyst

Type	Catalysts	E_a [kJ mol^{-1}]	Ref.
H-ZSM-5	H-ZSM-5	61	[1]
Fe-Zeolites	Fe/ZSM-5	46	[2]
	Fe/ZSM-5	45	[3]
	Fe-ZSM-5	54	[4]
	Fe-ZSM-5	35	[5]
	Fe-ZSM-5	42	[6]
Cu-Zeolites	Cu-SAPO	33.6	[7]
	Cu-Zeolite	35/40-42	[8]
	Cu-FAU	29	[9]
	Cu-MOR	35	[10]
MnO_x/TiO_2	MnO_x/TiO_2	38	[11]
V_2O_5-WO_3/TiO_2	V_2O_5–WO_3/TiO_2	80	[12]
	V_2O_5-WO_3	84	[13]
	VZWO_3-Ti	52-54	[14]

Reference

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The result of NH_3 oxidation kinetic experiments

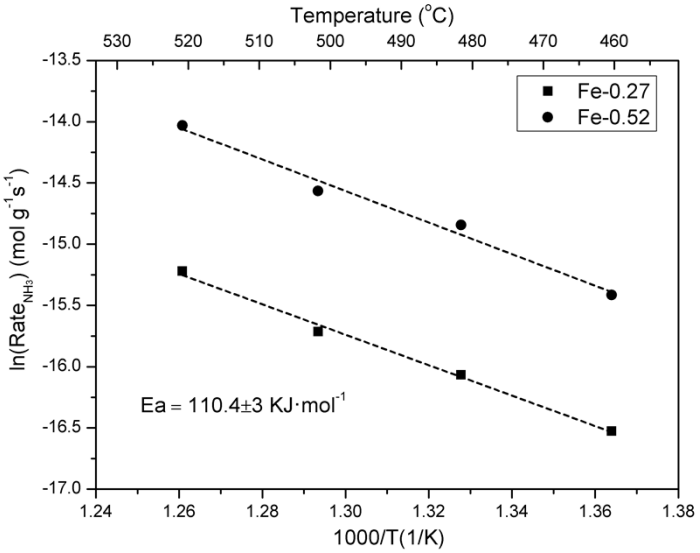

Fig.S5. Arrhenius plots of the NH_3 oxidation rates over Fe-Beta catalysts at 460-520 °C. Conditions: 500 ppmNH_3, 5% O_2, 8% CO_2, 5% H_2O balanced with N_2; flow rate: 1.5 L min^{-1}; GHSV: 420,000 h^{-1}.

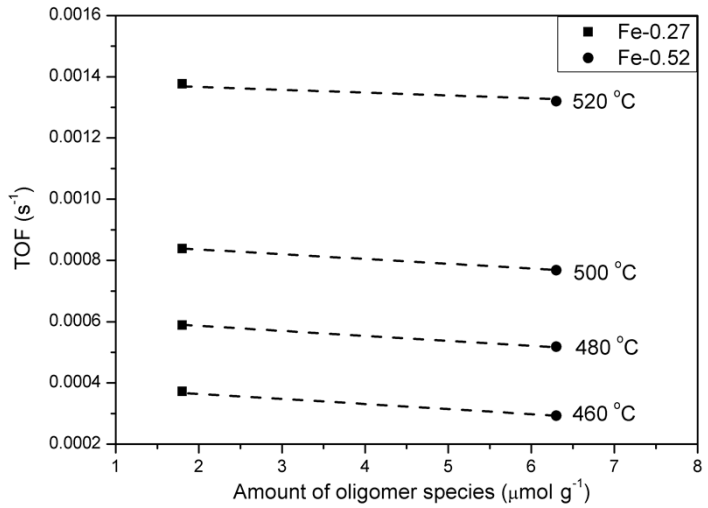

Fig.S6. Turnover frequency (TOF) for NH_3 oxidation with respect to the amount of oligomer species over Fe-Beta catalysts. Conditions: 500 ppmNH_3, 5% O_2, 8% CO_2, 5% H_2O balanced with N_2; flow rate: 1.5 L min^{-1}; GHSV: 420,000 h^{-1}.