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Supplementary Information

Study on the catalytic activity and hydrothermal stability of one-pot synthesized Fe-based FER zeolites for NH_3-SCR

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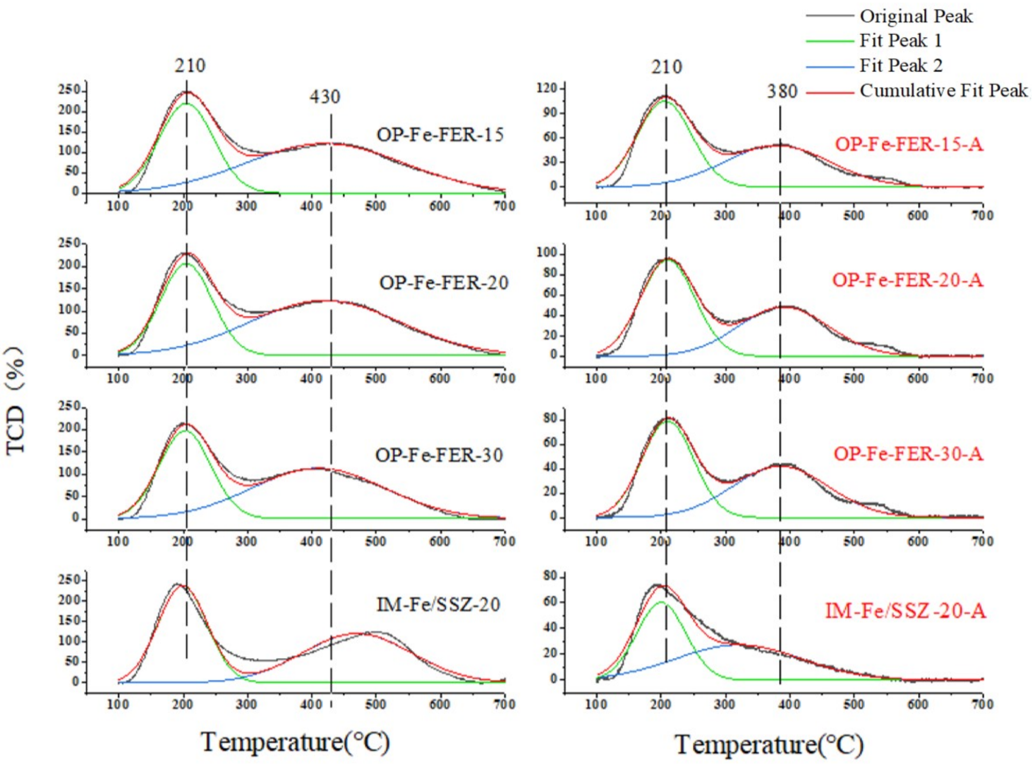

Figure S1 NH_3-TPD fitting results of fresh and aged OP-Fe-FER-x and IM-Fe/SSZ-20 zeolites.

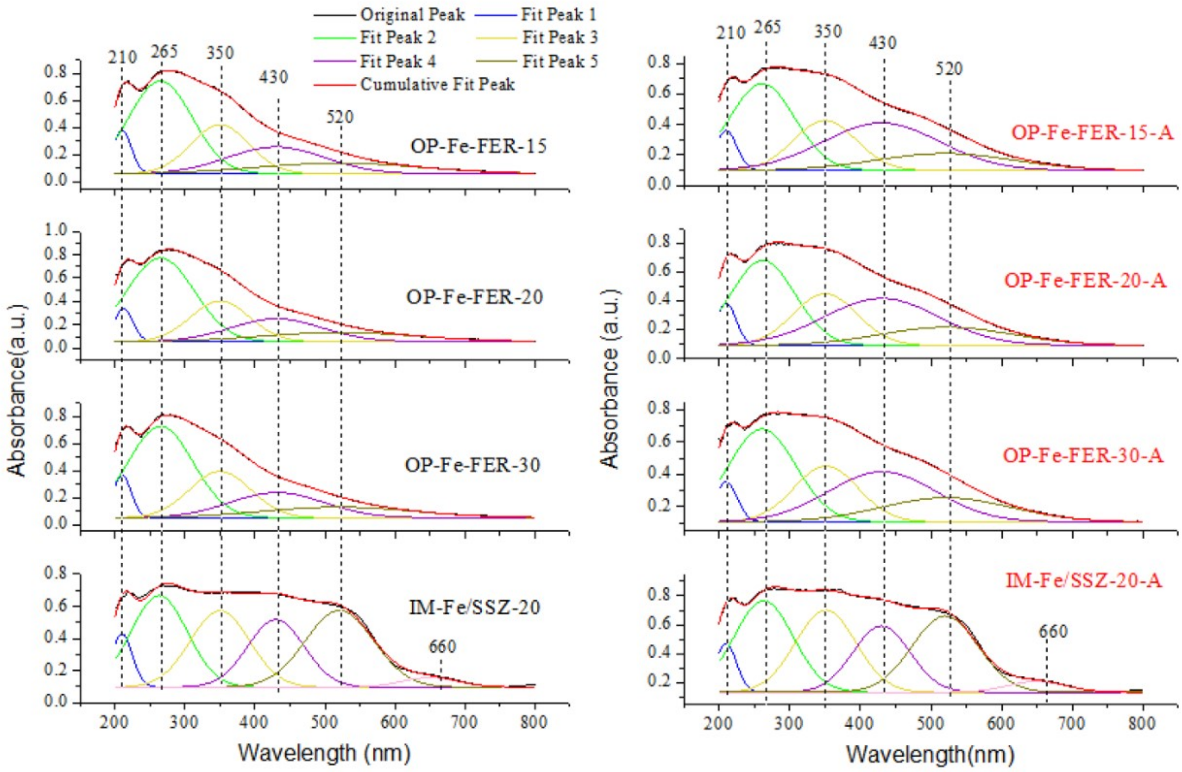

Figure S2 UV-vis fitting results of fresh and aged OP-Fe-FER-x and IM-Fe/SSZ-20 zeolites.

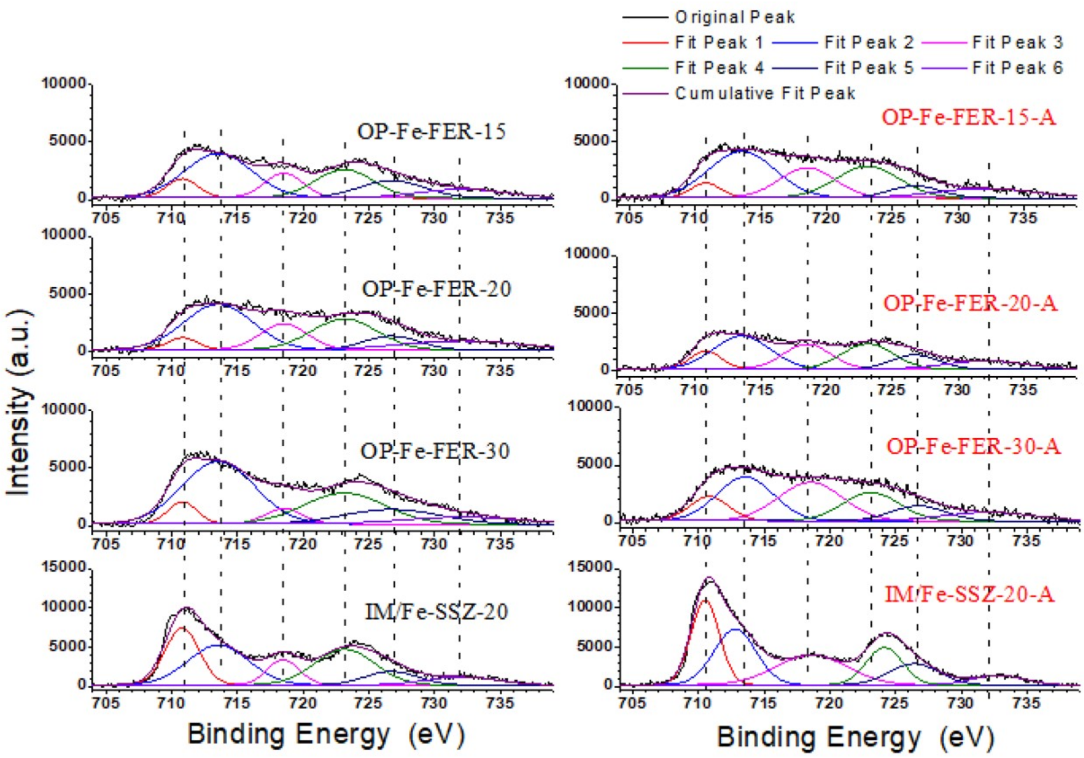

Figure S3. XPS spectra fitting results of fresh and aged OP-Fe-FER-x zeolites (the fit peaks 1-6 are centered at about 710.8 eV, 713.6 eV, 718.5 eV, 723.1 eV, 726.7 eV and 732.1 eV, respectively).

According to literatures[1-4], Fe^{3+} $2p_{1/2}$ and $2p_{3/2}$ signals are located at about 724 eV and 711 eV with satellite peaks at ca. 733 eV and 719 eV, while the Fe^{2+} $2p_{1/2}$ and $2p_{3/2}$ signals are located at ca. 723 eV and 710 eV with satellite peaks at ca. 729 eV and 715 eV, respectively. Therefore, the fit peak 1 and 4 are attributed to Fe^{2+} species, while the fit peak 2, 3, 5 and 6 are attributed to Fe^{3+} species and the corresponding satellite peaks.

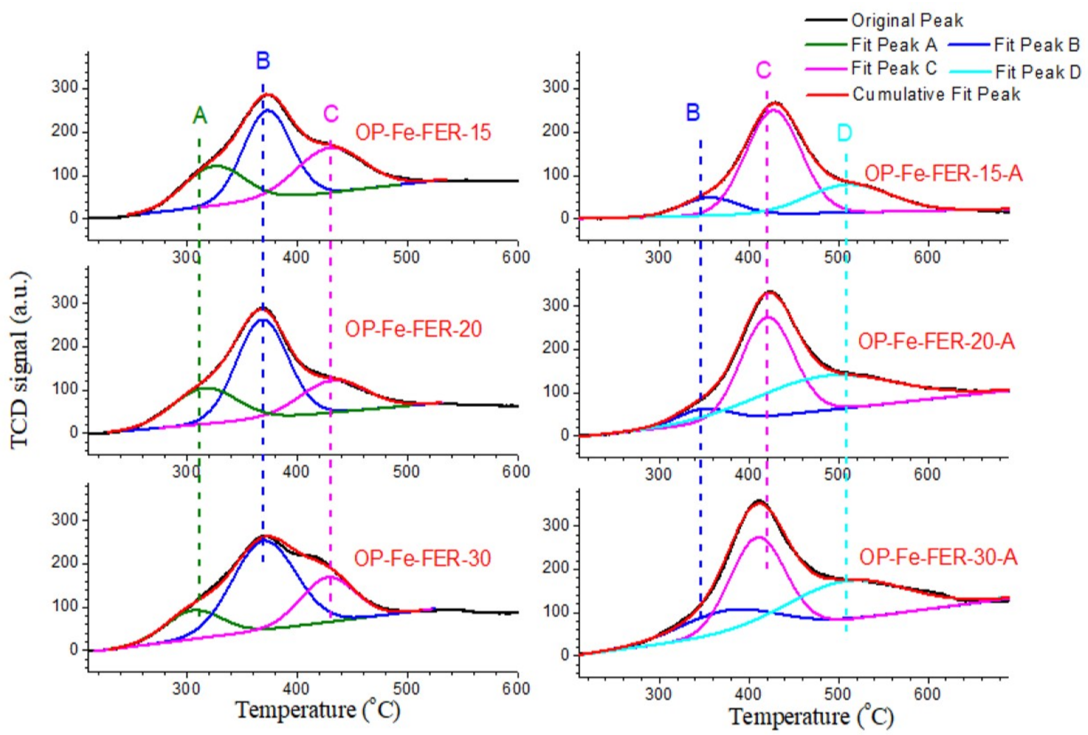

Figure S4. H_2-TPR fitting results of fresh and aged OP-Fe-FER-x zeolites.

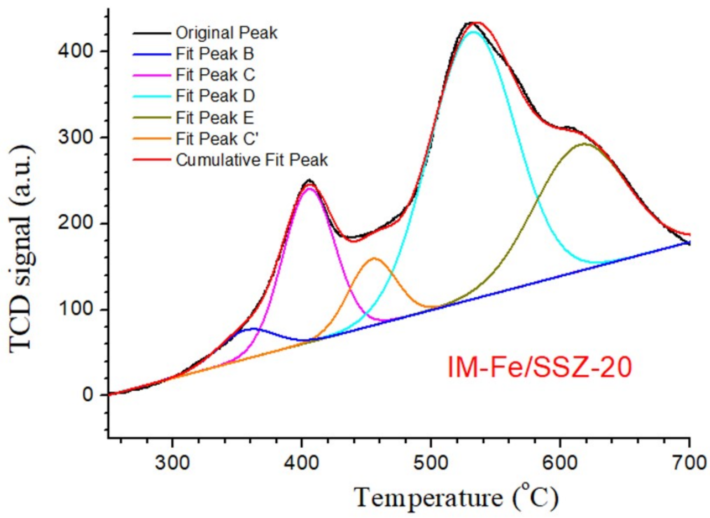

Figure S5. H_2-TPR fitting results of fresh IM-Fe/SSZ-20 zeolite.

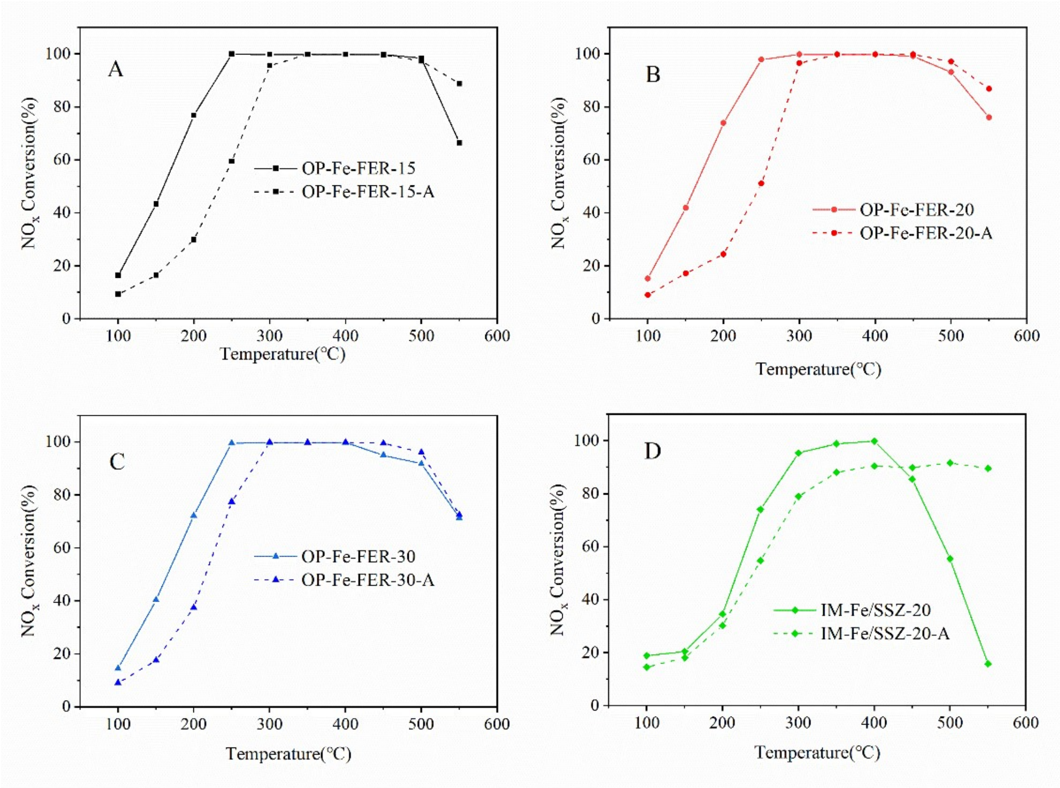

Figure S6 NO_x conversion in NH_3-SCR as a function of temperature over fresh and aged OP-Fe-FER-x and IM-Fe/SSZ-20 zeolites. Reaction conditions: 500 ppm NO, 600 ppm NH_3, 5.5% O_2 and balanced N_2, GHSV = 36000 h^{-1}.

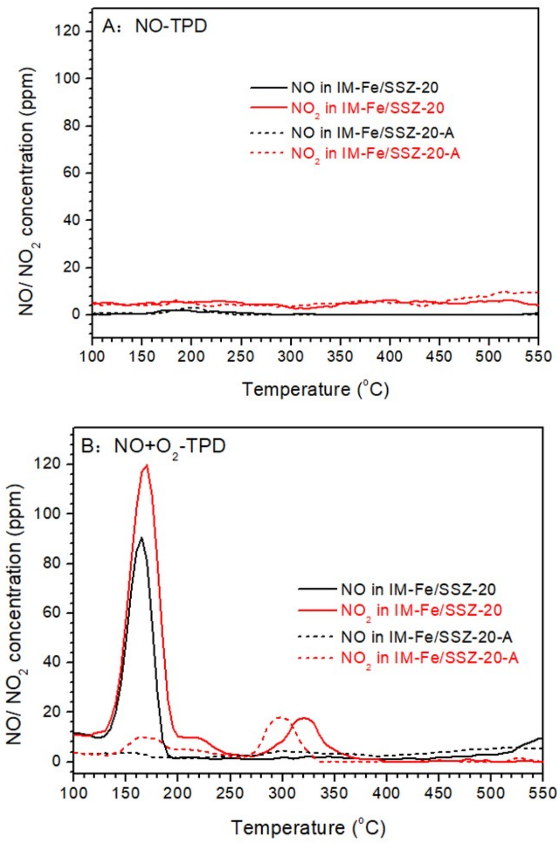

Figure S7 (A) NO-TPD and (B) NO+O_2-TPD results over fresh and aged IM-Fe/SSZ-20 zeolites.

Table S1 Representative Fe-based zeolite catalysts for NH_3-SCR

Catalysts	Framework topology	Preparation method [a]	Fe content (wt. %)	NH_3-SCR reaction condition	Temperature window (°C)	NO_x conversion	Reference
OP-Fe-FER-30	FER	OP	5.4	500 ppm NO, 600 ppm NH_3, 5.5 vol.% O_2, balanced N_2, GHSV = 3.6×10^4 h^{-1}	210 – 530	>80%	This work
IM-Fe/SSZ-20	CHA	IWI	5.0	500 ppm NO, 600 ppm NH_3, 5.5 vol.% O_2, balanced N_2, GHSV = 3.6×10^4 h^{-1}	264 – 460	>80%	This work
Fe/ZSM-5	MFI	IE	1.9	1000 ppm NO, 1000 ppm NH_3, 5 vol.% O_2, 6 vol.% H_2O and balanced He, GHSV = 1.9×10^5 h^{-1}	300 – 550	>80%	5
Fe/Beta	BEA	CVD	4.7	1000 ppm NO, 1200 ppm NH_3, 8 vol.% O_2, 8 vol.% H_2O, 10 vol.%CO_2, balanced N_2， GHSV = 2.1×10^5 h^{-1}	300 – 500	>90%	6
Fe/Mordenite	MOR	IE	2.3	500 ppm NO, 500 ppm NH_3, 5 vol.% O_2, balanced N_2, GHSV = 1.6×10^4 h^{-1}	350 – 500	100%	7
Fe/SSZ-13	CHA	IE	1.37	350 ppm NO, 350 ppm NH_3, 14 vol.% O_2, 2.5 vol.% H_2O, balanced N_2， GHSV = 2×10^5 h^{-1}	320 – 550	>80%	8
Fe-SAPO-34	CHA	OP	1.0	350 ppm NO, 350 ppm NH_3, 14 vol.% O_2, 5 vol.%CO_2， balanced Ar, GHSV = 3.0×10^4 h^{-1}	300 – 600	>80%	9
Fe/Ferrierite	FER	CVD	4.7	1000 ppm NO, 1200 ppm NH_3, 8 vol.% O_2, 8 vol.% H_2O, 10 vol.%CO_2, balanced N_2, GHSV = 2.1×10^5 h^{-1}	250 – 500	>90%	6
Fe-SSZ-39	AEI	OP	1.01	50 ppm NO, 60 ppm NH_3, 10 vol.% O_2, 10 vol.% H_2O, balanced N_2, GHSV = 4.5×10^5 h^{-1}	300 – 550	>90%	10
Fe-ERI	ERI	OP	1.03	500 ppm NO, 600 ppm NH_3, 10 vol.% O_2, 10 vol.% H_2O, balanced N_2, GHSV = 1×10^5 h^{-1}	450 – 550	>60%	11
Fe-SSZ-16	AFX	OP	0.95	500 ppm NO, 500 ppm NH_3, 5 vol.% O_2, 10 vol.% H_2O, balanced N_2, GHSV = 1×10^5 h^{-1}	400 – 550	>80%	11
Fe-MCM-22	MWW	OP	4.8	500 ppm NO, 500 ppm NH_3, 5 vol.% O_2 and balanced N_2， GHSV = 6×10^4 h^{-1}	190 – 490	>80%	12
Fe/LTA	LTA	IE	1.8	500 ppm NO, 500 ppm NH_3, 5 vol.% O_2, 10 vol.% H_2O and balanced N_2, GHSV = 1×10^5 h^{-1}	370 – 580	>90%	13
Fe/UZM-35	MSE	IE	1.9	500 ppm NO, 500 ppm NH_3, 5 vol.% O_2, 10 vol.% H_2O and balanced N_2, GHSV = 1×10^5 h^{-1}	250 – 570	>90%	14

[a] OP, IWI, IE and CVD represent one-pot synthesis method, incipient wetness impregnation method, ion-exchange method and chemical vapor deposition method, respectively.

References:

1. F. Mercier, N. Thromat and C. J. A. S. S. Beaucaire], *Appl. Surf. Sci.*, 2000, **165**, 2880302.
2. P. Boron, L. Chmielarz, J. Gurgul, K. Łatka, B. Gil, B. Marszałek and S. Dzwigaj, *Microporous Mesoporous Mater.*, 2015, **203**, 73-85.
3. T. Yamashita and P. Hayes, *Appl. Surf. Sci.*, 2008, **254**, 2441-2449.
4. D. D. Hawn and B. M. DeKoven, *Surf. Interface Anal.*, 1987, **10**, 63-74.
5. J. Li, R. Zhu, Y. Cheng, C. K. Lambert and R. T. Yang, *Environ. Sci. Technol.*, 2010, **44**, 1799-1805.
6. M. Iwasaki, K. Yamazaki and H. Shinjoh, *Appl. Catal. B: Environ.*, 2011, **102**, 302-309.
7. L. Ma, J. Li, Y. Cheng, C. K. Lambert and L. Fu, *Environ. Sci. Technol.*, 2012, **46**, 1747-1754.
8. F. Gao, M. Kollár, R. K. Kukkadapu, N. M. Washton, Y. Wang, J. Szanyi and C. H. Peden, *Appl. Catal. B: Environ.*, 2015, **164**, 407-419.
9. S. Andonova, S. Tamm, C. Montreuil, C. Lambert and L. Olsson, *Appl. Catal. B: Environ.*, 2016, **180**, 775-787.
10. N. Martin, P. N. R. Vennestrom, J. R. Thogersen, M. Moliner and A. Corma, *ChemCatChem*, 2017, **9**, 1754-1757.
11. N. Martín, C. Paris, P. N. R. Vennestrøm, J. R. Thøgersen, M. Moliner and A. Corma, *Appl. Catal. B: Environ.*, 2017, **217**, 125-136.
12. J. Chen, G. Peng, W. Zheng, W. Zhang, L. Guo and X. Wu, *Catal. Sci. Technol.*, 2020, **10**, 6583-6598.
13. T. Ryu, Y. Kang, I.-S. Nam and S. B. Hong, *React. Chem. Eng.*, 2019, **4**, 1050-1058.
14. T. Ryu and S. B. Hong, *Appl. Catal. B: Environ.*, 2020, **266**, 118622-118630.