Supplementary Material

Fe-doped Beta Zeolite from Organotemplate-free Synthesis for NH_3-SCR of NO_x

Yongjun Zhu[a], Bingbing Chen[a], Rongrong Zhao[a], Qi Zhao[a], Hermann Gies[b], Feng-Shou Xiao[c], Dirk De Vos[d], Toshiyuki Yokoi[e], Xinhe Bao[f], Ute Kolb[g], Mathias Feyen[h], Stefan Maurer[h], Ahmad Moini[i], Ulrich Müller[h], Chuan Shi[a,*], Weiping Zhang[a,*]

[a]*State Key Laboratory of Fine Chemicals, School of Chemistry, Dalian University of Technology, Dalian 116024, China*

[b]*Institute für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum, Germany*

[c]*Department of Chemistry, Zhejiang University, Hangzhou 310028, China*

[d]*Centre for Surface Chemistry and Catalysis, K. U. Leuven, Leuven, Belgium*

[e]*Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, Japan*

[f]*State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Dalian 116023, China*

[g]*Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany*

[h]*BASF SE, Process Research and Chemical Engineering, 67056 Ludwigshafen, Germany*

[i]*BASF Corporation, Catalysts LLC, Iselin, NJ 08830, USA*

Table S1 Compositions of the as-prepared catalysts.

Catalysts	Fe content (wt %)	Si/Al	Catalysts	Fe content (wt %)	Si/Al
H-Beta-9	—	9	H-Beta-19	—	19
Fe(0.2)-Beta-9	0.2	9	Fe(0.1)-Beta-19	0.1	19
Fe(1.3)-Beta-9	1.3	9	Fe(1.4)-Beta-19	1.4	19
Fe(2.1)-Beta-9	2.1	9	Fe(2.3)-Beta-19	2.3	19
Fe(5.4)-Beta-9	5.4	9	Fe(5.7)-Beta-19	5.7	19

Table S2 Comparison of NO conversion rate at 150 °C for the as-prepared and literature reported catalysts

Index	Catalyst	Conditions	Temperature/°C	Rate/$mol_{(NOx)}$ $g_{(cat.)}^{-1}$ s^{-1}
Our work	**Fe-Beta-9**	**500 ppm NO, 500 ppm NH_3, 10% O_2, N_2 balance**	**150**	**5.00×10^{-7}**
Our work	**Fe-Beta-19**	**500 ppm NO, 500 ppm NH_3, 10% O_2, N_2 balance**	**150**	**2.31×10^{-7}**
Applied Catalysis B: Environmental 164(2015)407-419	Fe-SSZ-13	350 ppm NO, 350 ppm NH_3, 14% O_2, N_2 balance	150	9.11×10^{-8}
Catalysis Science & Technology, 4(2014)1350-1356	Fe-BEA	500 ppm NO, 500 ppm NH_3, 5% O_2, 8% CO_2, 5% H_2O, N_2 balance	150	1.78×10^{-7}
Applied Catalysis B: Environmental 91(2009)587-595	Fe-BEA	500 ppm NO, 500 ppm NH_3, 5% O_2, N_2 balance	150	1.58×10^{-7}
Chemical Engineering Journal 209(2012)652-660	Fe-BEA	500 ppm NO, 500 ppm NH_3, 5% O_2, N_2 balance	150	4.46×10^{-7}
Applied Catalysis B: Environmental 85(2009)109-119	Fe-BEA	500 ppm NO, 500 ppm NH_3, 5% O_2, N_2 balance	150	1.58×10^{-7}
Catalysis Science & Technology, 4(2014)3917-3626	Fe-SSZ-13	400 ppm NO, 400 ppm NH_3, 8% O_2, Ar balance	150	5.67×10^{-8}
Catalysis Today 235(2014)210-225	Fe-BEA	[NO] = [NH_3] = 0.25 vol.%, [O_2] = 2.5 vol.% and [He] = 97 vol.%	150	0
Chemical Engineering Journal 262(2015)1199-1207	Fe-ZSM-5	1000 ppm NO_x, 1000 ppm NH_3, 5% O_2, N_2 balance	150	4.69×10^{-8}

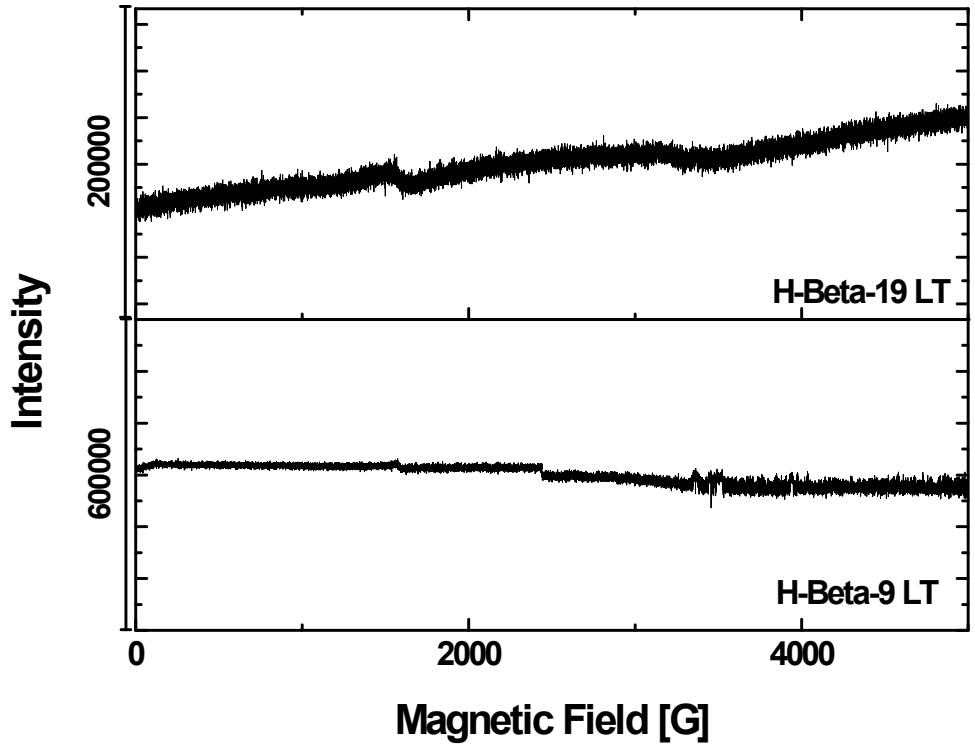

Fig. S1 EPR spectra of H-Beta-9 and H-Beta-19 catalysts measured at -196 °C.

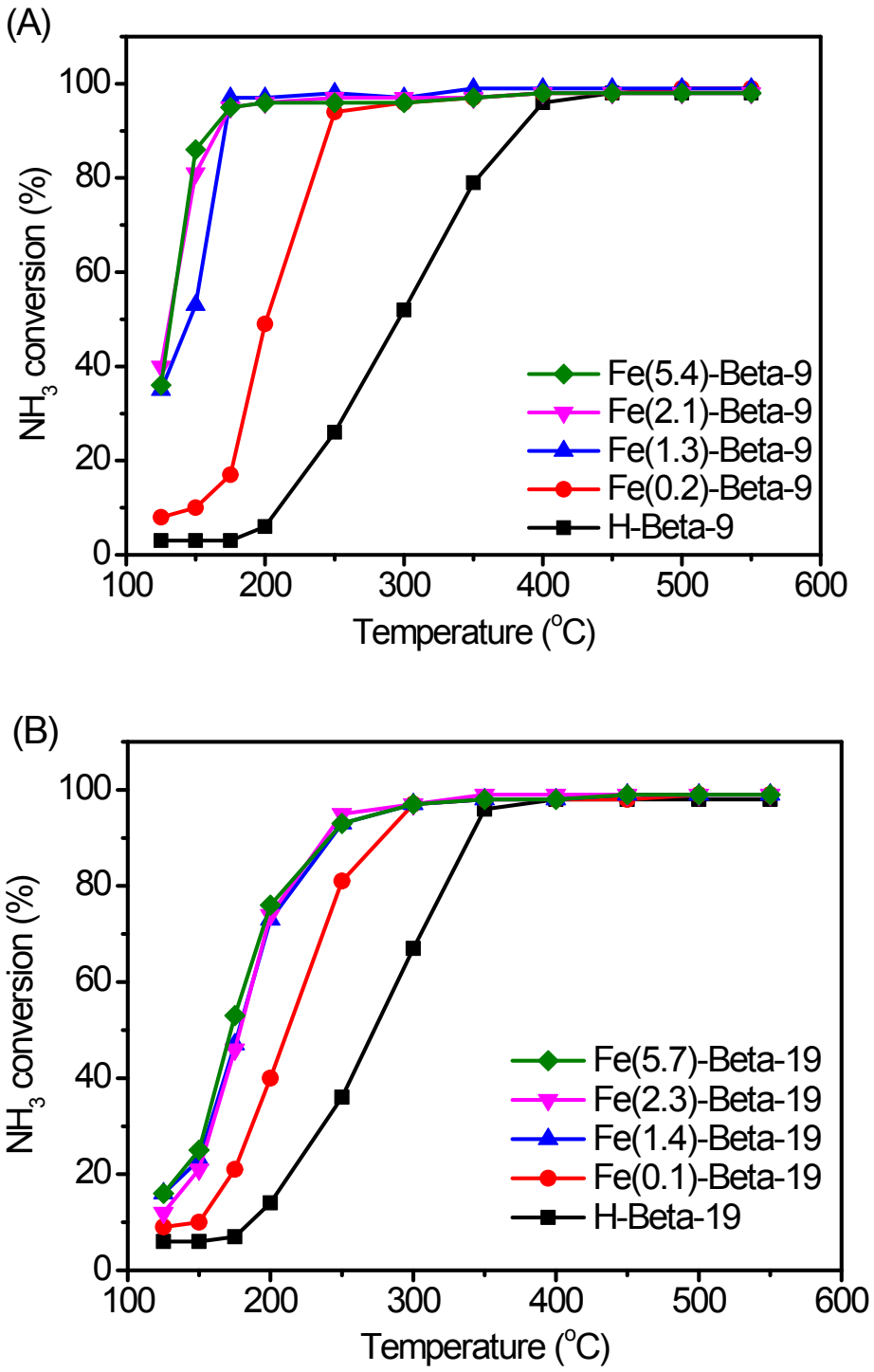

Fig. S2 NH_3 conversion as a function of temperature on both Fe-Beta-9(A) and Fe-Beta-19(B) series catalysts. Conditions: NO 500 ppm; NH_3 500 ppm, O_2 10%, balance N_2; GHSV=80000 h^{-1}.

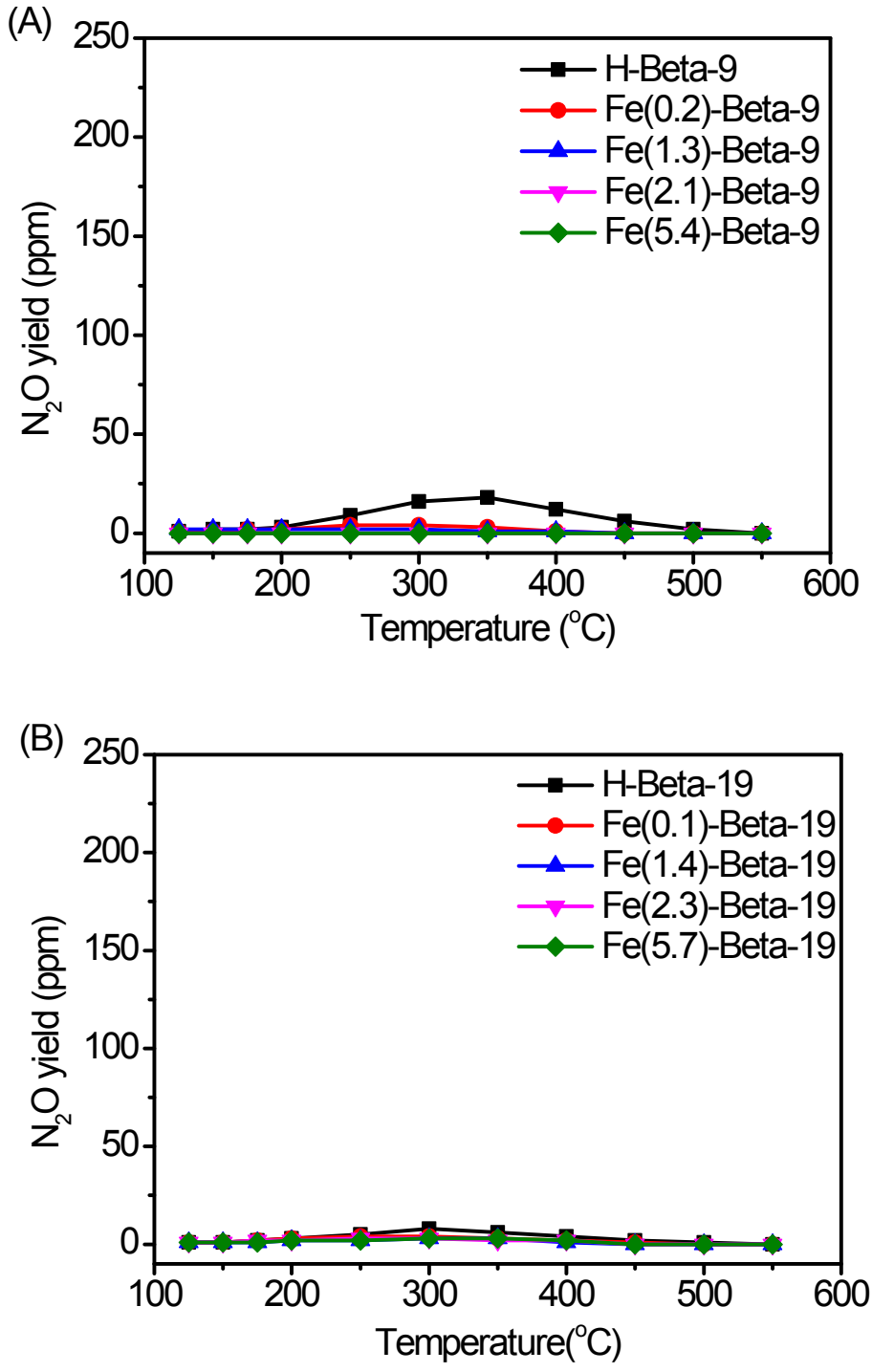

Fig. S3 N_2O yield as a function of temperature on both Fe-Beta-9(A) and Fe-Beta-19(B) series catalysts. Conditions: NO 500 ppm; NH_3 500 ppm, O_2 10%, balance N_2; GHSV=80000 h^{-1}.

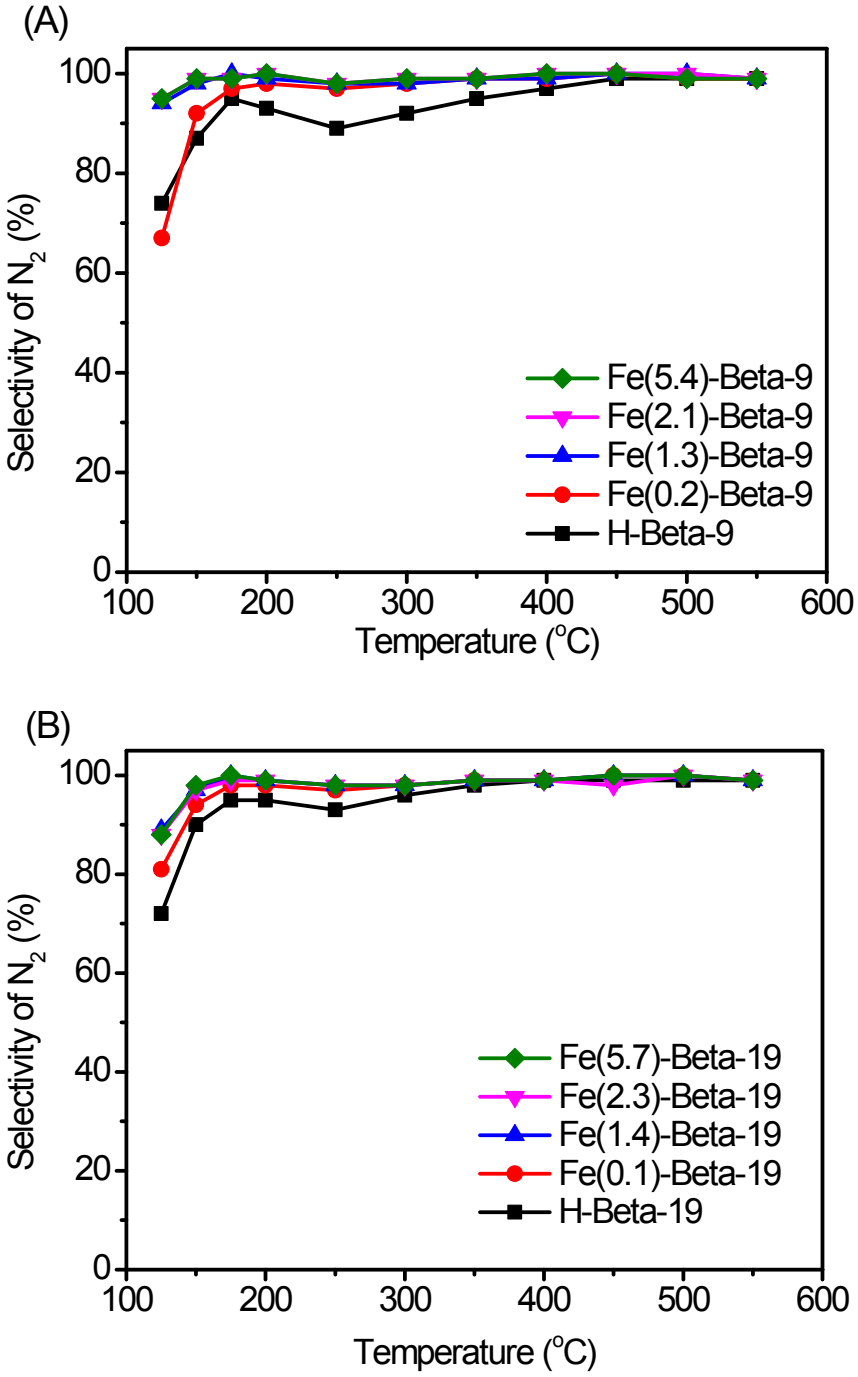

Fig. S4 Selectivity to N_2 in the course of the NH_3-SCR reaction over Fe-Beta-9 (A) and Fe-Beta-19 (B) series catalysts. Conditions: NO 500 ppm; NH_3 500 ppm, O_2 10%, balance N_2; GHSV=80000 h^{-1}.

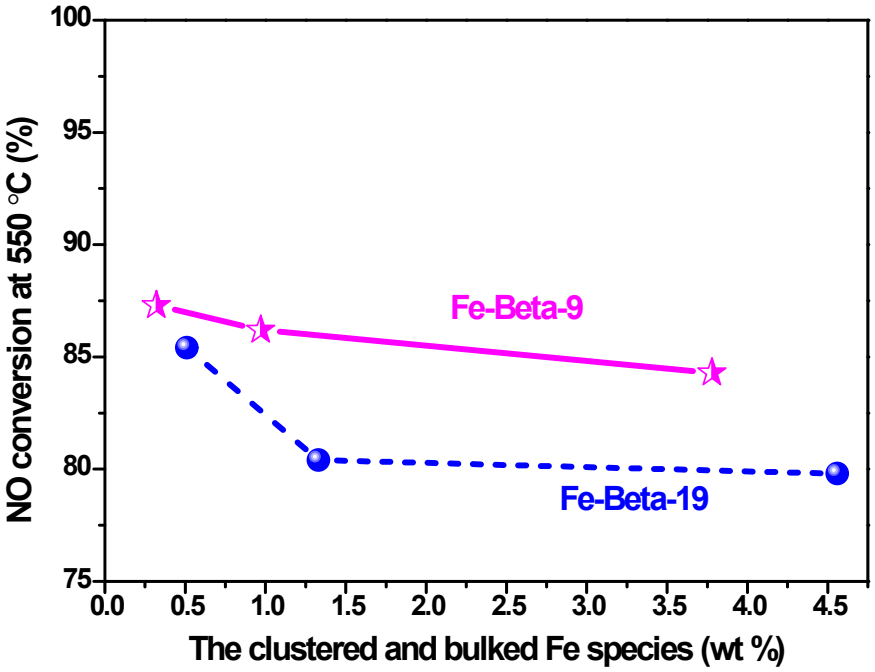

Fig. S5 Correlations of NO conversion at 550 °C as a function of clustered and bulked Fe species content of Fe-Beta-9 and Fe-Beta-19 series catalysts.

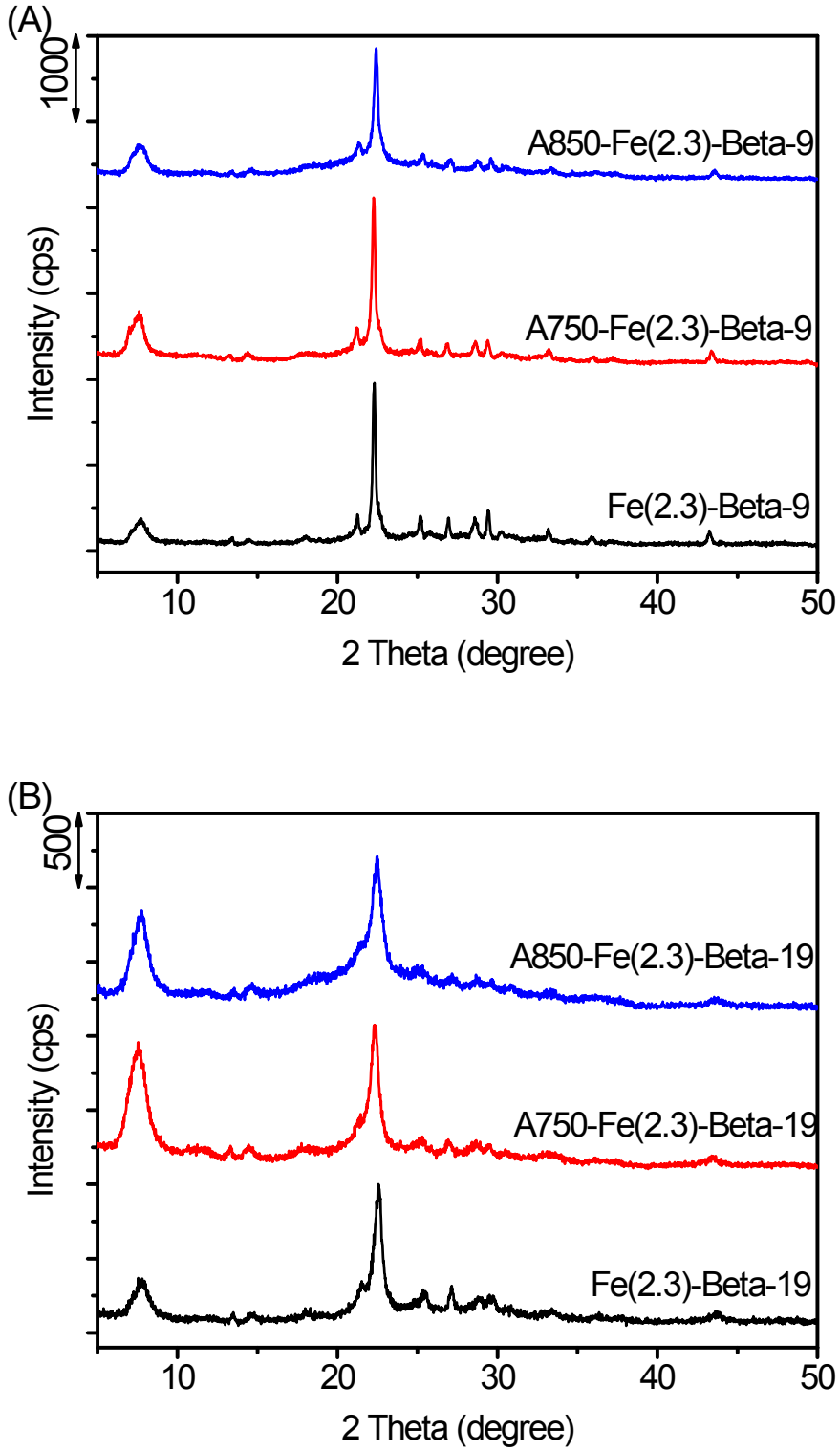

Fig. S6 XRD patterns of both Fe-Beta-9(A) and Fe-Beta-19(B) series catalysts. Where "A750, A850" are denoted that the catalyst have been treated under 10 % H_2O vapor /Ar at 750 °C and 850 °C for 10 h, respectively.

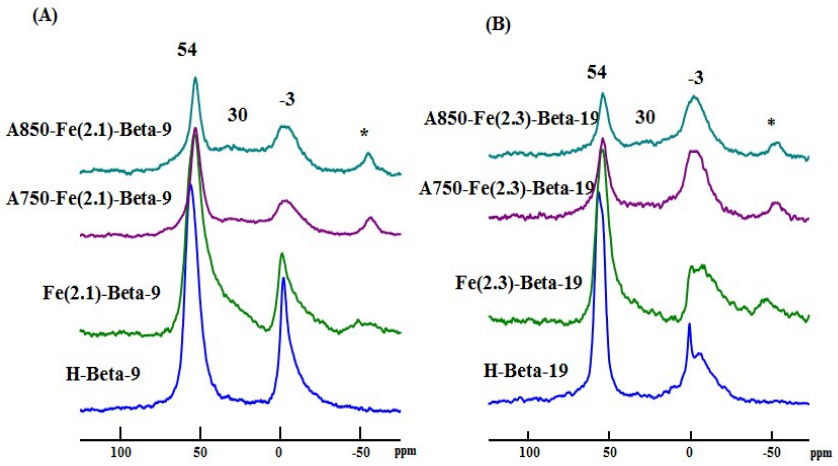

Fig. S7 ^{27}Al MAS NMR spectrum of Fe(2.1)-Beta-9(A) and Fe(2.3)-Beta-19 series catalysts. Where "A750, A850" are denoted that the catalyst have been treated under 10 % H_2O vapor /Ar at 750 °C and 850 °C for 10 h, respectively.

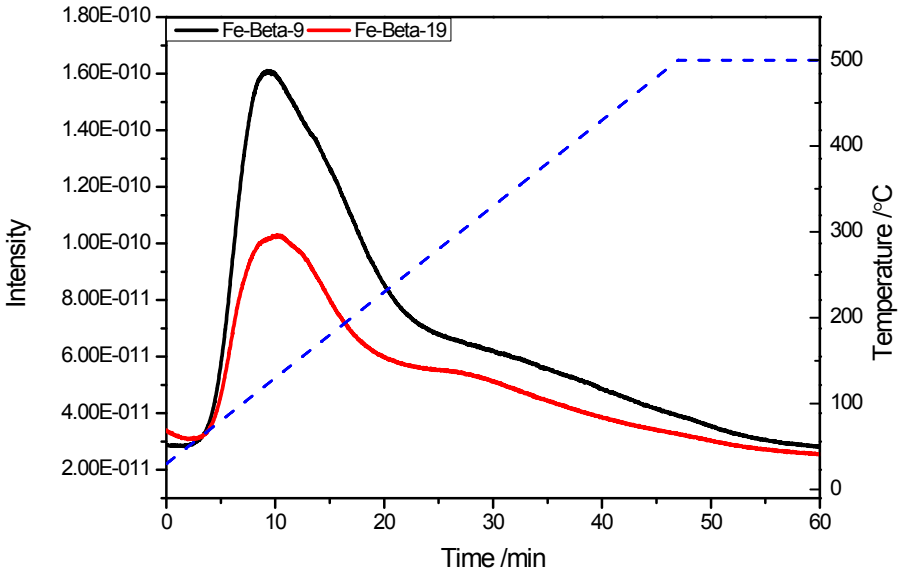

Fig. S8 NH_3-TPD profiles of the indicated catalysts with ammonia adsorbed at RT for 60 min, temperature ramping rate: 10 ^oC/min.