Iron-based composite oxide catalysts tuned by CTAB exhibit superior NH_3-SCR performance

Wenshuo Zhang [1,2], Xiaoyan Shi [1,2], Meng Gao [1,2], Jingjing Liu [1], Zhihui Lv [1,2], Yingjie Wang [4], Yanlong Huo [1,2], Chang Cui [1,2], Yunbo Yu [1,2,3,4,] and Hong He [1,2,3,*]*

[1] State Key Joint Laboratory of Environment Simulation and Pollution Control, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China

[2] University of Chinese Academy of Sciences, Beijing 100049, China

[3] Center for Excellence in Regional Atmospheric Environment, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China

[4] Ganjiang Innovation Academy, Chinese Academy of Sciences, Ganzhou 341000, China

Include 8 pages, 8 figures, 1 table.

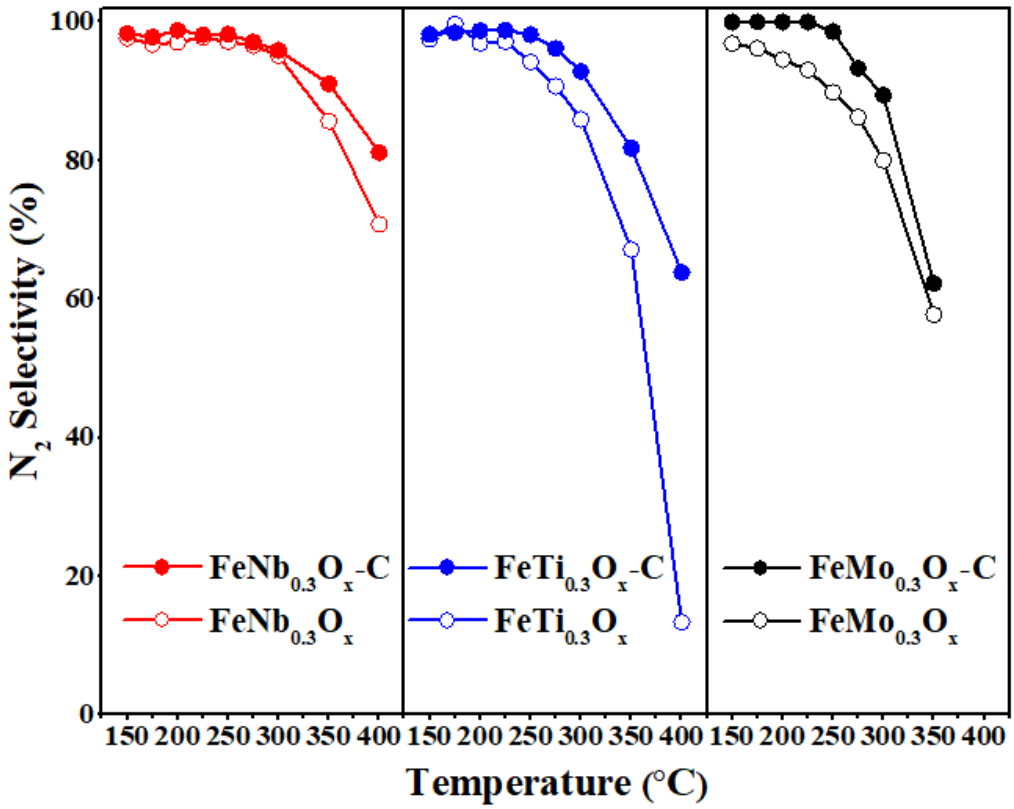

Figure S1. N_2 selectivity over all the $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples. Reaction conditions: [NO] = [NH_3] = 500 ppm, [O_2] = 5 vol%, N_2 balance, GHSV = 500 000 h^{-1}.

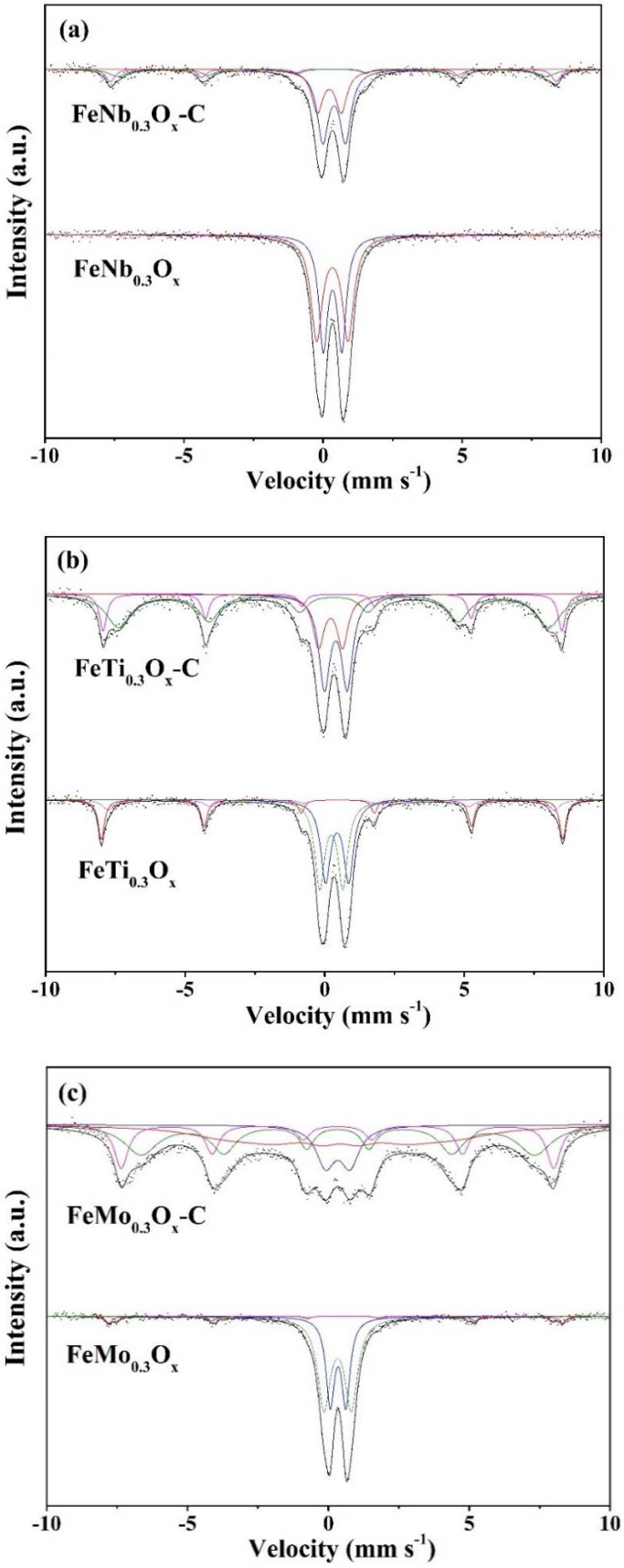

Figure S2. Mössbauer spectra of all the $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples at room temperature.

Table S1. Isomer shift (mm s^{-1}), quadrupole splitting (mm s^{-1}), internal hyperfine field (T), and area of sub-spectra from Mössbauer.

Sample	Sub Spectrum	Isomer Shift (mm s^{-1})	Quadrupole Splitting (mm s^{-1})	Internal Hyperfine Field (T)	Area (%)
$FeNb_{0.3}O_x$-C	Doublet	0.40	0.81	-	44.8
	Sextet	0.32	0.08	49.8	13.0
	Sextet	0.33	-	47.9	15.6
	Doublet	0.22	0.86	-	26.7
$FeNb_{0.3}O_x$	Doublet	0.34	0.66	-	45.4
	Doublet	0.33	1.13	-	54.6
$FeTi_{0.3}O_x$-C	Doublet	0.40	0.82	-	27.0
	Sextet	0.38	-0.21	51.1	14.1
	Sextet	0.32	-	49.8	43.5
	Doublet	0.21	0.86	-	15.3
$FeTi_{0.3}O_x$	Doublet	0.45	0.83	-	33.1
	Sextet	0.37	-0.21	51.4	21.4
	Sextet	0.37	-0.29	49.7	10.1
	Doublet	0.24	0.83	-	35.5
$FeMo_{0.3}O_x$-C	Doublet	0.33	0.87	-	12.6
	Sextet	0.32	0.00	47.7	20.6
	Sextet	0.33	-	43.4	34.4
	Sextet	0.43	-	24.7	32.3
$FeMo_{0.3}O_x$	Doublet	0.34	0.56	-	36.0
	Sextet	0.39	-0.28	50.06	4.6
	Sextet	0.36	-0.27	48.05	2.9
	Doublet	0.33	0.97	-	56.5

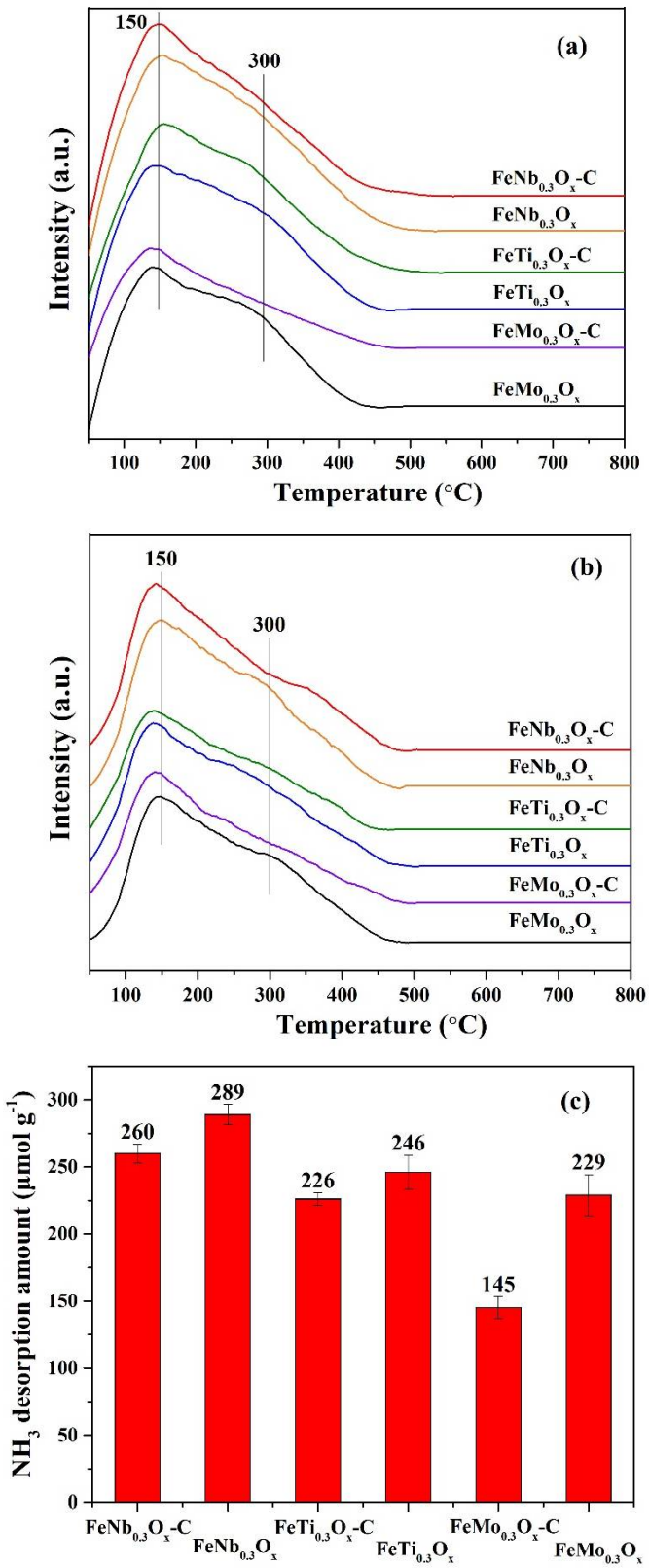

Figure S3. (**a**) NH_3-TPD results of all the $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples in a flow of N_2 with a heating rate of 10 °C min^{-1}. Before measurement, each sample was pretreated in 20 % O_2/N_2 at 350 °C for 0.5 h, then exposed to 500 ppm NH_3/N_2 at 50 °C for 0.5 h, and purged by N_2 for 0.5 h. (**b**) Repeated NH_3-TPD results and (**c**) NH_3 desorption amount of all the $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples with error bars.

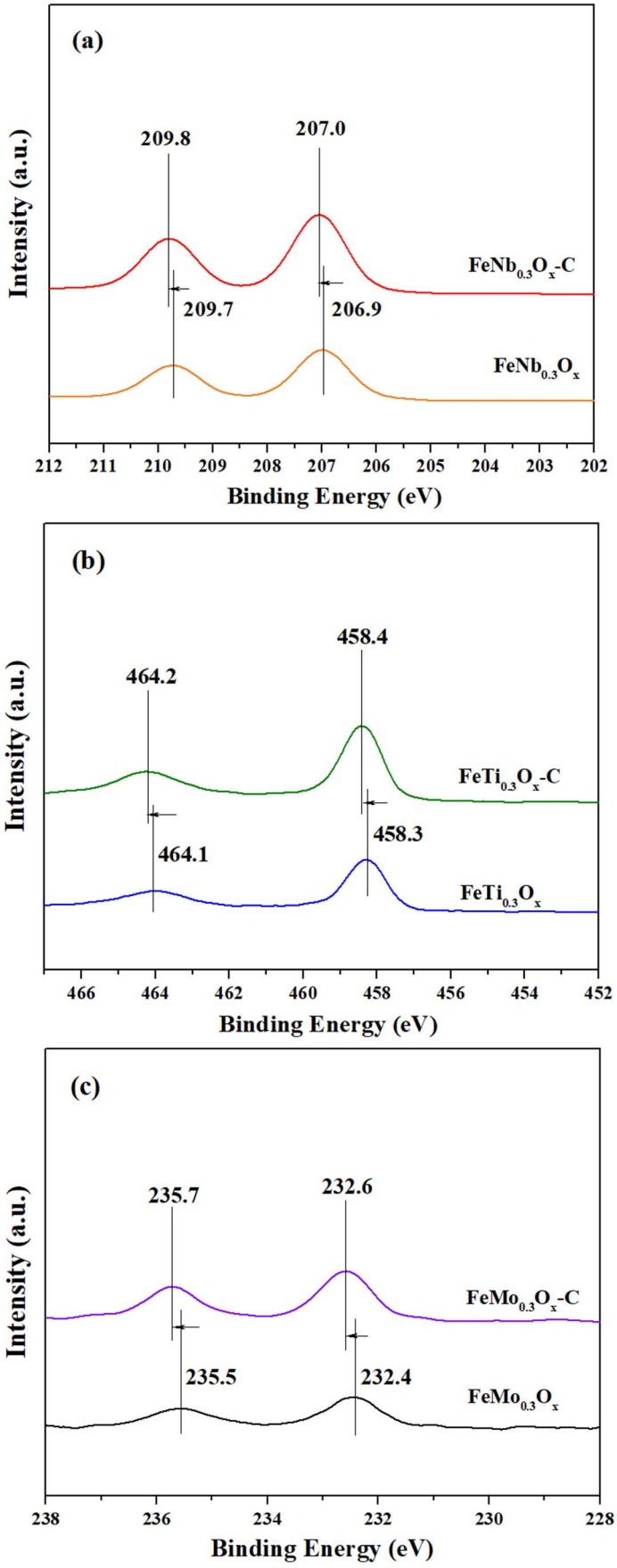

Figure S4. XPS spectra of (**a**) Nb 3d; (**b**) Ti 2p; and (**c**) Mo 3d over $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples.

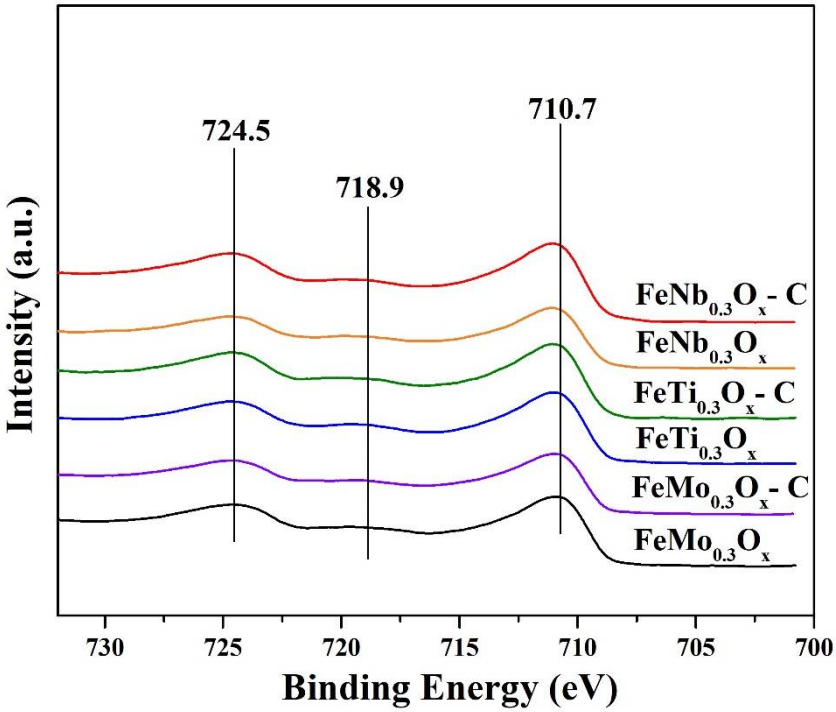

Figure S5. XPS spectra of Fe 2p over $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples.

The NH_3 conversion and NO conversion were calculated as follow:

$$NH_3\ \text{conversion}(\%) = \left(1 - \frac{[NH_3]_{out}}{[NH_3]_{in}}\right) \times 100\%$$

$$NO\ \text{conversion}(\%) = \left(1 - \frac{[NO]_{out}}{[NO]_{in}}\right) \times 100\%$$

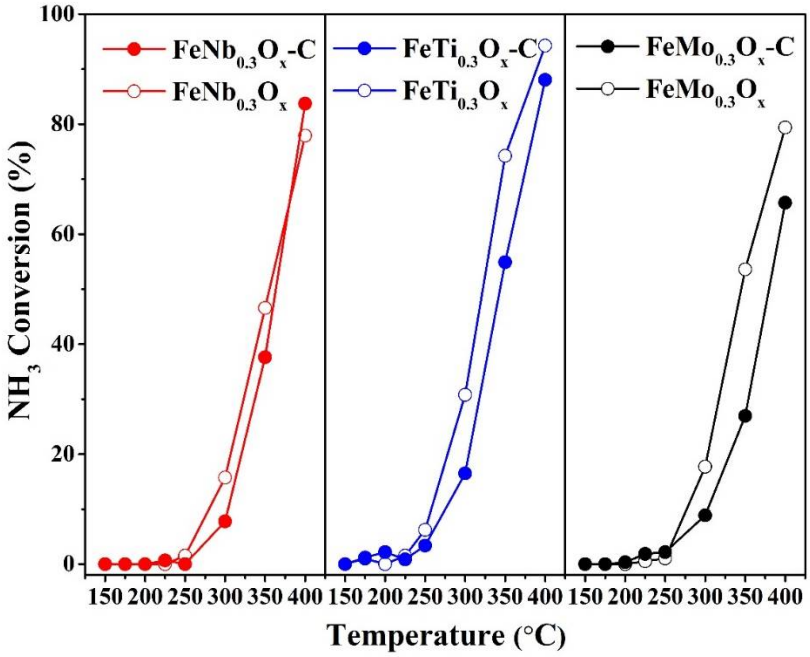

Figure S6. Direct oxidation of NH_3 over all the $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples. Reaction conditions: [NH_3] = 500 ppm, [O_2] = 5 vol%, N_2 balance, GHSV = 250,000 h^{-1}.

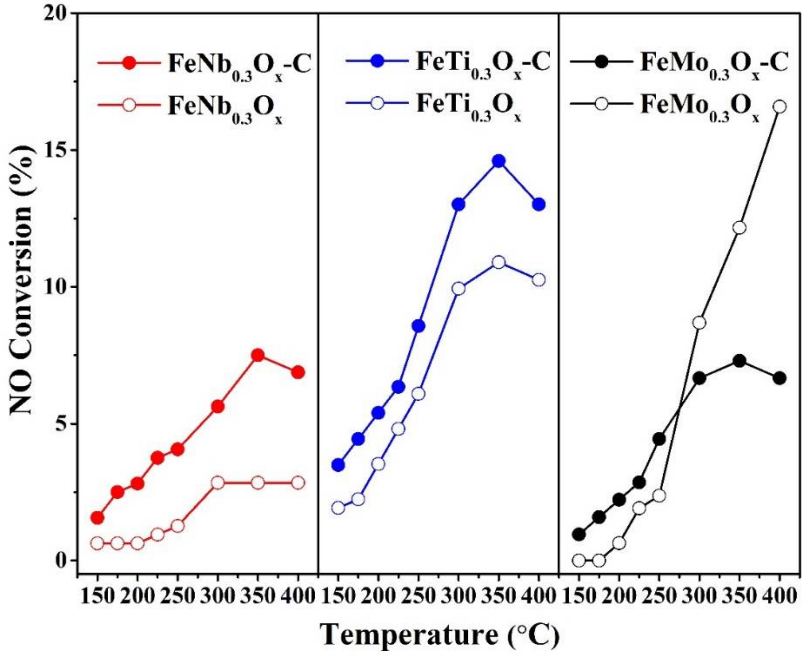

Figure S7. Direct oxidation of NO over all the $FeM_{0.3}O_x$-C and $FeM_{0.3}O_x$ (M = Nb, Ti, Mo) samples. Reaction conditions: [NO] = 500 ppm, [O_2] = 5 vol%, N_2 balance, GHSV = 250,000 h^{-1}.

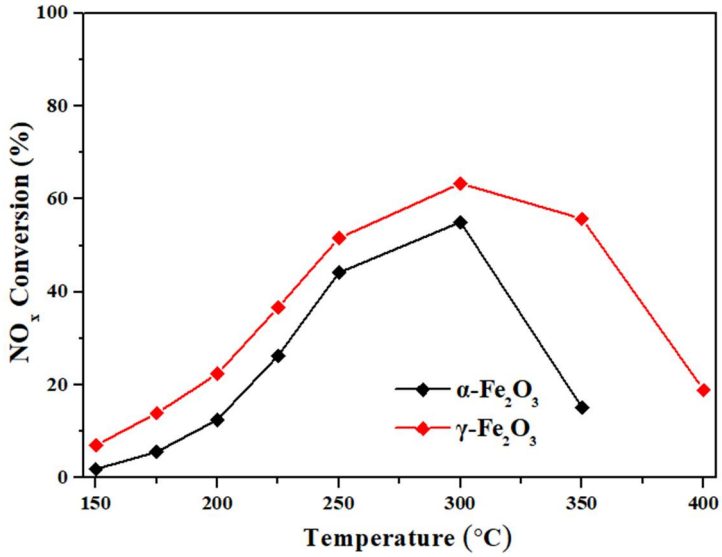

Figure S8. NO_x conversion over pure γ-Fe_2O_3 and pure α-Fe_2O_3. Reaction conditions: [NO] = [NH_3] = 500 ppm, [O_2] = 5 vol%, N_2 balance, GHSV=500 000 h^{-1}.