

Promotion effect of cerium doping on iron-titanium composite oxide catalyst for selective catalytic reduction of NO_x with NH₃

Wenshuo Zhang,^{a,b} Xiaoyan Shi,^{a,b} Yulong Shan,^{a,b} Jingjing Liu,^{a,b} Guangyan Xu,^{a,b}

Jinpeng Du,^{a,b} Zidi Yan,^{a,b} Yunbo Yu^{a,b,c} and Hong He*^{a,b,c}*

^a State Key Joint Laboratory of Environment Simulation and Pollution Control, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China.

^b University of Chinese Academy of Sciences, Beijing 100049, China.

^c Center for Excellence in Regional Atmospheric Environment, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China.

Include 6 pages, 6 figures, 4 tables.

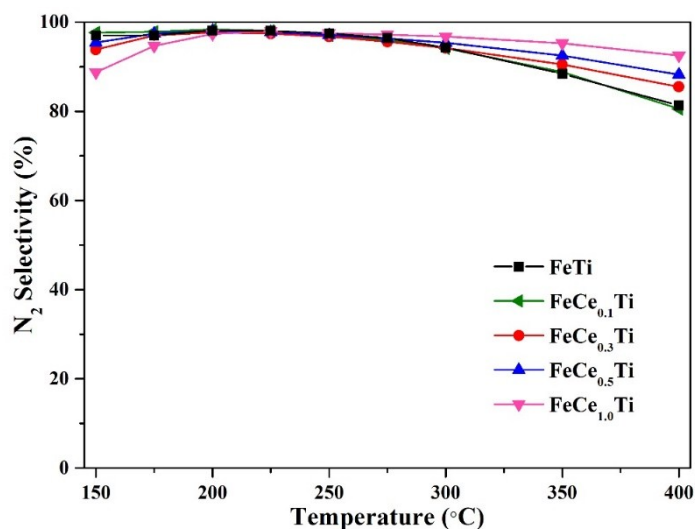


Fig. S1 N_2 selectivity over FeTi and $FeCe_aTi$ catalysts calcined at 500 °C. Reaction conditions: $[NO] = [NH_3] = 500$

ppm, $[O_2] = 5$ vol.%, N_2 balance, and GHSV=250,000 h^{-1} .

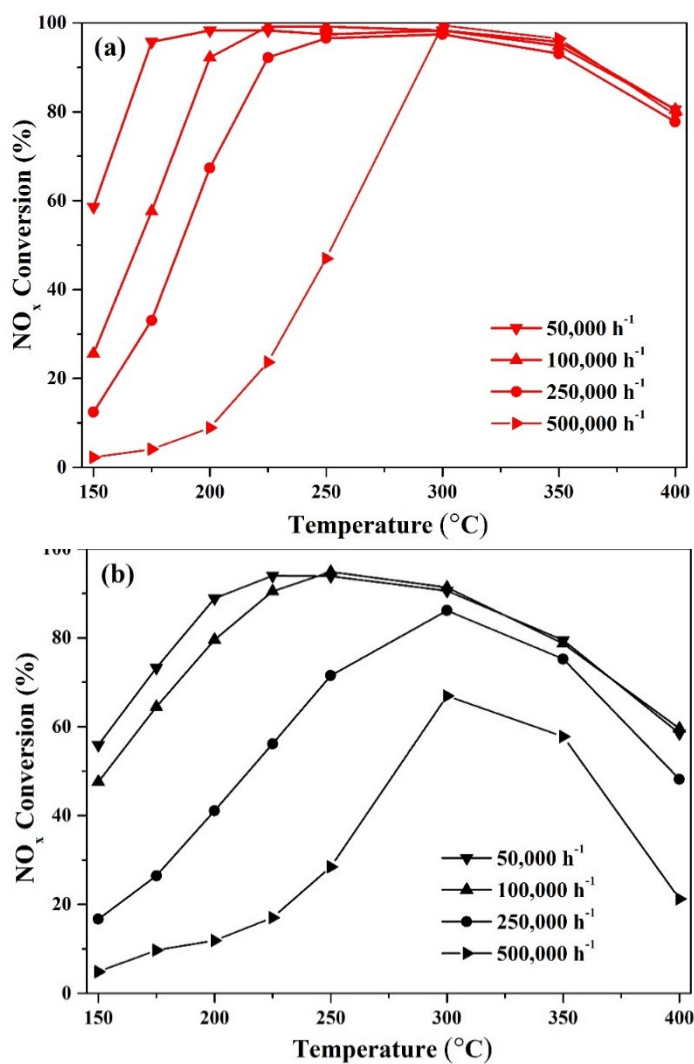


Fig. S2 NO_x conversion over (a) $FeCe_{0.3}Ti$ and (b) FeTi catalysts calcined at 500 °C. Reaction conditions: $[NO] =$

$[NH_3] = 500$ ppm, $[O_2] = 5$ vol.%, N_2 balance, and GHSV from 50,000 to 500,000 h^{-1} .

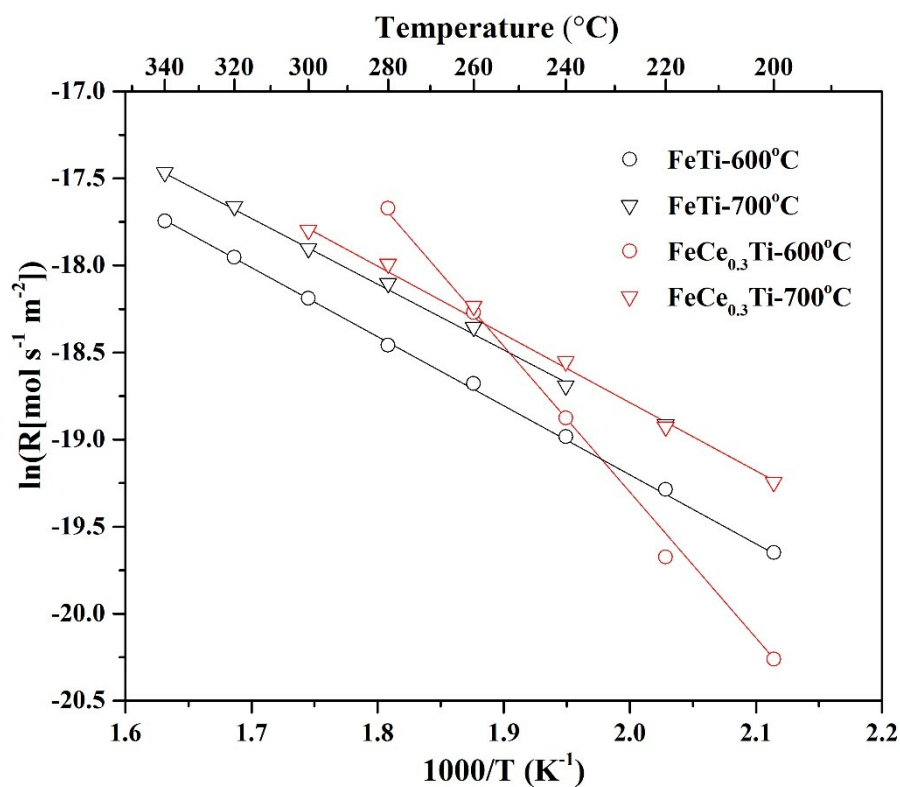


Fig. S3 Arrhenius plots of the reaction rates over FeTi and FeCe_{0.3}Ti catalysts calcined at 600 °C and 700 °C, respectively. Reaction conditions: [NO] = [NH₃] = 500 ppm, [O₂] = 5 vol.%, N₂ balance.

Table S1 Activation energy, pre-exponential factor and R² of FeTi and FeCe_{0.3}Ti catalysts calcined at 500 °C, 600 °C, and 700 °C, respectively.

	E_a (kJ mol ⁻¹)	A (molecules per m ² s)	R ²
FeTi	28.8	7.2×10^{18}	0.994
FeTi-600 °C	32.6	7.1×10^{18}	0.999
FeTi-700 °C	30.8	1.1×10^{18}	0.998
FeCe _{0.3} Ti	47.5	1.9×10^{21}	0.991
FeCe _{0.3} Ti-600 °C	71.6	1.2×10^{22}	0.997
FeCe _{0.3} Ti-700 °C	36.1	1.8×10^{19}	0.996

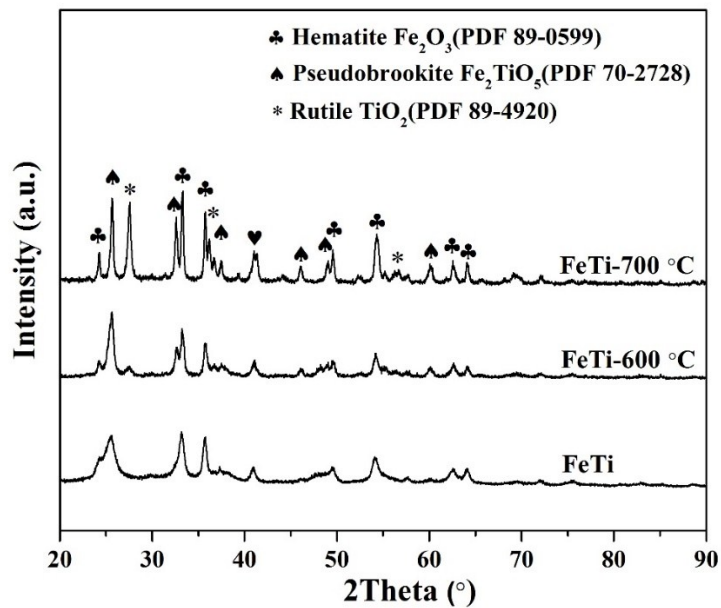


Fig. S4 XRD patterns of FeTi catalysts calcined at 500 °C, 600 °C, and 700 °C.

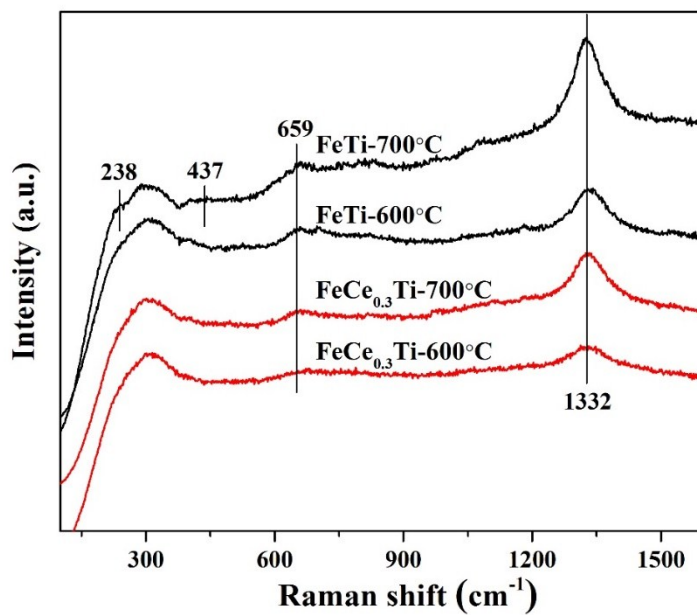


Fig. S5 Raman spectra of FeTi and FeCe_{0.3}Ti catalysts calcined at 600 °C and 700 °C, respectively.

Table S2 XRF results of FeTi and FeCe_aTi catalysts calcined at 500 °C.

	Fe (Wt %)	Ti (Wt %)	Ce (Wt %)
FeTi	35.92	28.60	-
FeCe _{0.1} Ti	32.34	25.87	7.82
FeCe _{0.3} Ti	26.42	21.30	19.55
FeCe _{0.5} Ti	22.99	18.58	27.10
FeCe _{1.0} Ti	17.60	14.02	39.21

Table S3 Atom ratios in near-surface region of FeTi and FeCe_aTi catalysts calcined at 500 °C from XPS.

	Fe 2p (%)	Ti 2p (%)	Ce 3d (%)	O 1s (%)
FeTi	30.60	3.85	-	50.23
FeCe _{0.1} Ti	30.68	3.60	0.51	49.34
FeCe _{0.3} Ti	29.62	2.92	0.86	49.68
FeCe _{0.5} Ti	26.60	2.00	1.79	50.50
FeCe _{1.0} Ti	23.68	1.53	4.11	51.49

Table S4 XPS binding energies of individual peaks of the Ce 3d spectra for FeCe_aTi catalysts calcined at 500 °C.

	Ce ⁴⁺						Ce ³⁺	
	v	v ₂	v ₃	u	u ₂	u ₃	v ₁	u ₁
FeCe_{0.1}Ti	882.6	890.0	898.5	901.2	907.2	915.0	885.0	903.0
FeCe_{0.3}Ti	882.6	890.0	898.5	901.0	907.2	916.8	885.7	904.0
FeCe_{0.5}Ti	882.6	889.0	898.5	901.2	907.1	916.9	885.0	903.0
FeCe_{1.0}Ti	882.6	888.7	898.5	901.2	907.2	916.9	885.0	903.0

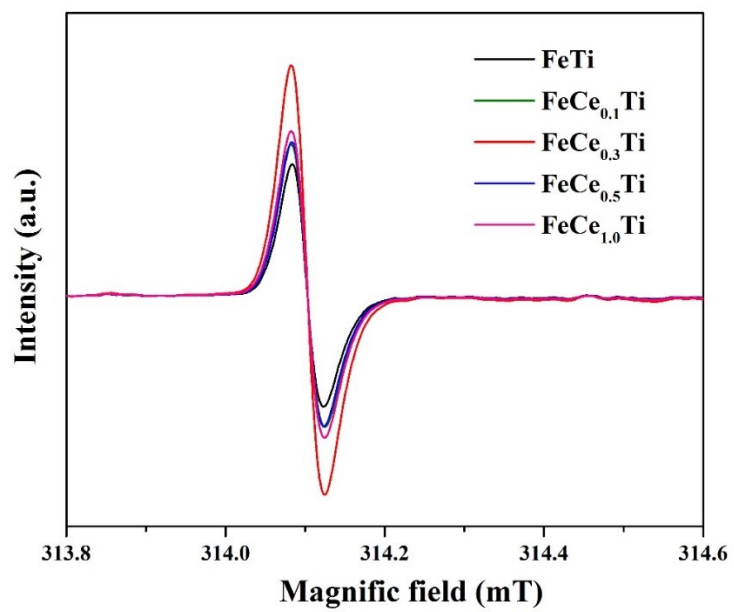


Fig. S6 EPR spectra of FeTi and FeCe_aTi catalysts calcined at 500 °C.