

Decorated CrO_x on Fe/TiO₂ with tunable and stable Oxygen Vacancy for Selective Oxidation of Glycerol to Lactic Acid

Dawang Chu ^{a, b}, Hui Zhou ^c, Zhicheng Luo* ^a

^a MOE Key Laboratory of Energy Thermal Conversion & Control, School of Energy and Environment, Southeast University, Nanjing 210096, China, 202162.

^b School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China, 200062.

^c Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Beijing Key Laboratory of CO₂ Utilization and Reduction Technology, Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, P.R. China.

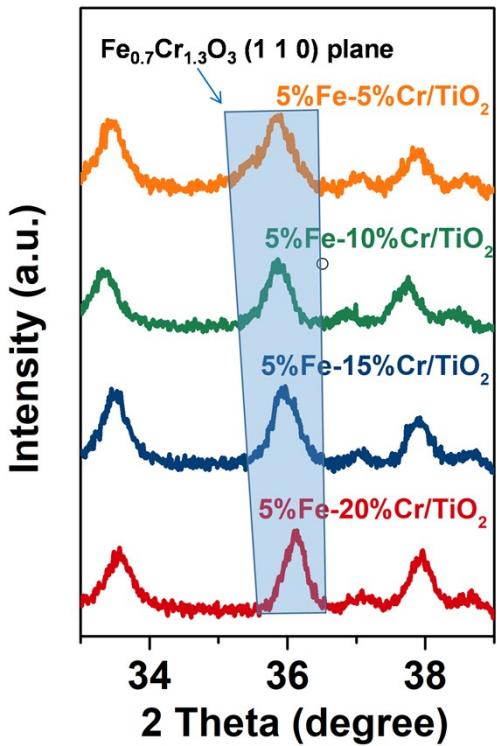


Figure S1. Zoomed area ranging from 33° to 39° in Figure 2a.

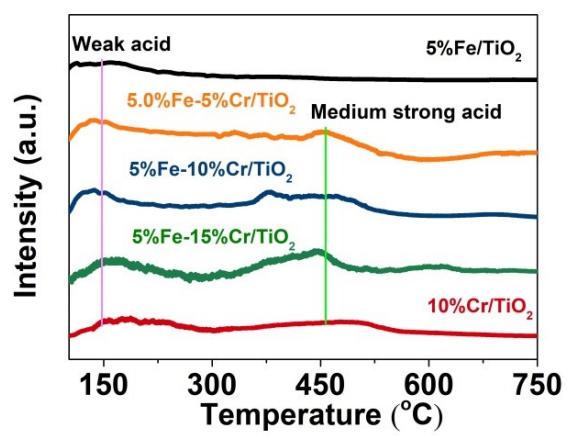


Figure S2. NH₃-TPD for various Fe-Cr/TiO₂ catalysts.

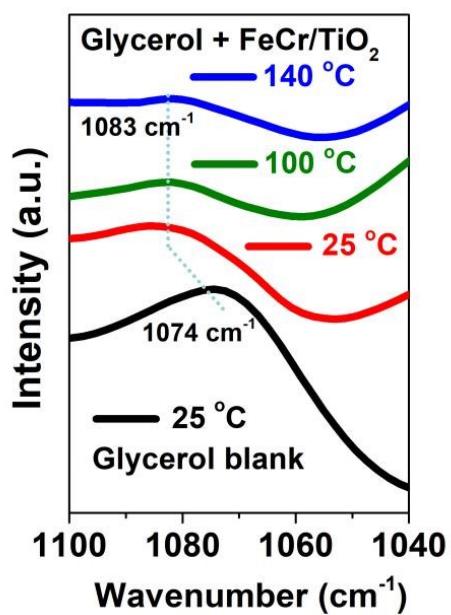


Figure S3. Zoomed area ranging from 1110 cm^{-1} to 1040 cm^{-1} in Figure 5.

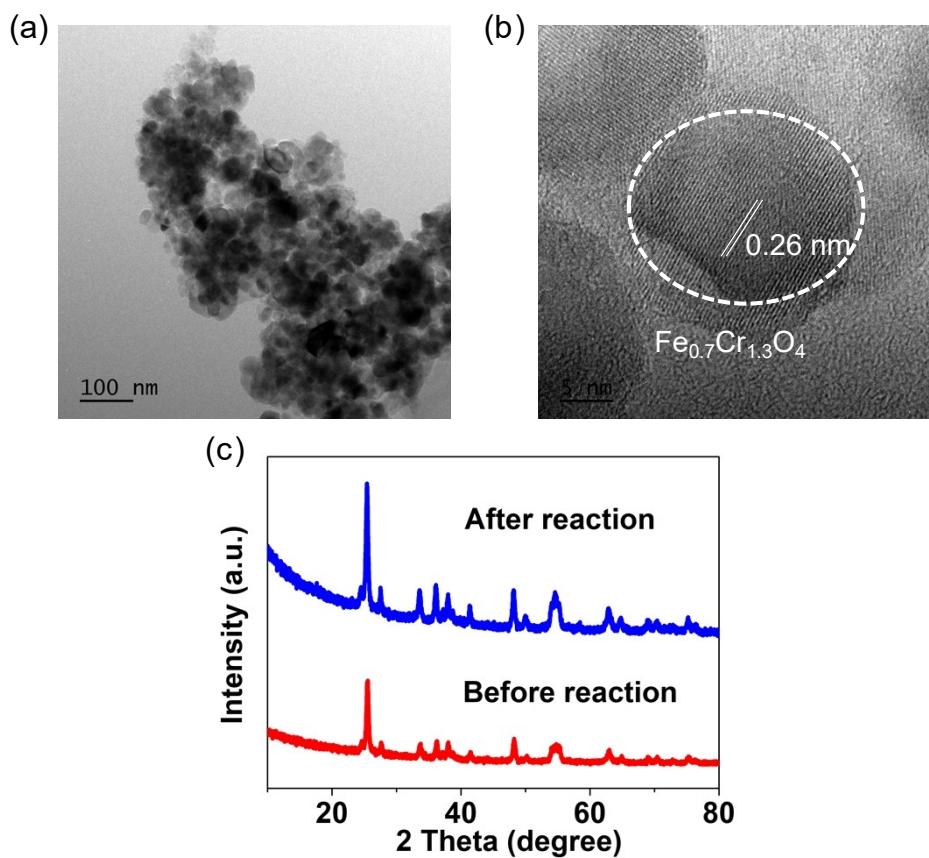


Figure S4. Characterization of the used 5%Fe-10%Cr/TiO₂ catalyst. (a) TEM image, (b) HRTEM image and (c) XRD pattern.

Table S1. Effect of catalysts on one-pot conversion of glycerol into LA.

Catalyst	Conv. (%)	Selectivity (C%)					Carbon balance (C%)
		Lactic acid	Glyceraldehyde	Acetic acid	Formic acid	Others	
TiO ₂	72.1	15.1	6.5	3.1	3.3	11.5	39.5
Fe/TiO ₂	55.3	40.7	5.5	1.3	3.2	14.3	65.0
Co/TiO ₂	45.5	35.1	13.7	4.2	3.5	9.7	66.2
Ni/TiO ₂	55.1	23.3	37.2	5.1	3.0	8.4	77.0
Cu/TiO ₂	48.4	29.4	19.0	2.5	2.2	13.6	66.7
Zn/TiO ₂	36.7	34.4	9.0	3.7	2.9	7.3	57.3
Ga/TiO ₂	46.4	30.7	11.5	4.5	3.0	9.5	59.2

Reaction condition: 1.0 g glycerol, 0.2 g catalyst, 0.5 g NaOH, 50 ML H₂O, 140 °C, 1 Mpa initial pressure of O₂, 6 h.

Table S2. Acidity of 5%Fe-x%Cr/TiO₂ catalysts calculated from NH₃-TPD.

Catalysts	Total acid amount (μmol/g) ^a
5%Fe/TiO ₂	3.0
5%Fe-5%Cr/TiO ₂	8.1
5%Fe-10%Cr/TiO ₂	14.6
5%Fe-15%Cr/TiO ₂	16.2
10%Cr/TiO ₂	12.8

^a measured by NH₃-TPD.

Table S3. Acidity of 5%Fe-10%Cr/TiO₂ catalysts reduced at different temperatures calculated from pyridine-adsorbed FT-IR.

Reduction temperature (°C)	Lewis acid amount (μmol/g) ^a	Brönsted acid amount (μmol/g) ^a
300	13.9	2.5
450	11.2	1.1
600	6.9	0.5
750	1.5	0.1

^a measured by Py-FTIR.

Table S4. Effect of temperature on one-pot conversion of glycerol into LA over 5%Fe-10%Cr/TiO₂ catalysts..

Temperature (°C)	Conv. (%)	Selectivity (C%)				Carbon balance (C%)	
		Lactic acid	Glyceraldehyde	Acetic acid	Formic acid		
120	10.4	27.3	10.0	22.5	7.1	11.2	78.1
140	60.5	60.4	6.7	2.3	2.9	6.5	78.8
160	97.4	7.1	1.2	8.7	6.6	9.7	33.3
180	99.2	7.8	0.6	10.4	17.4	8.4	44.6

Reaction condition: 1.0 g glycerol, 0.2 g catalyst, 0.5 g NaOH, 50 ML H₂O, 1 Mpa initial pressure of O₂, 6 h.