Heterogeneous Conversion of SO₂ on Nano α-Fe₂O₃: the Effect of Morphology, Light Illumination and Relative Humidity

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Preparation of α-Fe₂O₃ samples

Synthesis of nanocapsule-like α -Fe₂O₃ (α -Fe₂O₃-A): according to the reported procedure,¹ 0.2 mmol SDS was added into 40 mL deionized water under magnetic stirring. Then 2.0 mmol FeCl₃·6H₂O and 2.0 mmol CH₃COONa were added to the SDS solution orderly under stirring. The colorless transparent SDS solution transferred to turbid solution immediately after the FeCl₃·6H₂O and CH₃COONa were added. After being stirred for 20 min, the slurry was treated at 140 °C for 24 h in 50-mL Teflon-lined autoclave, and then cooled to room temperature naturally. The precipitate was centrifuged for 5 min under 4000 rpm. The obtained product was washed with deionized water and ethanol for 3 times, and then dried at 80 °C for 12 h. The obtained powders were finely ground and collected for experiments.

Synthesis of hollow nanoring-like α -Fe₂O₃ (α -Fe₂O₃-B): in a typical procedure,² 1.62 g FeCl₃·6H₂O was added into 300 mL deionized water with stirring to form a transparent solution. Then 0.0062 g NH₄H₂PO₄ and 0.023 g Na₂SO₄ were added respectively under stirring. After being stirred for 10 min, the solution was transferred into three 100-mL Teflon-lined autoclaves and maintained at 220 °C for 48 h. After the autoclave cooled to room temperature, the precipitate was separated by centrifugation, washed with deionized water and ethanol for 3 times. The product was dried at 80 °C for 12 h and finely ground for following experiments.

Synthesis of hexagonal nanoplate-like α -Fe₂O₃ (α -Fe₂O₃-C): according to previous work,³ 4 mmol FeCl₃·6H₂O was dissolved in 40.0 mL ethanol with a trace addition of deionized water (2.8 mL) under magnetic stirring. After dissolution, 3.2 g of CH₃COONa was added while stirring. The solution was transferred into 50-mL Teflon-lined autoclave and maintained at 180 °C for 12 h. Following natural cooling to room temperature, the products were centrifuged and washed with

distilled water and ethanol for 3 times. Then the product was dried at 80 °C for 12 h and finely ground.

Synthesis of agglomerated nanoparticle-like α -Fe₂O₃ (α -Fe₂O₃-D): according to the previously reported procedure,⁴ 40.4 g Fe(NO₃)₃ \bigcirc 39H₂O, 4.2 g NaHCO₃, 33.6 g KOH were added into 500, 50, 300 mL deionized water under stirring, respectively, and then the three solutions were heated to 363 K with water bath. Then mixed them together in a polyethylene bottle and the pH is adjusted to 8.0~8.5 before aging at 363 K for 48 h. After cooling to room temperature, the precipitate was centrifuged and washed with distilled water and ethanol for 3 times. Then the product was dried at 80 °C for 12 h and finely ground.

Table S1.	Parameters for	r uptake coe	efficient of	calculation

Parameter (unit)	Value	
Sulfate formation rate: d[SO ₄ ²⁻]/dt (ion·s ⁻¹)	According to reactions	
$A_{BET} \left(m^2/g \right)$	Shown in Table 1	
A_{geo} (m ²)	7.85×10 ⁻⁵	
Reactant concentration: c_{SO_2} (molecule·m ⁻³)	7.37×10 ¹⁹	
Gas constant: R (J·mol ⁻¹ ·K ⁻¹)	8.314	
Temperature: T (K)	298	
Molar mass: M_{SO_2} (Kg·mol ⁻¹)	6.4×10 ⁻²	
π (dimensionless)	3.14	



Figure S1. In situ DRIFTS spectra of different samples (1400~900 cm⁻¹) under light illumination. a, α-Fe₂O₃-A.

b, α -Fe₂O₃-B. c, α -Fe₂O₃-C. d, α -Fe₂O₃-D.



Figure S2. In situ DRIFTS spectra of collected on α -Fe₂O₃ samples (3720-3560 cm⁻¹) under light illumination.

a, α -Fe₂O₃-A. b, α -Fe₂O₃-B. c, α -Fe₂O₃-C. d, α -Fe₂O₃-D.



Figure S3. Calculated ions of sulfates on different α-Fe₂O₃ samples under light illumination.



Figure S4. The spectrum of the Xe lamp with optical fiber (model CEL-TCX250, Beijing Jin Yuan Science and

Technology Co., Ltd.).



Figure S5. In-situ DRIFTS spectra collected at 120 min on α-Fe₂O₃-C under different 68% RH saturation time.

Supplementary References

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