Supplementary information

Effect of the feed impurities on catalytic performance of $CuFe_2O_4$/β–SiC for SO_3 decomposition in the sulfur–iodine cycle

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ESI1 WHSV is defined as ratio of mass flow rate of feed (g/h) to catalyst mass (g).[1]

$$\text{WHSV} = \frac{F_{feed}}{W_{cat}} \ \text{h}^{-1}$$

ESI2 XRD of fresh $CuFe_2O_4$/β–SiC

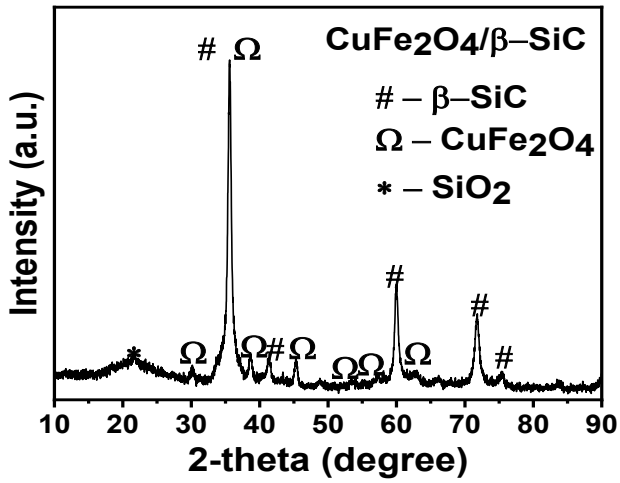

Fig. ESI2 XRD of fresh $CuFe_2O_4$/β–SiC.[2]

ESI3 Adsorption–desorption isotherms of fresh $CuFe_2O_4$/β–SiC

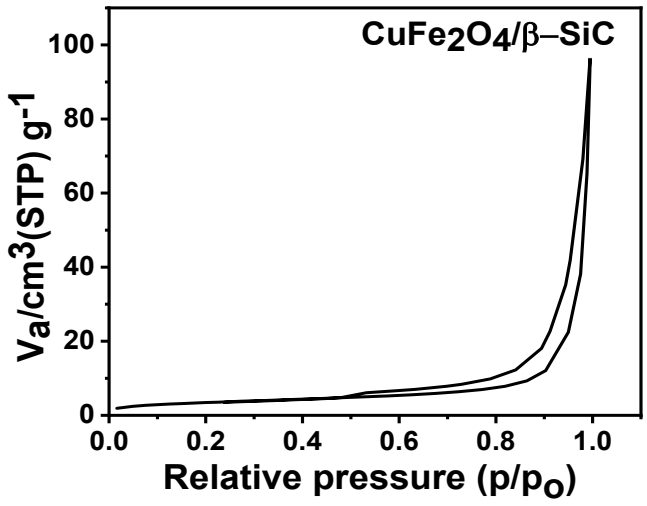

Fig. ESI3 Adsorption–desorption isotherms of fresh $CuFe_2O_4$/β–SiC.[2]

ESI4 Plausible reaction mechanism

Plausible reaction mechanism of sulfuric acid decomposition in presence of the feed impurities is discussed in this section. Potassium iodide (KI) reacts with sulfuric acid (H_2SO_4) to form potassium bisulfate ($KHSO_4$) and hydrogen iodide (HI) as shown in the equation Seq1. Hydrogen iodide, which is a strong reducing agent reacts with H_2SO_4 and gets oxidised to free iodine, sulfur dioxide (SO_2) and water (H_2O) which is a reverse Bunsen reaction as given in the equation Seq2. The product steam containing SO_2 and water vapour were trapped using concentrated sodium hydroxide, calcium oxide and silica gel. In the equation Seq3, thermal decomposition of potassium bisulfate takes place in the temperature range of 370–840 ˚C and it converts into potassium pyrosulfate ($K_2S_2O_7$) and water.[3] Potassium pyrosulfate either converts into potassium metabisulfite (K_2SO_5) and sulfur dioxide (SO_2) as shown in the equation Seq4 or it may be converted into potassium sulfate (K_2SO_4) and sulfur trioxide (SO_3) between 470–700 ˚C as shown in the equation Seq5.[3–5] In the equation Seq6, potassium metabisulfite further converts into potassium sulfate and oxygen.[3] Potassium sulfate converts into potassium oxide and sulfur trioxide as shown in the equation Seq7. Sulfur trioxide produced in Seq5 and Seq7 converts into sulfur dioxide and oxygen over the catalytic system as shown in the equation Seq8.

$$2\ KI + 2\ H_2SO_4 \rightarrow 2\ KHSO_4 + 2\ HI$$

(Seq1)

$$2\ HI + H_2SO_4 \rightarrow I_2 + SO_2 + 2\ H_2O$$

(Seq2)

$$2\ KHSO_4 \rightarrow K_2S_2O_7 + H_2O \quad \text{(Seq3)}$$

$$K_2S_2O_7 \rightarrow K_2SO_5 + SO_2 \quad \text{(Seq4)}$$

$$K_2S_2O_7 \rightarrow K_2SO_4 + SO_3 \quad \text{(Seq5)}$$

$$K_2SO_5 \rightarrow K_2SO_4 + \frac{1}{2}O_2 \quad \text{(Seq6)}$$

$$K_2SO_4 \rightarrow K_2O + SO_3 \quad \text{(Seq7)}$$

$$SO_3 \rightarrow SO_2 + \frac{1}{2}O_2 \quad \text{(Seq8)}$$

ESI5 SAED patterns of the spent catalysts

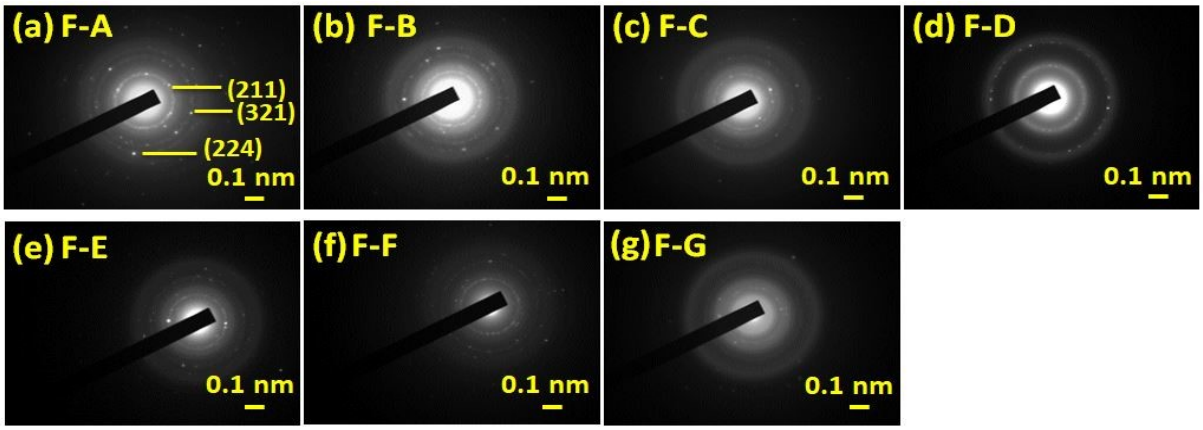

Fig. ESI5 SAED of the spent $CuFe_2O_4$/β–SiC with the different feed compositions: (a) F–A: 98 wt % H_2SO_4; (b) F–B: 98 wt % H_2SO_4 – 1 wt % HI; (c) F–C: 50 wt % H_2SO_4 – 1 wt % HI – H_2O solution; (d) F–D: 50 wt % H_2SO_4 – 10 wt % HI – H_2O solution; (e) F–E: 98 wt %

H_2SO_4 – 1 wt % KI; (f) F–F: 50 wt % H_2SO_4 – 1 wt % KI – H_2O solution; (g) F–G: 50 wt % H_2SO_4 – 10 wt % KI – H_2O solution.

ESI6 Model validation plot

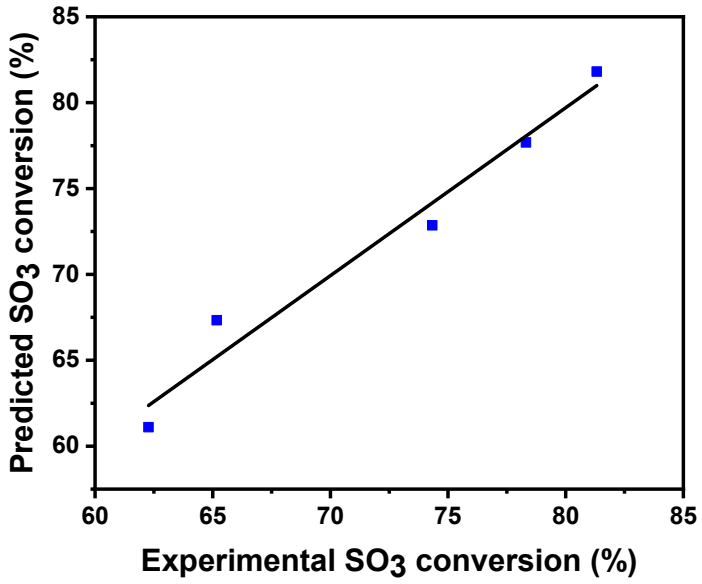

Fig. ESI6 Model validation plot of experimental and predicted SO_3 conversion (R^2 = 0.96).

References

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