

Supplementary Information

Surface self-reconstructed amorphous/crystalline hybrid iron disulfide for high-efficiency water oxidation electrocatalysis

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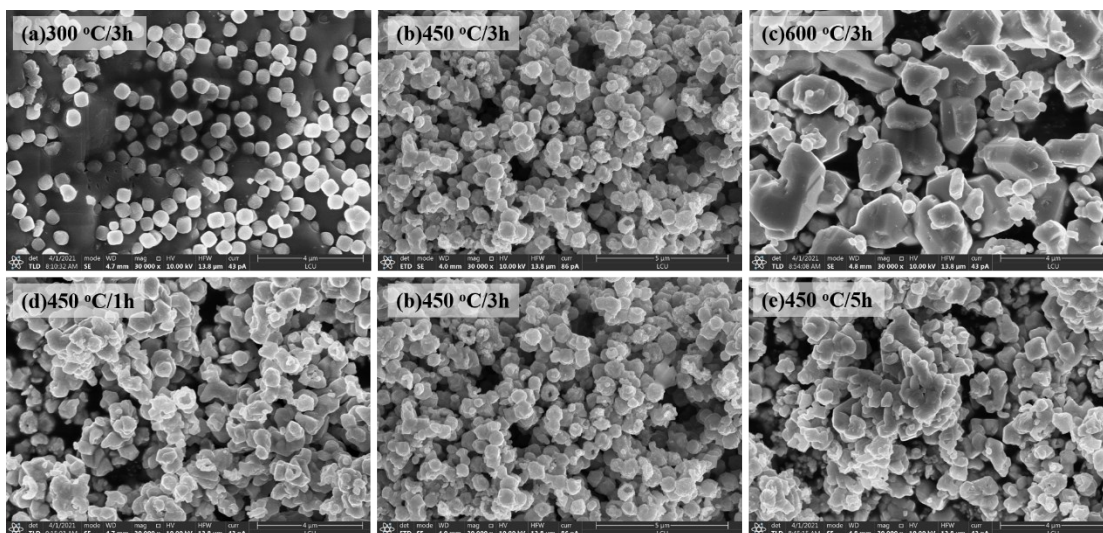


Figure S1 SEM images of the samples synthesized at different temperatures and time

(a)300 °C/3h (b)450 °C/3h (c)600 °C/3h (d)450 °C/1h (e)450 °C/5h

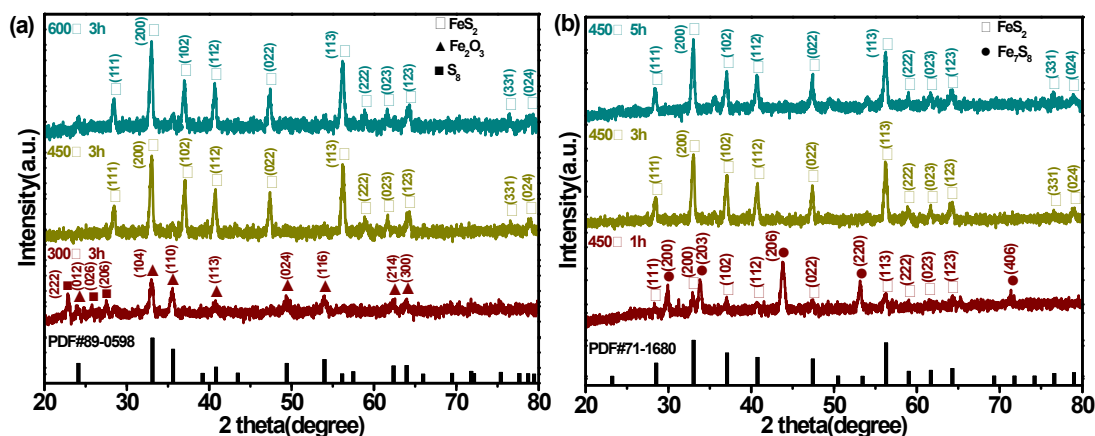


Figure S2 XRD patterns of the samples synthesized (a) at different temperatures for 3 hours and (b) at 450 °C for different hours

TOF calculation:

In order to better understand the intrinsic activity, the turnover frequency (TOF) of all the samples for OER at the same potential had been provided. Figure S3 is the turnover frequency (TOF) of the samples for OER at the same overpotential (332.8 mV)

To calculate the per-site turnover frequency (TOF), we used the following formula¹:

$$TOF \text{ per site} = \frac{\#Total \text{ Oxygen Turn Overs}/cm^2}{Sites (Catalyst)/cm^2}$$

The total number of oxygen turn overs was calculated from the current density

according to the following conversion:

$$\left(\frac{j}{\text{cm}^2}\right)\left(\frac{1\text{A}}{1000\text{mA}}\right)\left(\frac{1\text{C/s}}{1\text{A}}\right)\left(\frac{1\text{mol } e^-}{96485.3\text{ C}}\right)\left(\frac{1\text{ mol } O_2}{4\text{ mol } e^-}\right)\left(\frac{6.02214 \times 10^{23}\text{ molecules } O_2}{1\text{ mol } O_2}\right)$$

$$= 1.56 \times 10^{15} \frac{O_2/s}{\text{cm}^2} \text{ per } \frac{\text{mA}}{\text{cm}^2}$$

Since the exact oxygen binding site is not known, we estimate the number of sites as the number of sample molecular calculated based on the mass of the samples used in the electrochemical measurements according to the following conversion:

Site (FeS₂)

$$= \left(1\text{mg} \times \frac{1}{\text{cm}^2}\right) \left(\frac{6.02214 \times \frac{10^{23}}{\text{mol}} \text{FeS}_2 \text{ sties}}{119.967 \times \frac{10^3\text{mg}}{\text{mol}}}\right) = 5.01983 \times 10^{18} \text{ sites/cm}^2$$

Sites (Fe₂O₃)

$$= \left(1\text{mg} \times \frac{1}{\text{cm}^2}\right) \left(\frac{6.02214 \times \frac{10^{23}}{\text{mol}} \text{Fe}_2\text{O}_3 \text{ sties}}{159.688 \times \frac{10^3\text{mg}}{\text{mol}}}\right) = 3.77119 \times 10^{18} \text{ sites/cm}^2$$

Sites (RuO₂)

$$= \left(1\text{mg} \times \frac{1}{\text{cm}^2}\right) \left(\frac{6.02214 \times \frac{10^{23}}{\text{mol}} \text{RuO}_2 \text{ sites}}{133.07 \times \frac{10^3\text{mg}}{\text{mol}}}\right) = 4.52554 \times 10^{18} \text{ sites/cm}^2$$

Based on the current density at the same overpotential (332.8 mV), the per site TOF is determined as follows:

TOF per FeS₂ (332.8 mV)

$$= \frac{\# \text{Total Oxygen Turn Overs/cm}^2}{\text{Sites (Catalyst)/cm}^2} = \frac{1.56 \times 10^{15} \frac{O_2/s}{\text{cm}^2} \text{ per } \frac{\text{mA}}{\text{cm}^2}}{5.01983 \times 10^{18} \text{ sites/cm}^2}$$

$$= 0.031 \frac{O_2/s}{\text{site}}$$

TOF per Fe_2O_3 (332.8 mV)

$$\begin{aligned}
 &= \frac{\#Total\ Oxygen\ Turn\ Overs/cm^2}{Sites\ (Catalyst)/cm^2} = \frac{1.56 \times 10^{15} \frac{O_2/s}{cm^2} per \frac{mA}{cm^2}}{3.77119 \times 10^{18} site} \\
 &= 0.013 \frac{O_2/s}{site}
 \end{aligned}$$

TOF per RuO_2 (332.8 mV)

$$\begin{aligned}
 &= \frac{\#Total\ Oxygen\ Turn\ Overs/cm^2}{Sites\ (Catalyst)/cm^2} = \frac{1.56 \times 10^{15} \frac{O_2/s}{cm^2} per \frac{mA}{cm^2}}{4.52554 \times 10^{18} site} \\
 &= 0.015 \frac{O_2/s}{site}
 \end{aligned}$$

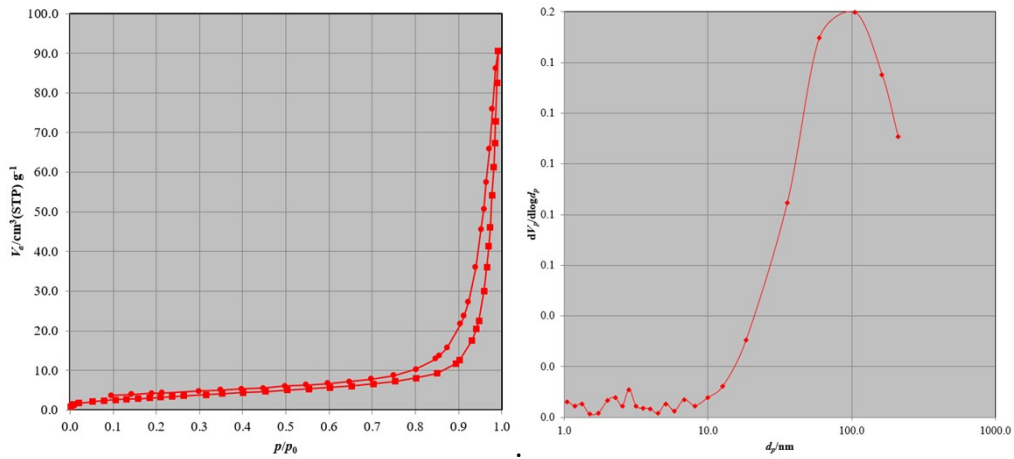


Figure S3 Nitrogen adsorption-desorption isotherms and pore size distribution of the pre-catalyst of amorphous/crystalline hybrid iron disulfide

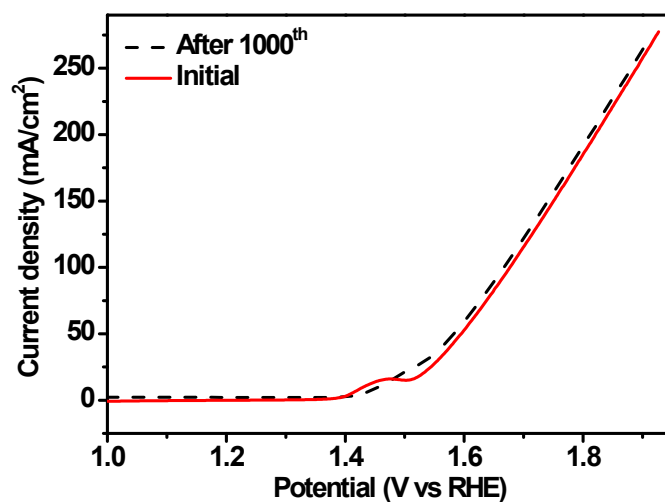


Figure S4 the polarization curve of FeS₂ after 1000 cycles of CV

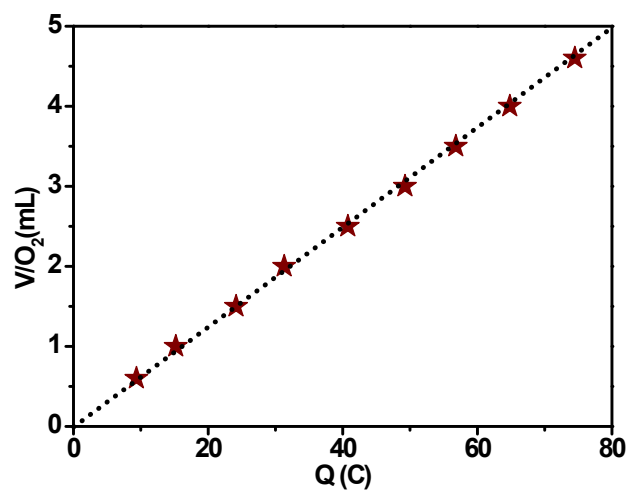


Figure S5 Plot showing the volume of oxygen evolved as a function of the passed charge. The data points for FeS₂/NF//Pt/C/NF fall on the dotted line representing 100 % Faradaic efficiency as calculated from Faraday's law of electrolysis and the ideal gas law

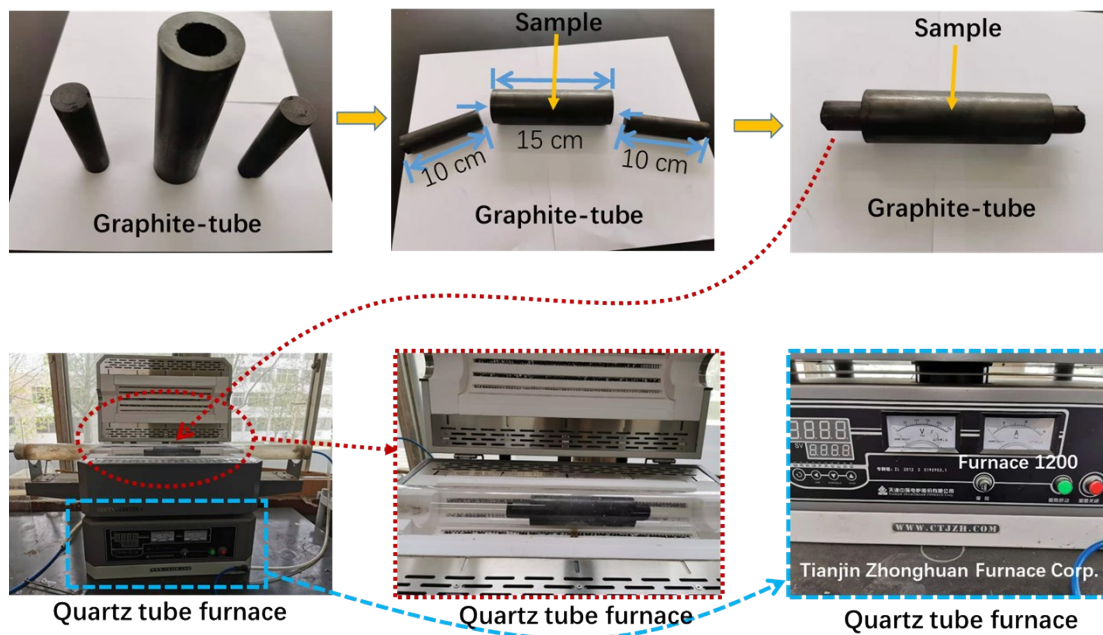


Figure S6 Dimensions of graphite-tube and type of tube furnace