

Supporting Information

Synthesis and study of the application of Iron, Nitrogen-doped high surface area carbon for Li-S batteries

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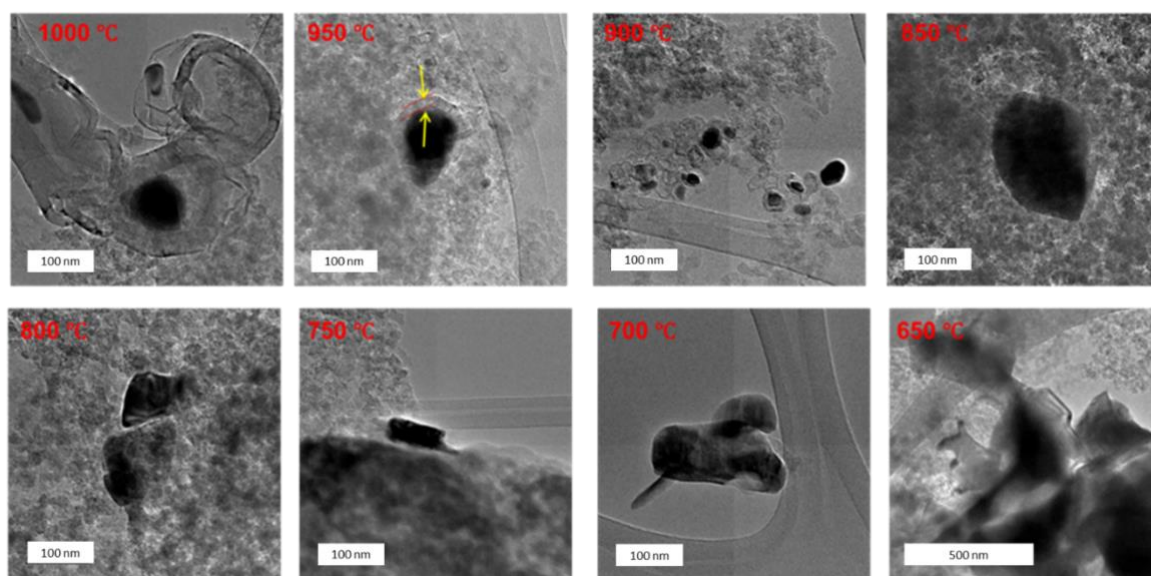


Figure S1. TEM images of the iron-based structures obtained with the same pyrolysis route but with different temperatures, from 650 °C to 1000 °C. As it is shown, by increasing the temperature from 650°C, to 1000 °C, the size of the iron-based particles becomes smaller and at the temperature higher than 850 °C a carbon-based layer surrounds the Fe-based particles which grows with temperature.

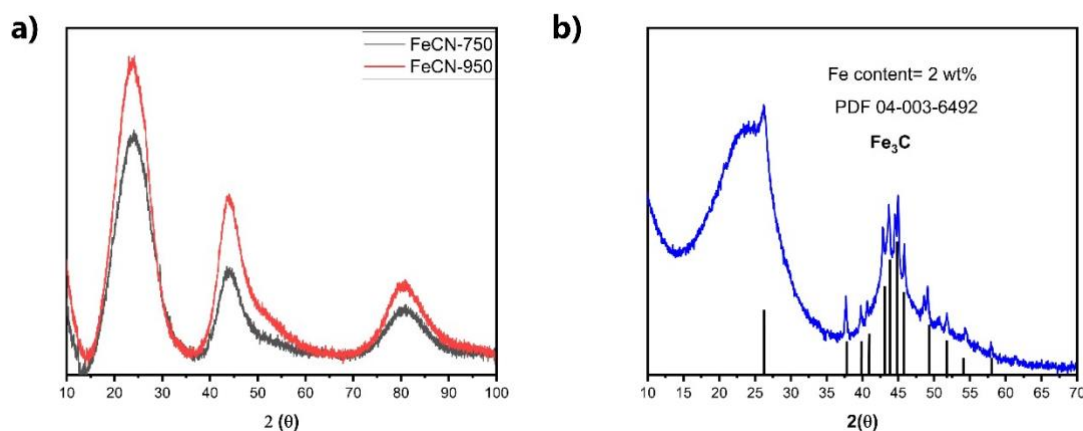


Figure S2. **a)** XRD patterns of FeCN-750 and FeCN-950, with 0.5 wt% of iron in the precursor, representing peaks only for amorphous carbon, without presence of any crystalline peaks from Iron-based phases. **b)** XRD pattern of FeCN-950 with 2 wt% of iron in the precursor, highlighting that by increasing the iron ratio in the precursor at 950°C under N_2 , formation of iron-carbide particles is favorable.

Note S1

The Raman spectra for FeCN-750 and FeCN-950 were deconvoluted into four distinct peaks. The D1 peak, attributed to carbon atoms at the edges of graphene layers with A_{1g} symmetry, appears at 1338 cm^{-1} . The G peak, observed at 1603 cm^{-1} , corresponds to the ideal graphitic lattice vibration with E_{2g} symmetry. The D2 peak, located at 1534.8 cm^{-1} , may be associated with the vibration of non-sandwiched graphene layers with E_{2g} symmetry or may originate from functional groups, molecular fragments, or organic molecules within the amorphous carbon. The final peak, labeled D4 and arising at 1178.6 cm^{-1} , is related to the stretching vibrations of C–C and C=C bonds in polyene-like structures¹ (**Figure 3 c**).

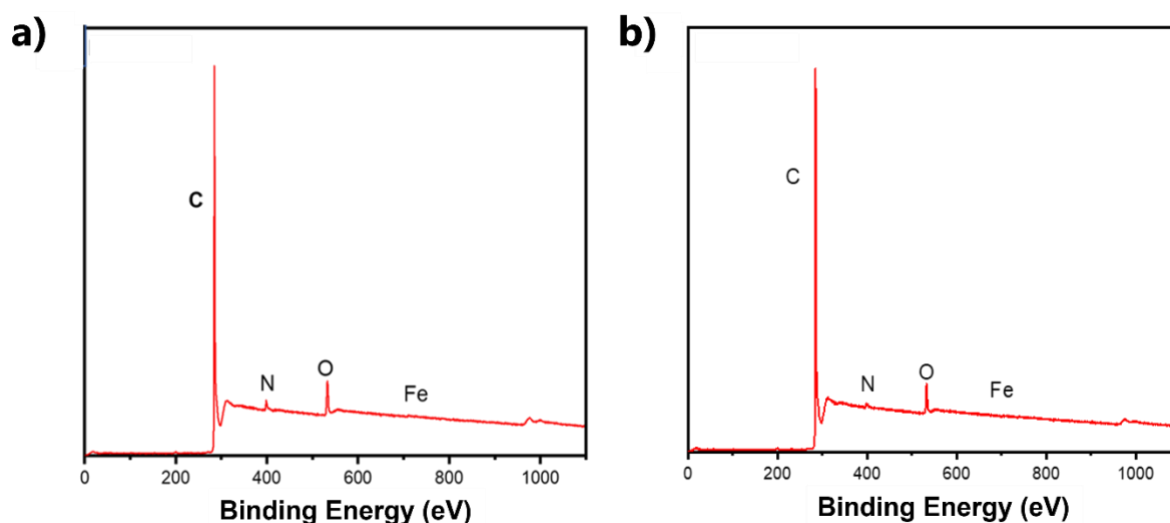


Figure S3. XPS survey of **a)** FeCN-750, and **b)** FeCN-950 sulfur hosts.

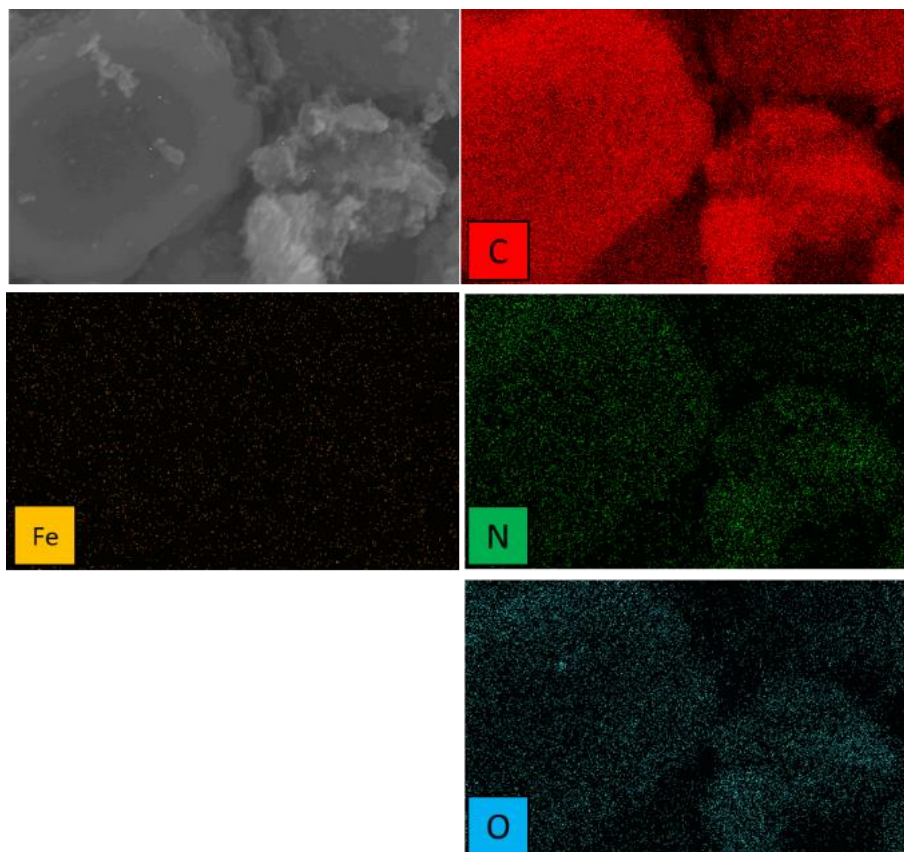


Figure S4. EDX elemental mapping of the FeCN materials representing carbon, nitrogen and oxygen and low amount of iron.

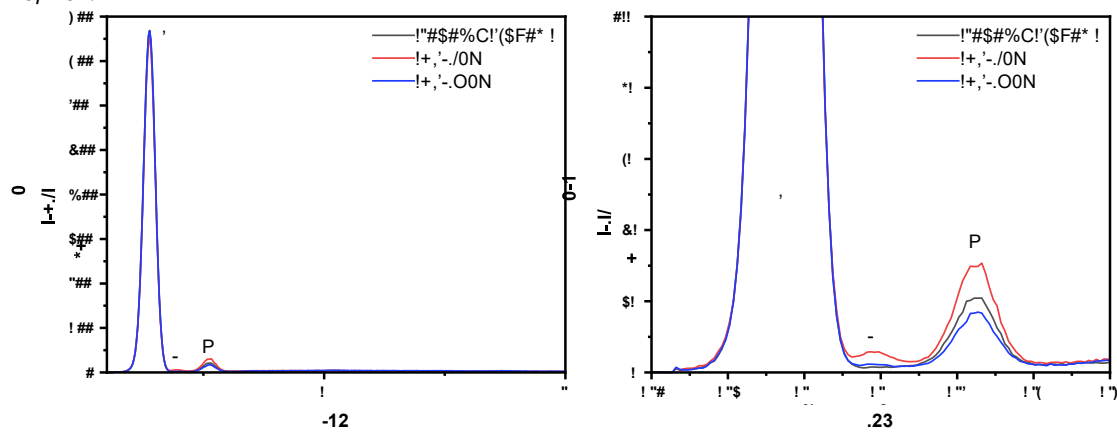


Figure S5. EDX quantitative analysis of the porous carbon xerogel (pristine), FeCN-750, and FeCN-950 sulfur hosts performed in representative zones.

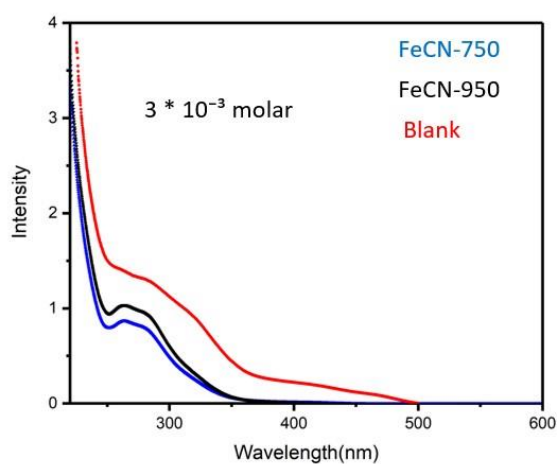


Figure S6. UV-visible spectroscopy and adsorption test results of the synthesized materials, compared with a blank Li_2S_6 solution at a concentration of $3 \times 10^{-3} \text{ mol l}^{-1}$.

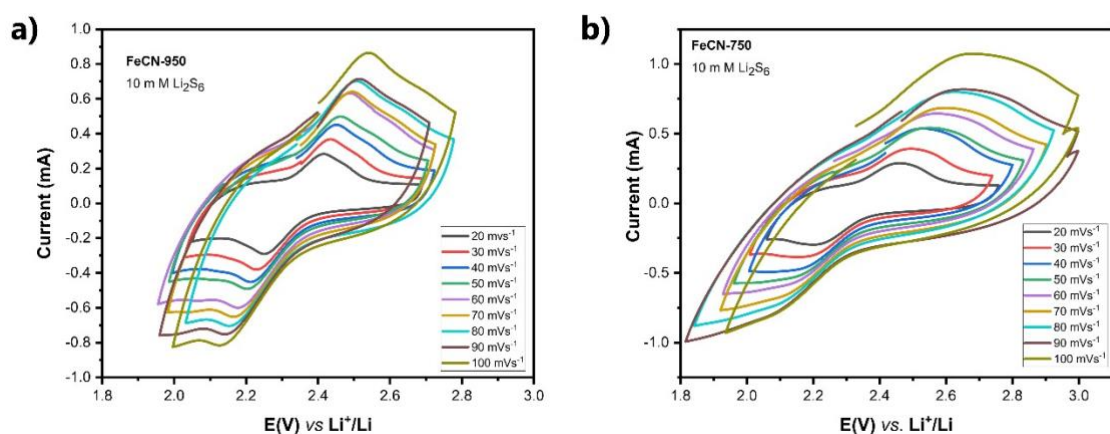


Figure S7. CV of **a)** FeCN-750, and **b)** FeCN-950 at different scan rates in 10 mM of Li_2S_6 in three electrode configurations, versus lithium metal as the reference and counter electrodes.

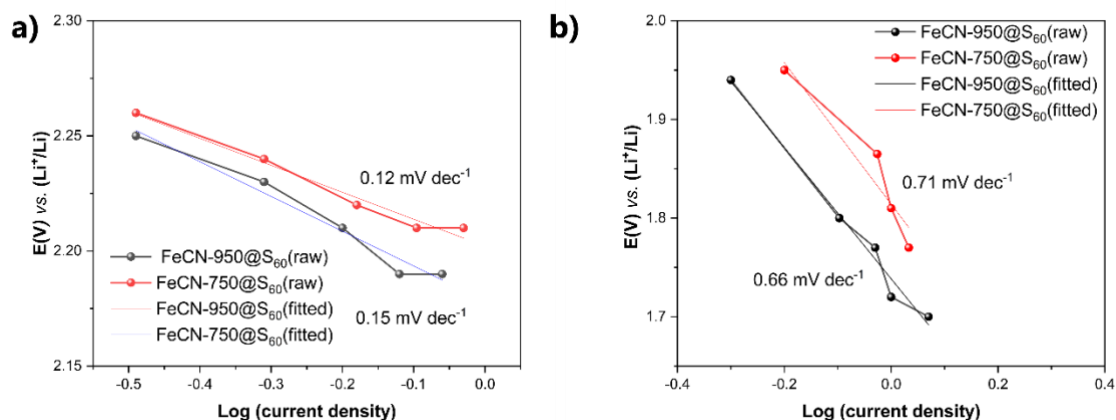


Figure S8. Tafel curves of **a)** first reduction peak at 2.2 V vs Li^+/Li and **b)** second reduction peak (1.9-1.8 V vs Li^+/Li) of FeCN-750@ S_{60} and FeCN-950@ S_{60} electrode in two electrode system vs. lithium metal negative electrode.

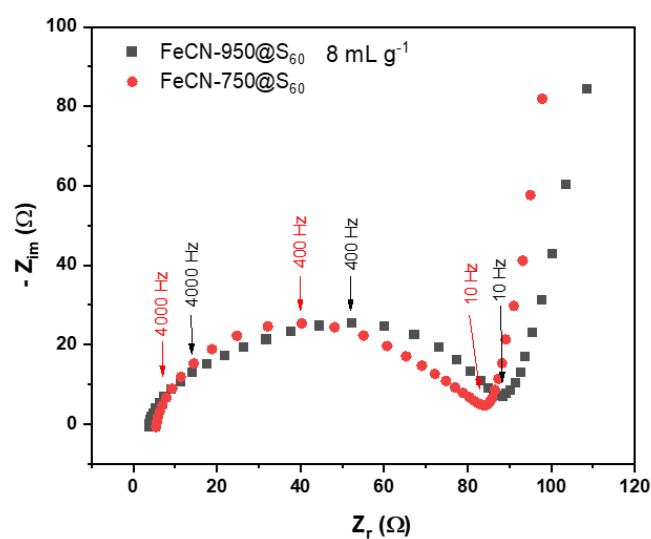


Figure S9. The Nyquist plot of FeCN-750@S₆₀ and FeCN-950@S₆₀ with the sulfur loading of 2 mg cm⁻² at 8 mL g⁻¹ of electrolyte.

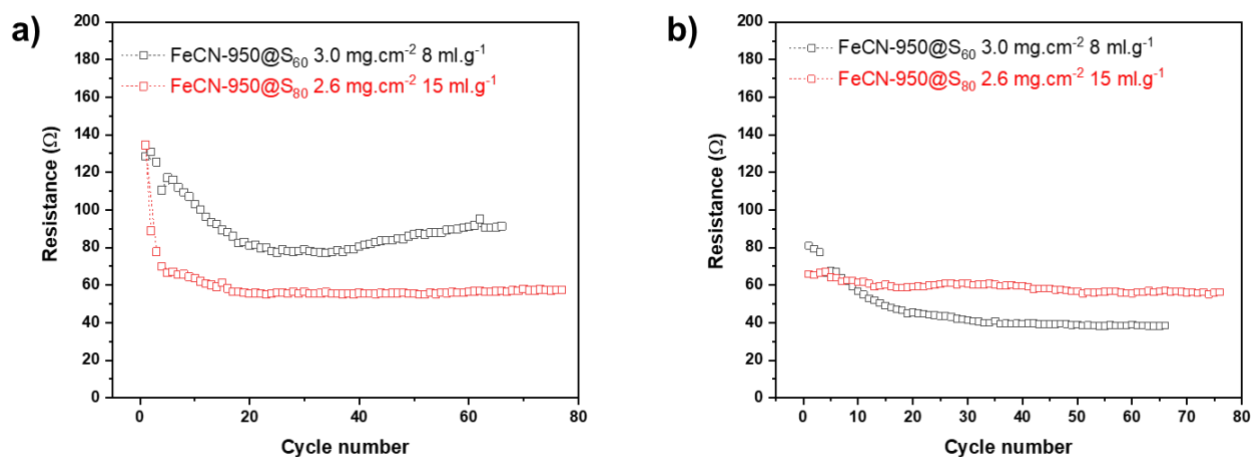


Figure S10. Resistance value evolutions of FeCN-750@S₆₀ E/S=8 mL.g⁻¹ and FeCN-750@S₆₀ E/S=6 mL.g⁻¹ with the sulfur loading of 3 mg cm⁻² a) at the end of the discharge, b) at the end of the charge.

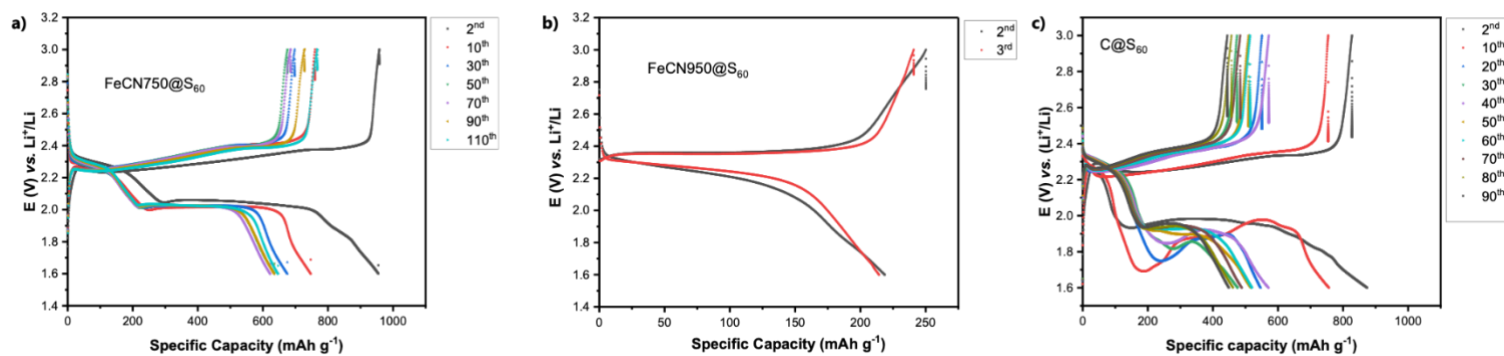


Figure S11. GCPL curves (0.1C) of the electrodes made of sample **a)** FeCN-750@S₆₀, **b)** FeCN-950@S₆₀, and **c)** C@S₆₀ with $\sim 3 \text{ mg cm}^{-2}$ loading and $E/S = 6 \text{ mL g}^{-1}$.

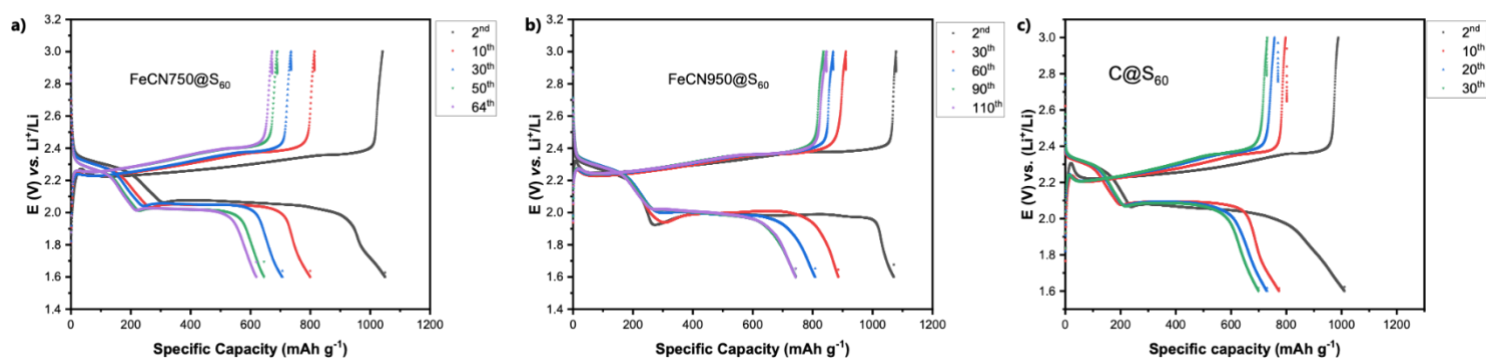


Figure S12. GCPL curves (0.1C) of the electrodes made of sample **a)** FeCN-750@S₆₀, **b)** FeCN-950@S₆₀, and **c)** C@S₆₀ with $\sim 3 \text{ mg cm}^{-2}$ loading and $E/S = 8 \text{ mL g}^{-1}$.

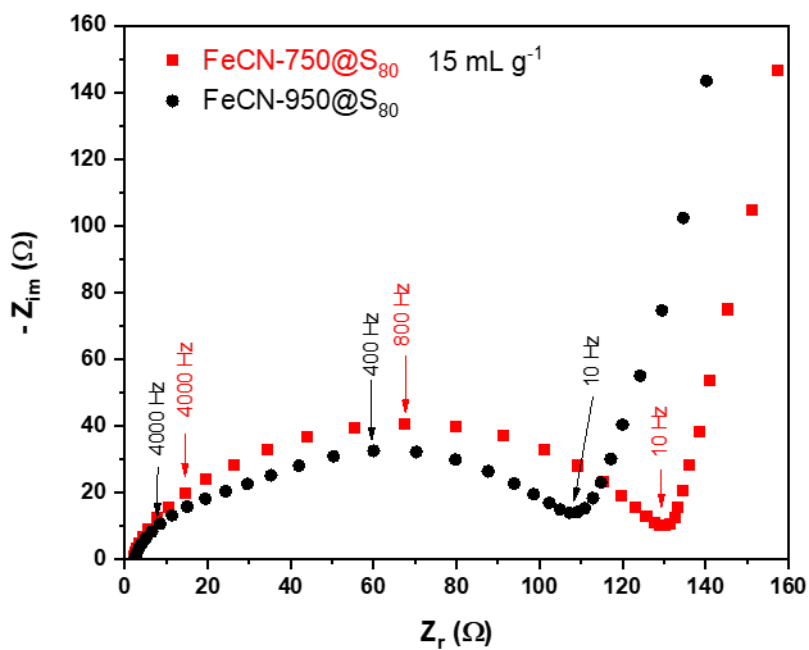


Figure S13. The Nyquist plot of FeCN-750@S₈₀ and FeCN-950@S₈₀ with the sulfur loading of $\sim 2 \text{ mg cm}^{-2}$ at 15 mL g^{-1} of electrolyte.

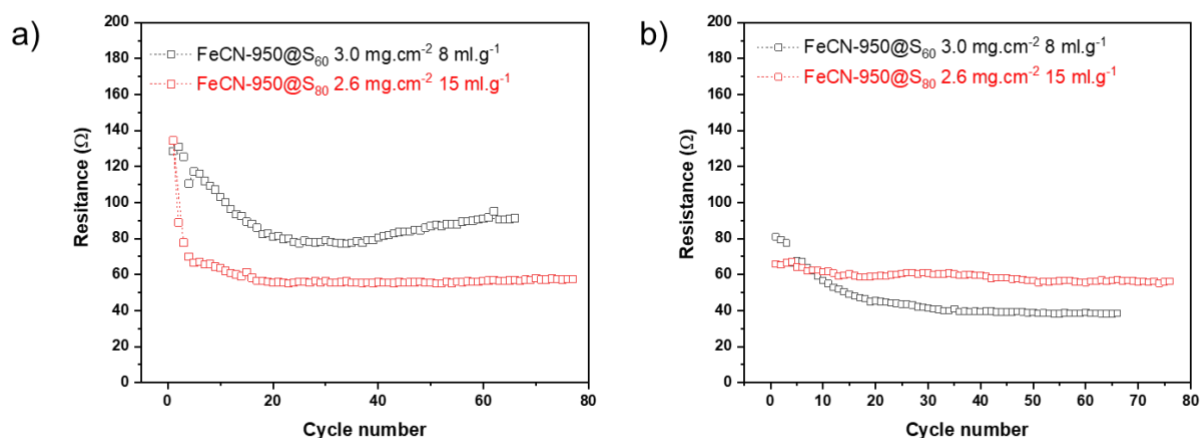


Figure S14. Resistance value evolution of FeCN-950@S₆₀ 3 mg.cm⁻² E/S=8 ml.g⁻¹ and FeCN-950@S₆₀ 2.6 mg.cm⁻² E/S=15 ml.g⁻¹ a) at the end of the discharge, b) at the end of the charge.

Table S1, The comparison of this work with other literature highlights the promising electrochemical performance of the developed sulfur electrodes under challenging conditions.

Ref.	Sulfur loading (mg cm ⁻²)	Sulfur content	Cycling rate	E/S (mL g ⁻¹)	Capacity, cycle number
²	3.5	70 wt.%	0.1C	8.5	496 mAh g ⁻¹ , 100 cycles
³	3.7	70 wt.%	0.5C	7	720 mAh g ⁻¹ , 70 cycles
⁴	4.0	60 wt.%	0.2C	5	700 mAh g ⁻¹ , 100 cycles
⁵	1.2	65 wt.%	0.1C	14.2	860 mAh g ⁻¹ , 100 cycles
⁶	2.0	78 wt.%	1C	15	500 mAh g ⁻¹ , 400 cycles
⁷	1.0	75 wt.%	0.2C	15	1000 mAhg ⁻¹ , 400cycles
⁸	0.5-0.7	80 wt.%	2C	60	543 mAh g ⁻¹ , 400 cycles
⁹	-----	60 wt.%	0.2C	----	728 mAh g ⁻¹ , 100 cycles
¹⁰	3.3	70 wt.%	1C	10	670 mAhg ⁻¹ , 100 cycles
¹¹	---	75 wt.%	1C	-----	291 mAhg ⁻¹ , 300 cycles
¹²	3.5	-----	1C	12	576 mAhg ⁻¹ , 400 cycles
¹³	3.7	74 wt.%	1C	10	----, 400 cycles
¹⁴	3	----	0.5C	18	600 mAhg ⁻¹ , 200 cycles
¹⁵	2	~73wt.%	1C	-----	526 mAhg ⁻¹ , 200 cycles

This work	3.5	>80wt.%	0.1C	7.5	576 mAhg ⁻¹ , 100 cycles
This work	3.0	>60wt.%	0.1C	8	700 mAhg ⁻¹ , 140 cycles
This work	3.0	>60wt.%	0.1C	6	650 mAh ⁻¹ , 100 cycles

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