

Supporting Information

Efficient Fe₃C-CF cathode catalyst based on the formation/decomposition of Li_{2-x}O₂ for Li-O₂ batteries

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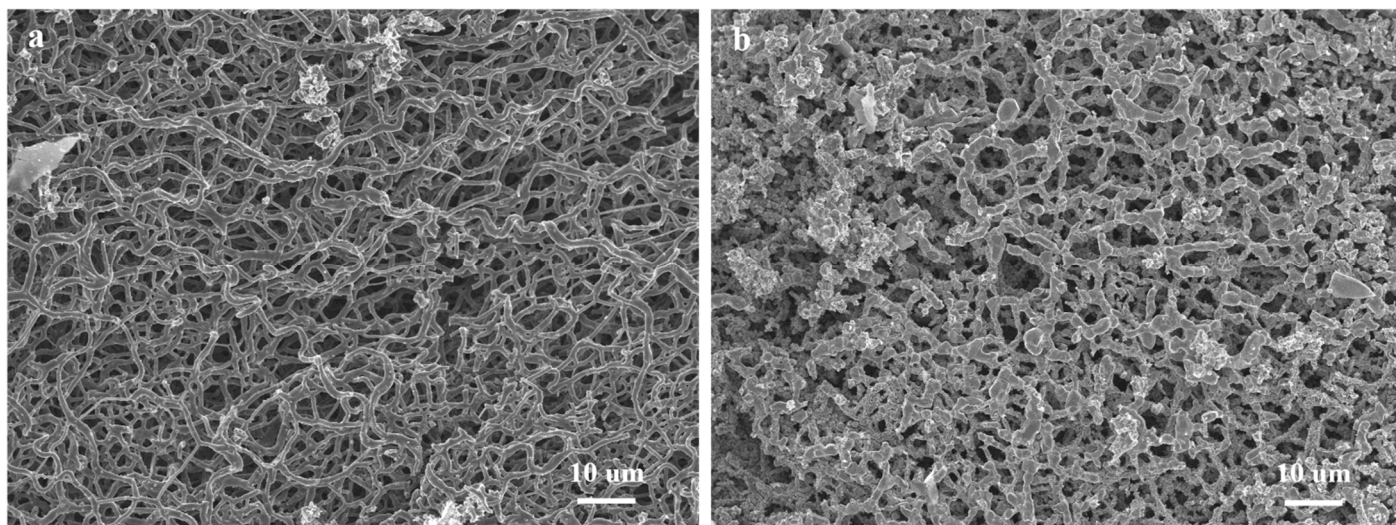


Figure S1. The SEM images of Fe₃C-600 (a) and Fe₃C-800 (b) after carbonization.

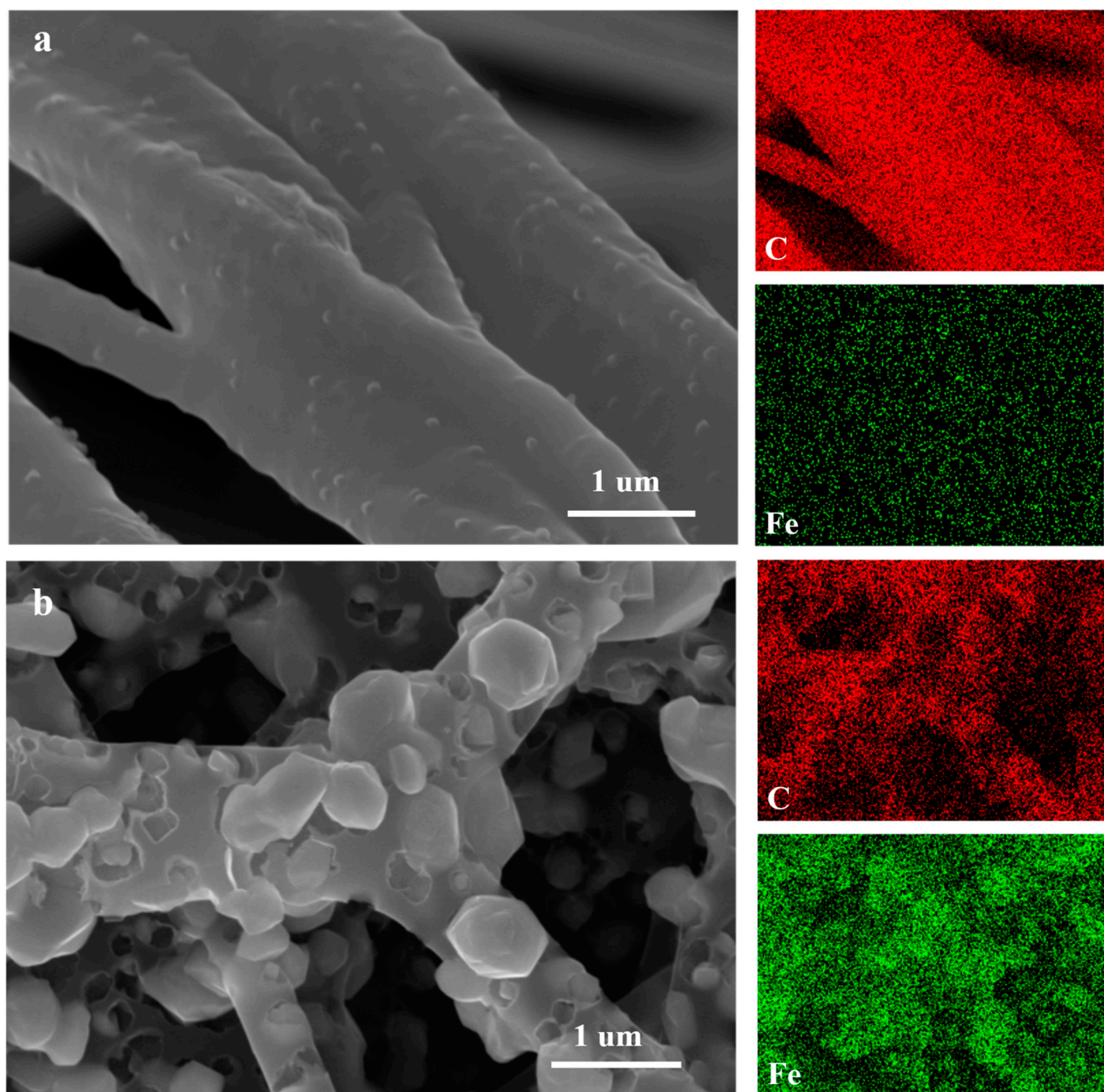


Figure S2. SEM images and elemental mapping of Fe and C in Fe₃C-600 (a), and Fe₃C-800 (b).

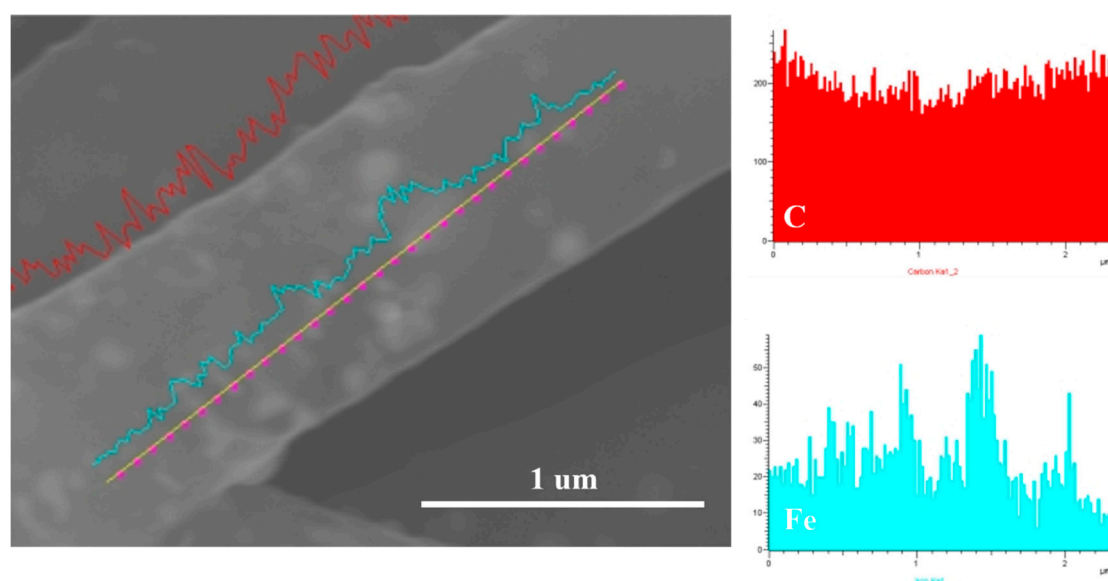


Figure S3. Line SEM images and elemental mapping of the Fe₃C-700.

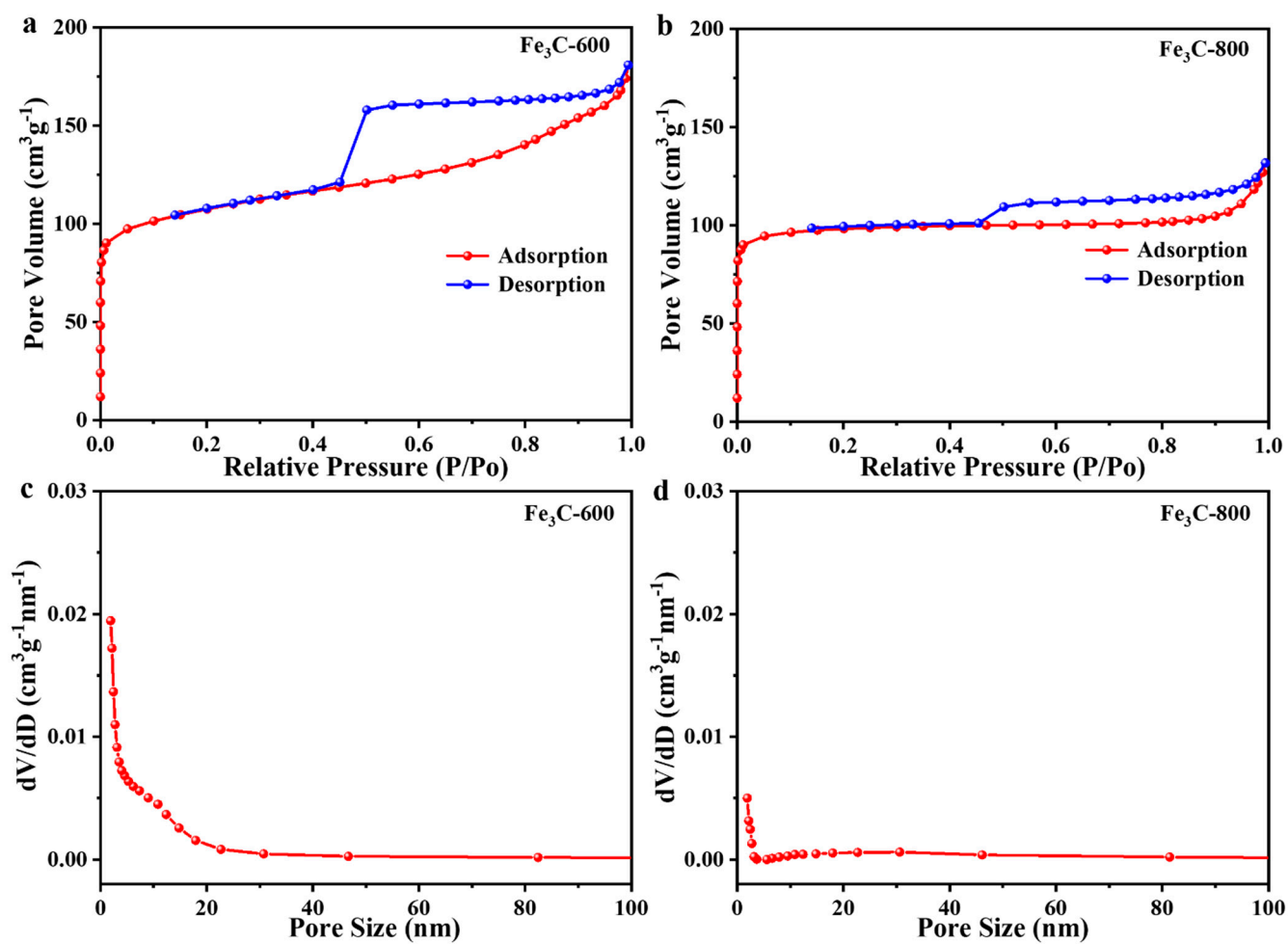


Figure S4. Nitrogen adsorption/desorption isotherms of Fe₃C-600 (a) and Fe₃C-800 (b); The pore size distribution of Fe₃C-600 (c) and Fe₃C-800 (d).

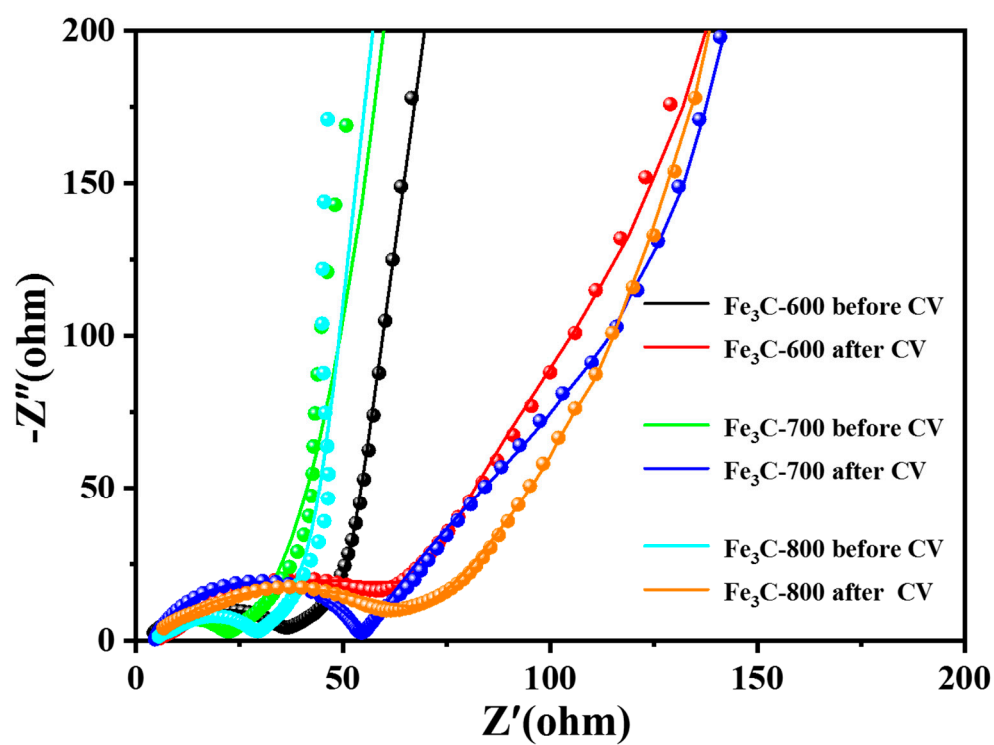


Figure S5. EIS spectrums of Fe₃C-CF electrodes before and after CV.

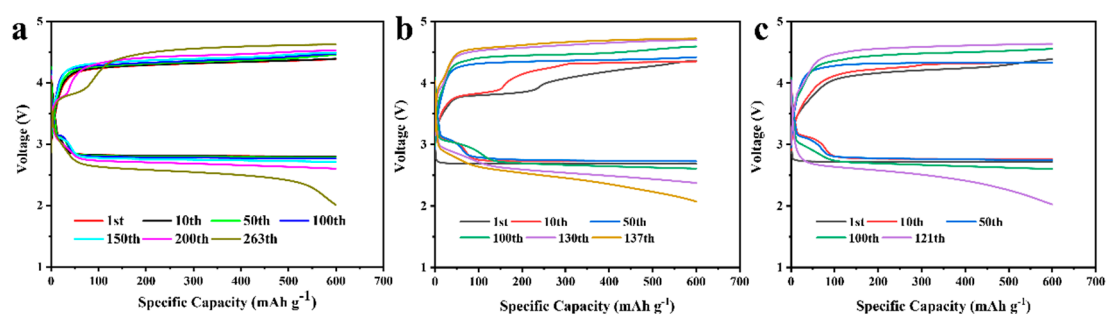


Figure S6. Galvanostatic discharge/charge curves of Fe₃C-700 within an upper-limited specific capacity of 600 mAh g⁻¹ at a current density of 200 mA g⁻¹(a), 800 mA g⁻¹(b), 1000 mA g⁻¹(c).

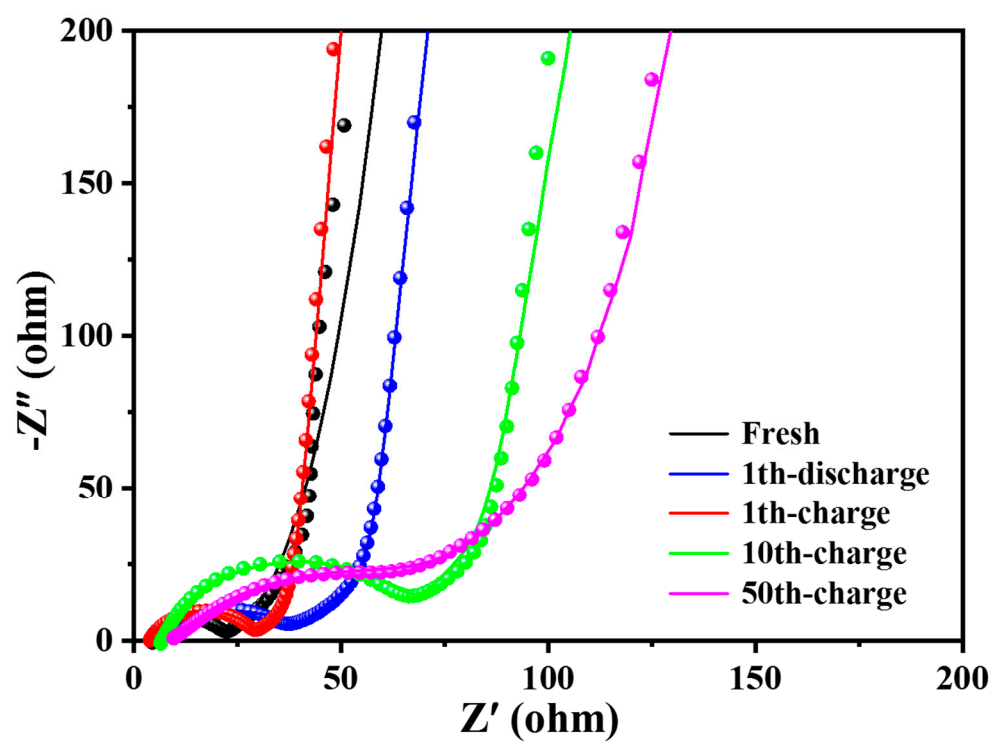


Figure S7. Electrochemical impedance spectra of Fe₃C-700 at different stages.

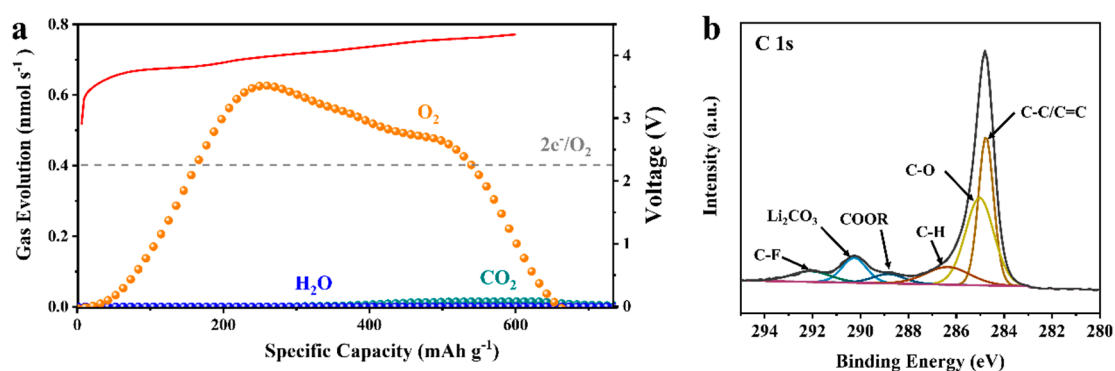



Figure S8. (a) In-situ DEMS curves of the Fe₃C-700 catalyst, which were collected during the charging process with a specific capacity of 600 mAh g⁻¹, at a current density of 500 mA g⁻¹; (b) High-resolution XPS spectra of C 1s core level of the Fe₃C-700 electrode after 50th recharged.

Table S1. Overpotentials of the ORR and OER processes of two paths on the different surfaces.


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	(002) Li-PATH	(002) O ₂ -PATH	(121) Li-PATH	(121) O ₂ -PATH
U_{DC}(V)	0.91	1.48	1.32	1.51
U₀(V)	4.52	4.52	3.79	3.79
U_C(V)	5.72	11.06	4.62	5.48
η_{ORR}(V)	3.61	3.04	2.47	2.28
η_{OER}(V)	1.20	6.54	0.83	1.69
η_{TOT}(V)	4.81	9.58	3.30	3.97

Table S2. Adsorption energy (E_{ads}) between different adsorbates and surface of Fe_3C .

$E_{\text{ads}}(\text{eV})$	(002)	(121)
Li	-0.90897	-1.32169
O₂	3.49652	-2.27596
LiO₂	-7.09868	-7.29455
Li₂O₂	-7.06259	-7.29278

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