

Supporting Information

Multicore-shell Iron Fluoride @ Carbon Microspheres as Long-life Cathode for High-Energy Lithium Battery

Ziang Jiang[‡], Yujie Wang[‡], Xuanfeng Chen, Fulu Chu, Xuansi Jiang, Felix Kwofie, Qianfan Pei, Shunrui Luo*, Jordi Arbiol and Feixiang Wu*

Table S1. Comparison between the experimental and the theoretical bulk plane spacing distances and angles between planes.

Spot	Experimental (nm)	FeF ₃ (R-3c) [1-11]
1	0.136	0.134 (242)
2	0.178 (45.61° vs Spot 1)	0.187 (45.86°) (022)
3	0.248 (87.92° vs Spot 1)	0.260 (90,00°) (10-1)

Table S2. The corresponding R_s and R_{ct} fitted values.

Cathode	R_s (Ω)	R_{ct} (Ω)
FeF ₃ @C	20.55	129.5
Commercial FeF ₃	26.96	190.8

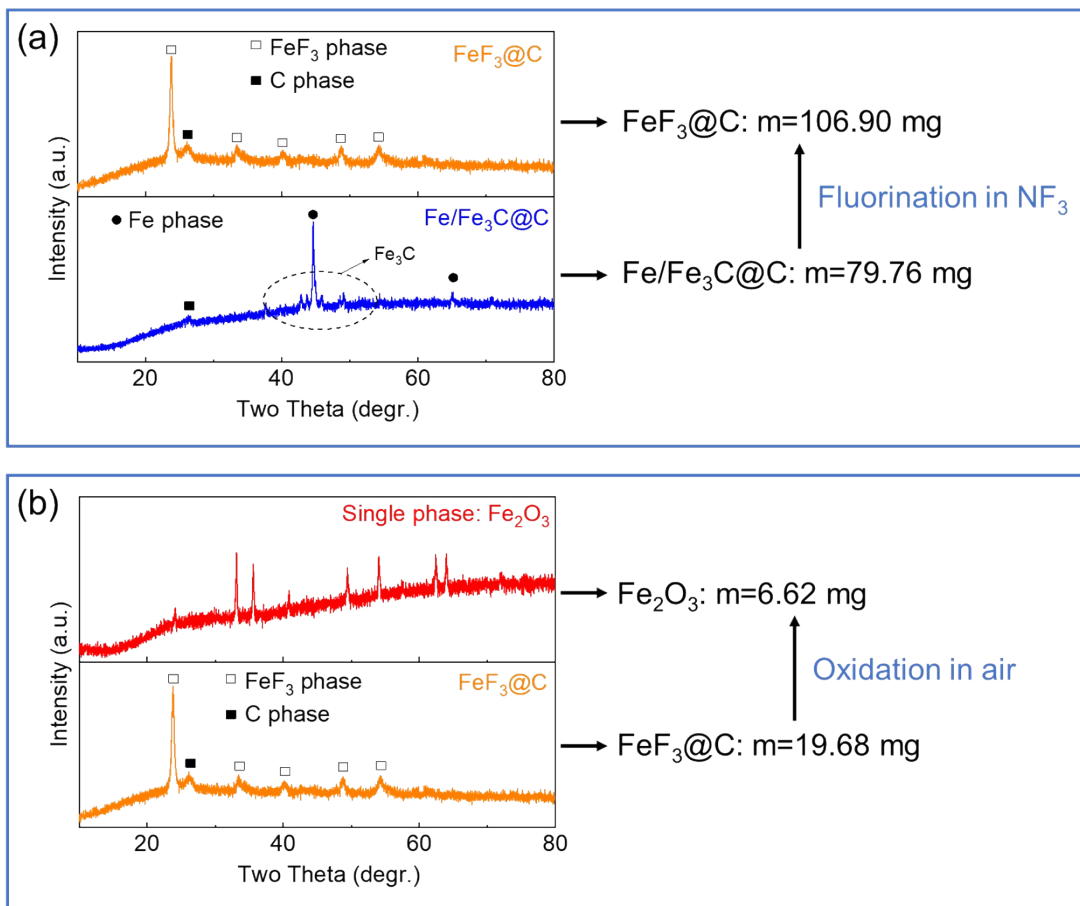


Fig. S1 the phase and mass change of samples (a) before and after fluorination in NF_3/Ar (from $\text{Fe}/\text{Fe}_3\text{C}@C$ to $\text{FeF}_3@C$) or (b) thermogravimetric analysis in air (from $\text{FeF}_3@C$ to Fe_2O_3)

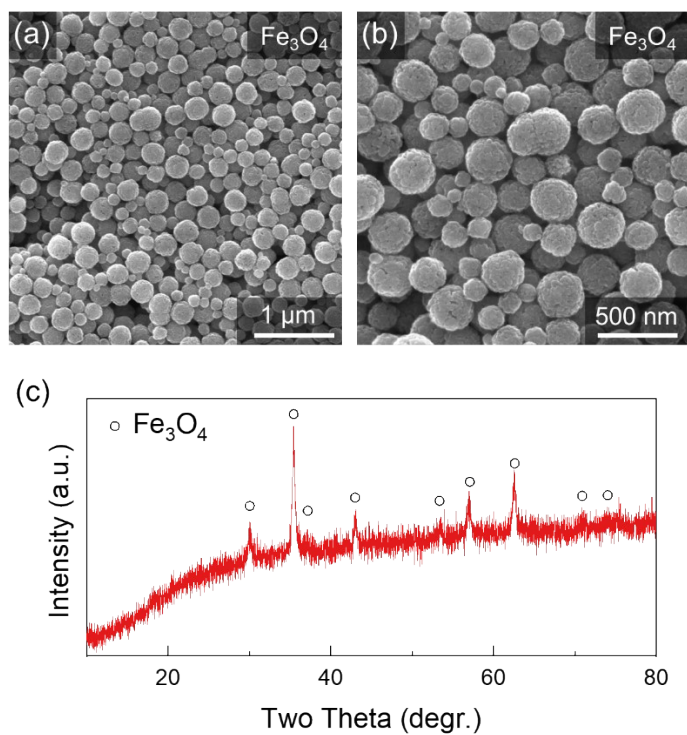


Fig. S2 (a, b) SEM images and XRD pattern of Fe_3O_4 microspheres.

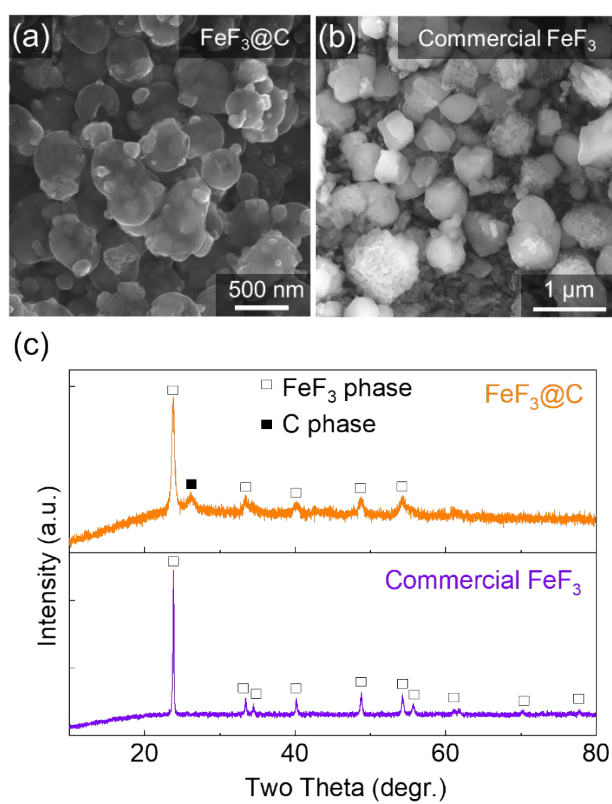


Fig. S3 SEM images of (a) $\text{FeF}_3@C$ composite and (b) commercial FeF_3 particles; (c) Comparison of XRD patterns of the $\text{FeF}_3@C$ composite and commercial FeF_3 particles.

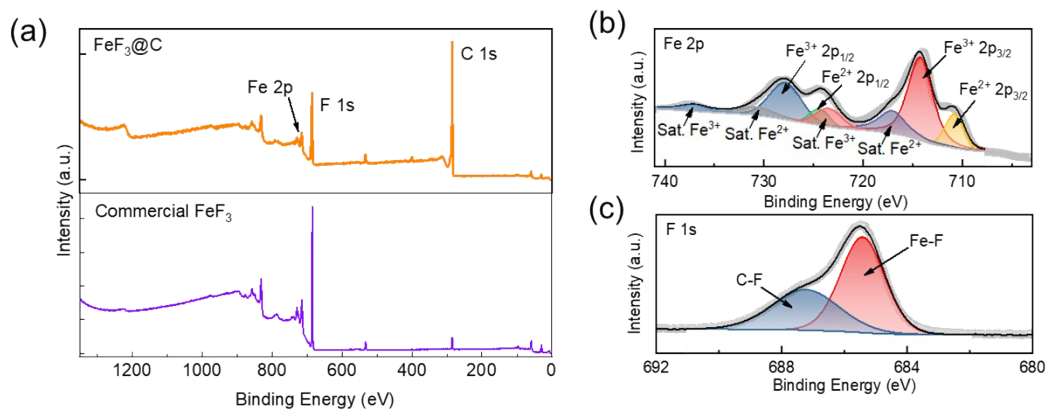


Fig. S4 XPS spectra. (a) Full XPS analysis of the $\text{FeF}_3@C$ and commercial FeF_3 particles; (b) Fe 2p of the commercial FeF_3 and (c) C 1s of the $\text{FeF}_3@C$ composites.

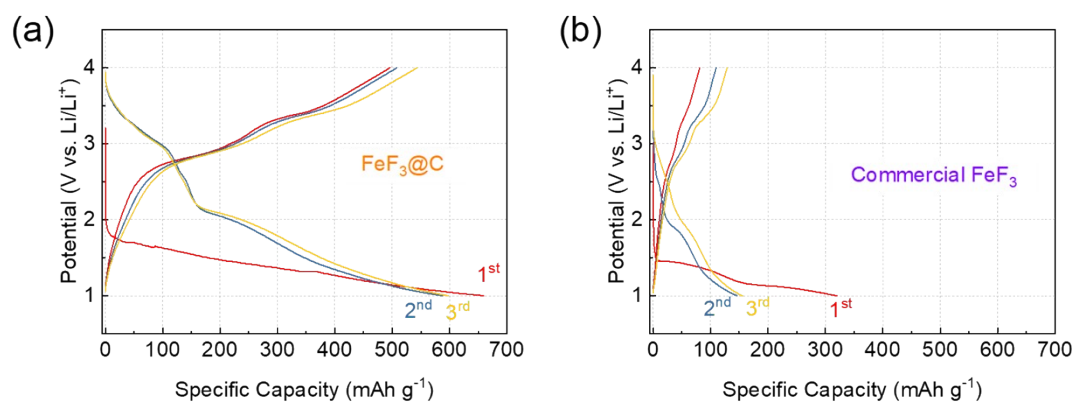


Fig. S5 The galvanostatic charge/discharge profiles of (a) the $\text{FeF}_3@C$ cathode in the first three cycles at 0.1C, the commercial FeF_3 cathode (b) in the first three cycles at 0.1C.

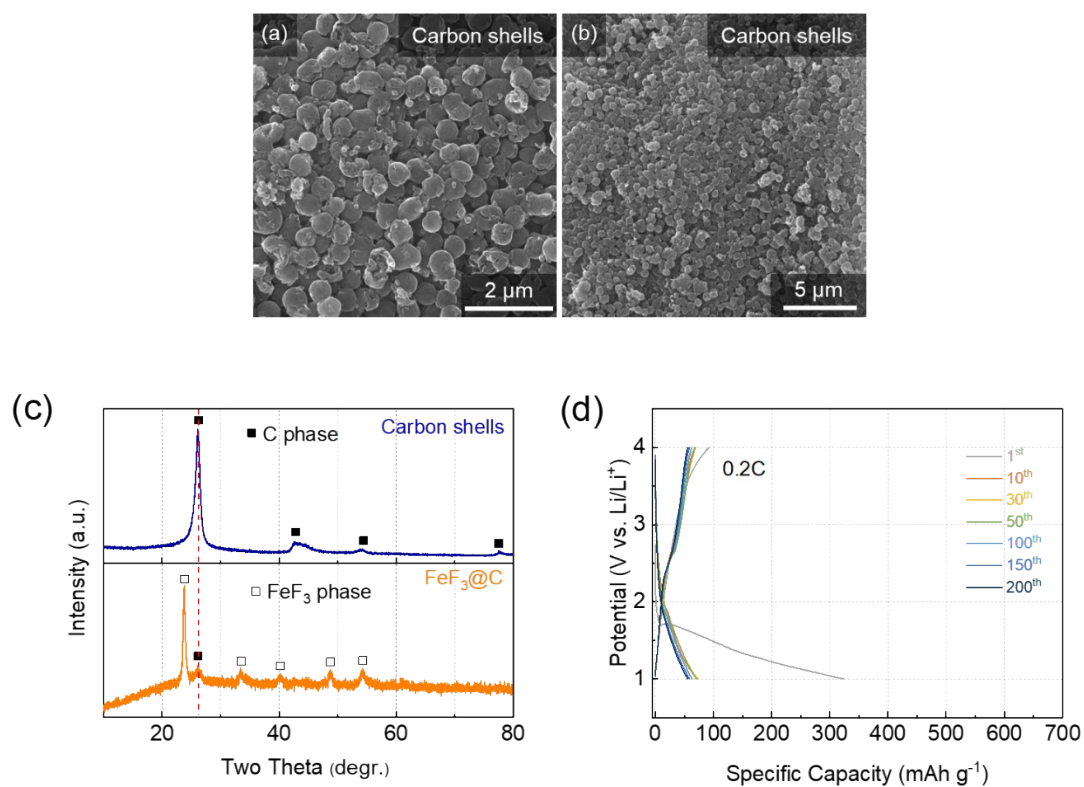


Fig. S6 (a, b) SEM images of the FeF₃@C particles after washing experiment using dilute HCl solution; (c) the XRD patterns of the FeF₃@C composite before and after acid washing; (d, e) discharge-charge voltage profiles of the blank carbon shells.

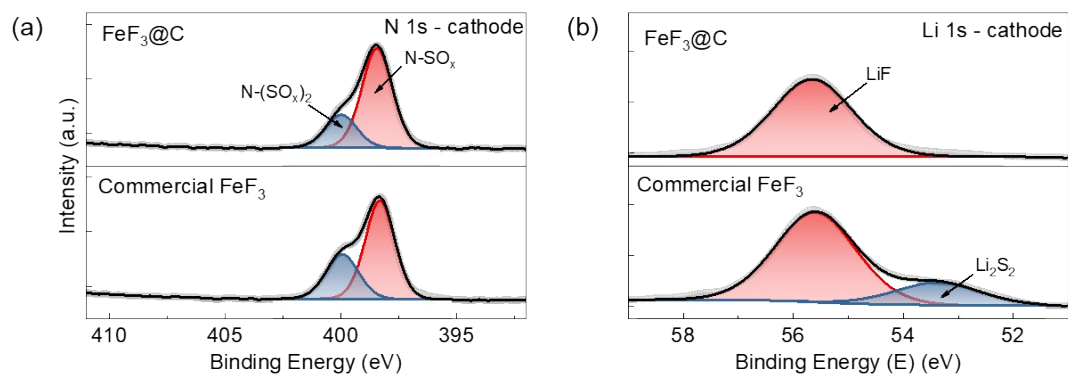


Fig. S7 XPS spectra of (a) N 1s, (b) Li 1s from cycled cathodes.

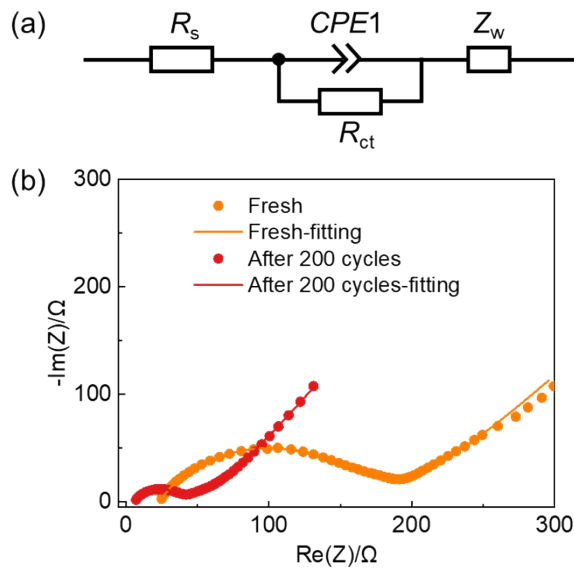


Fig. S8 (a) Equivalent circuit of the EIS fitted; (b) Comparison of electrical impedance in the fresh and after-200-cycles $FeF_3@C$ cathodes.

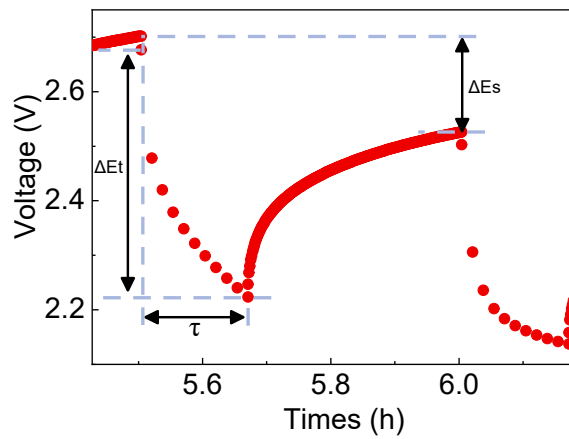


Fig. S9 Schematic of the diffusion coefficient via the GITT method.

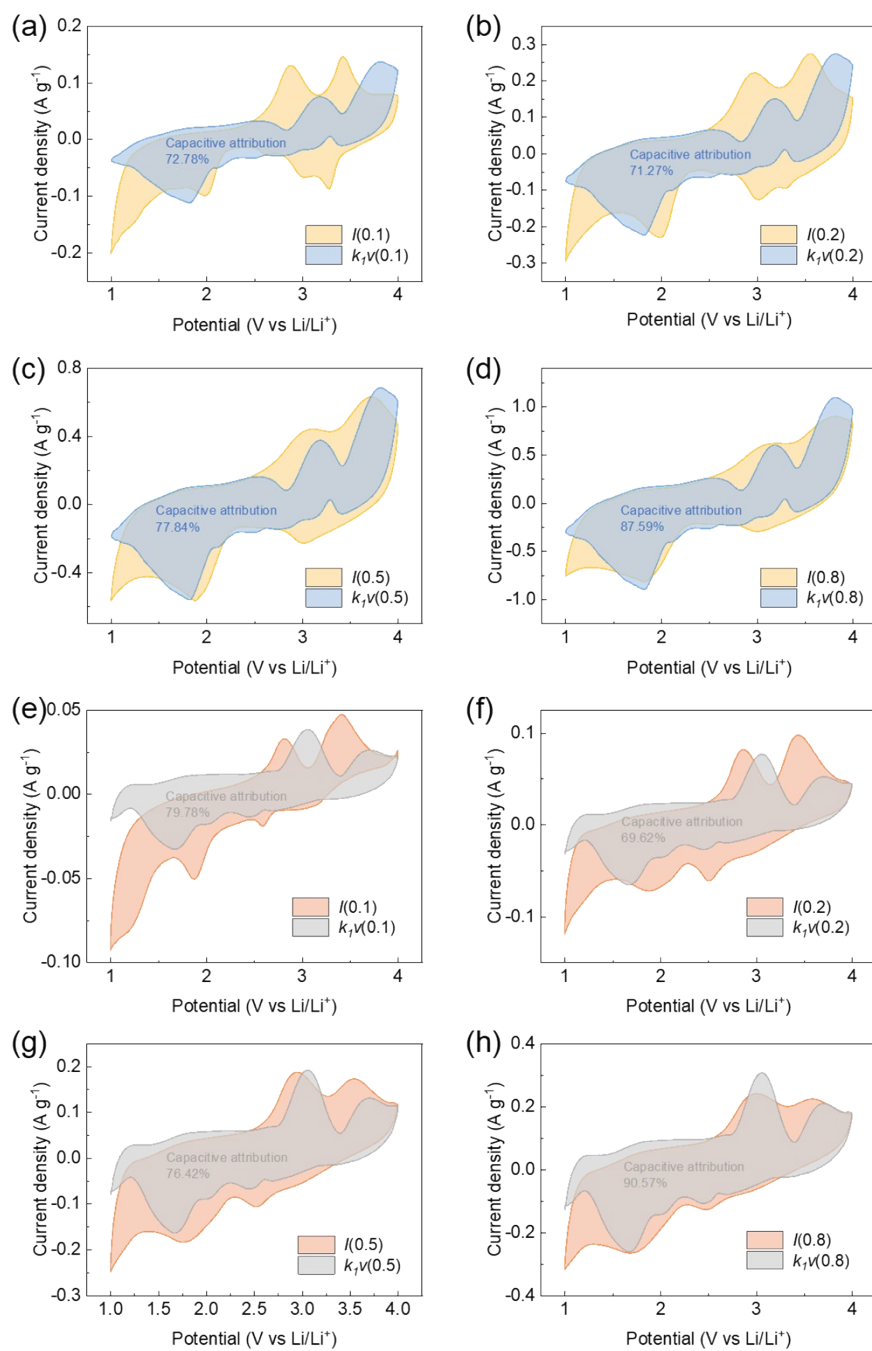


Fig. S10 capacitive contribution and diffusion contribution for $\text{FeF}_3@C$ cathode at (a) 0.1 mV s^{-1} , (b) 0.2 mV s^{-1} , (c) 0.5 mV s^{-1} and (d) 0.8 mV s^{-1} ; and for commercial FeF_3 cathode at (e) 0.1 mV s^{-1} , (f) 0.2 mV s^{-1} , (g) 0.5 mV s^{-1} and (h) 0.8 mV s^{-1} .