

Supporting Information

Doped modified nano-Si/C composites as high-Coulombic-efficiency anodes for lithium-ion batteries

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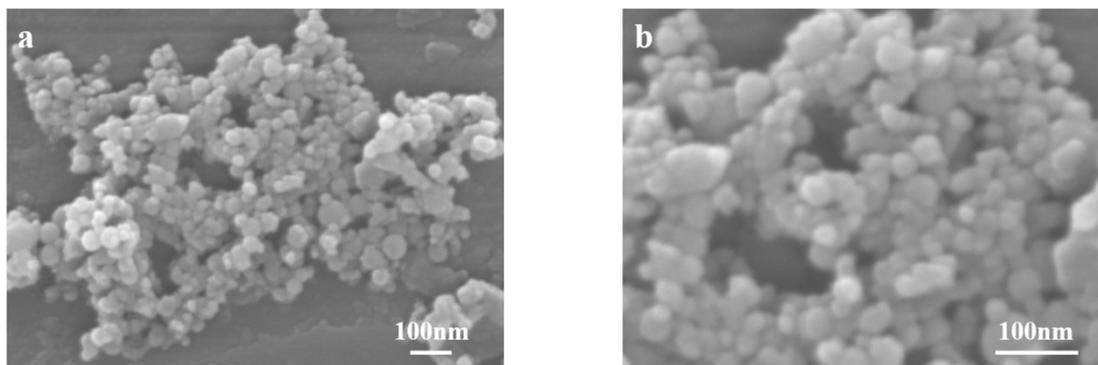


Fig. S1. SEM image of nano-silicon material.

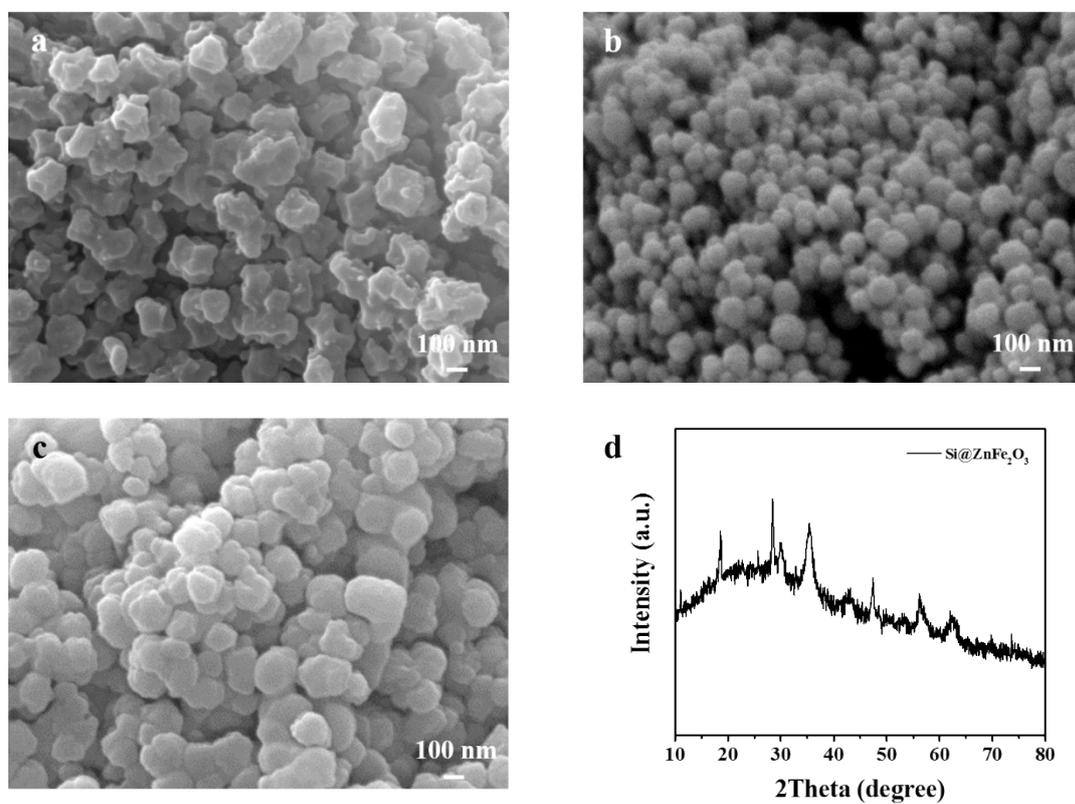


Fig. S2. Si@ZnFe₂O₃ produced by solvothermal reaction at different temperatures for 12 h. (a) 160°C, (b) 180°C, (c) 200°C, (d) XRD crystal diffraction pattern of Si@ZnFe₂O₃ samples.

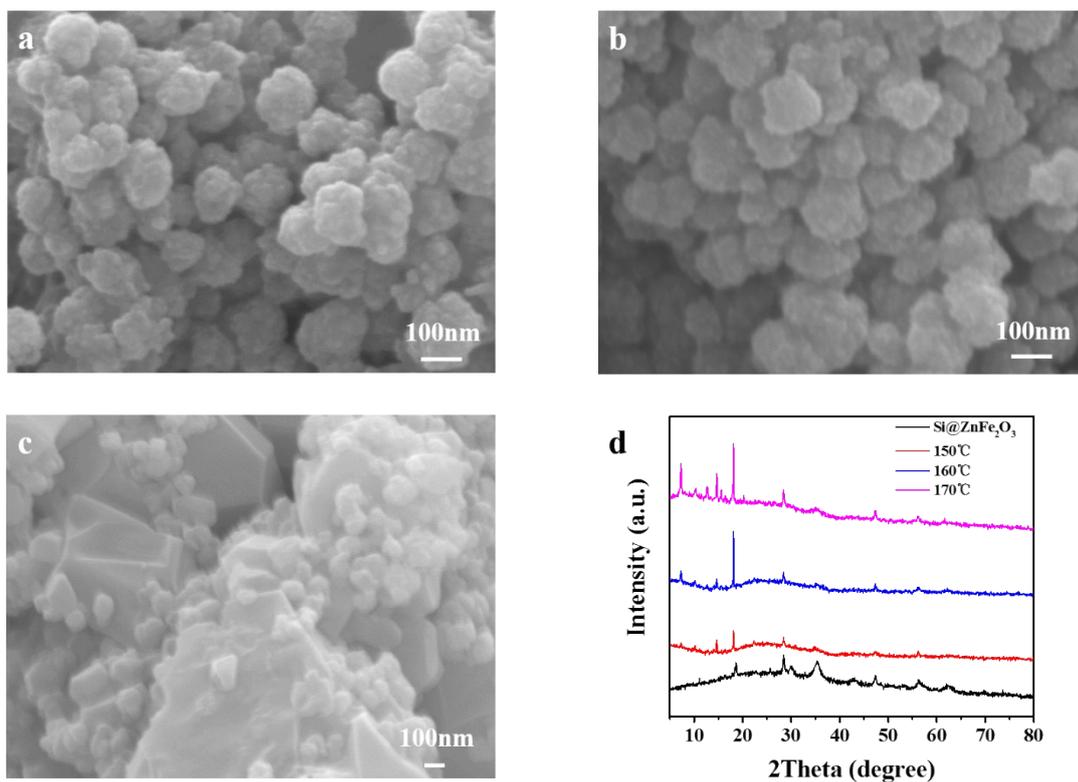


Fig. S3. The product of Si@ZnFe₂O₃ after 12h of low-pressure gas-solid reaction at different temperatures. (a) 150°C, (b) 160°C, (c) 170°C, (d) XRD patterns of Si@ZnFe₂O₃ and gas-solid reaction products at 150°C, 160°C, 170°C.

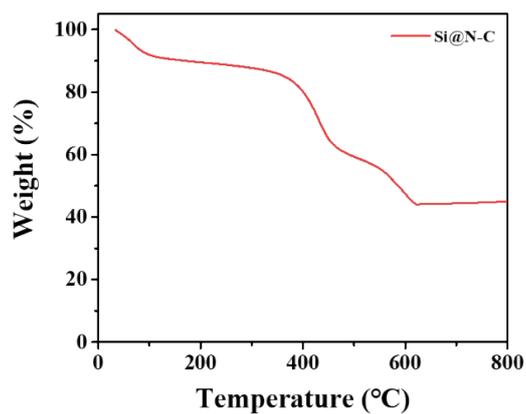


Fig. S4. The thermogravimetric (TG) curve of the Si@Fe₃C/N-C after pickling.

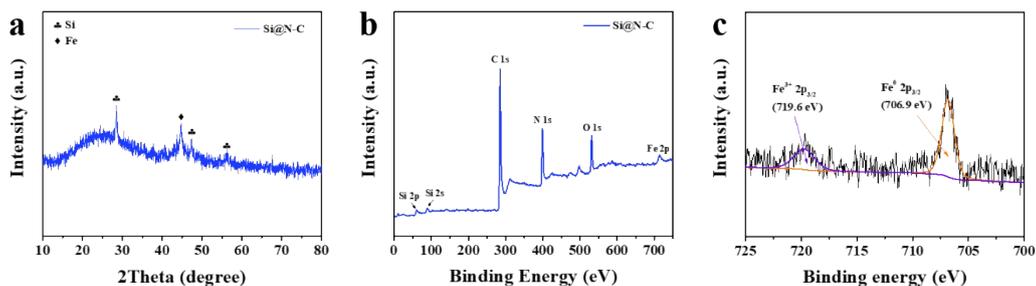


Fig. S5. The comparative sample Si@N-C was prepared by pickling with Si@Fe₃C/N-C products. (a) The XRD pattern of Si@N-C shows that there is no Fe₃C, and only a small amount of unremoved Fe metal. (b) XPS spectrum of Si@N-C. (c) Fe 2p high-resolution XPS diagram of Si@N-C samples show that only a small amount of Fe⁰ was detected. This is consistent with the XRD test results.

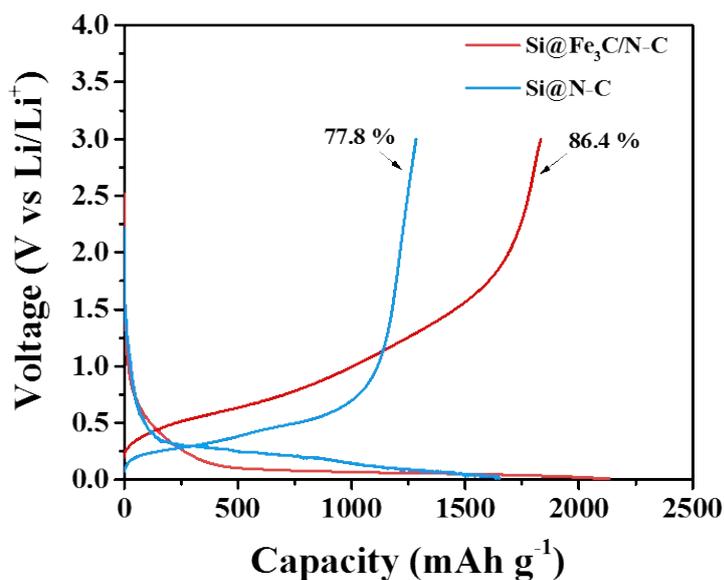


Fig. S6. Capacity-voltage curves of Si@Fe₃C/N-C and Si@N-C electrodes at 0.2 A g⁻¹ current density

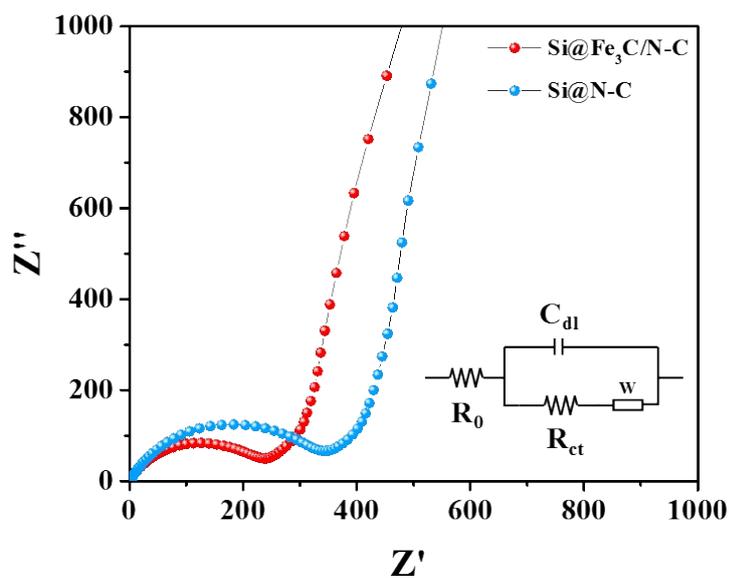


Fig. S7. EIS test of Si@Fe₃C/N-C and Si@N-C electrodes before cycling. The equivalent circuit diagram is embedded in the Fig.

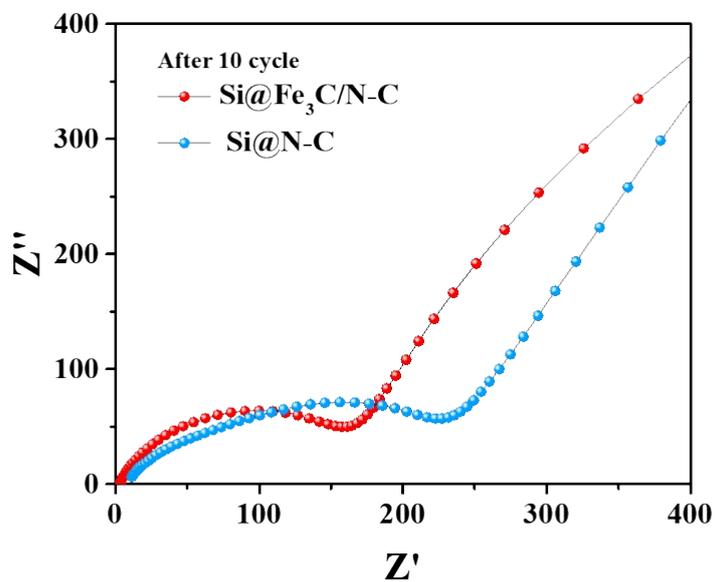


Fig. S8. The EIS test of Si@Fe₃C/N-C and Si@N-C electrodes after 10 cycles. The results show that Si@Fe₃C/N-C electrodes have better dynamic properties.

Table S1. The fitted impedance values of Si@Fe₃C/N-C electrodes before cycling, after 1 cycle and after 10 cycles.

Si@Fe ₃ C/N-C	Before cycle	After 1 cycle	After 10 cycle
R₀ (Ω)	2.42	6.54	3.13
R_{SEI} (Ω)	0	32.50	84.76
R_{ct} (Ω)	249.3	96.84	164.6

Table S2. The fitted impedance values of Si@N-C electrodes before cycling, after 1 cycle and after 10 cycles.

Si@N-C	Before cycle	After 1 cycle	After 10 cycle
R₀ (Ω)	2.65	5.28	5.06
R_{SEI} (Ω)	0	124.50	265.8
R_{ct} (Ω)	365.4	204.70	675.5

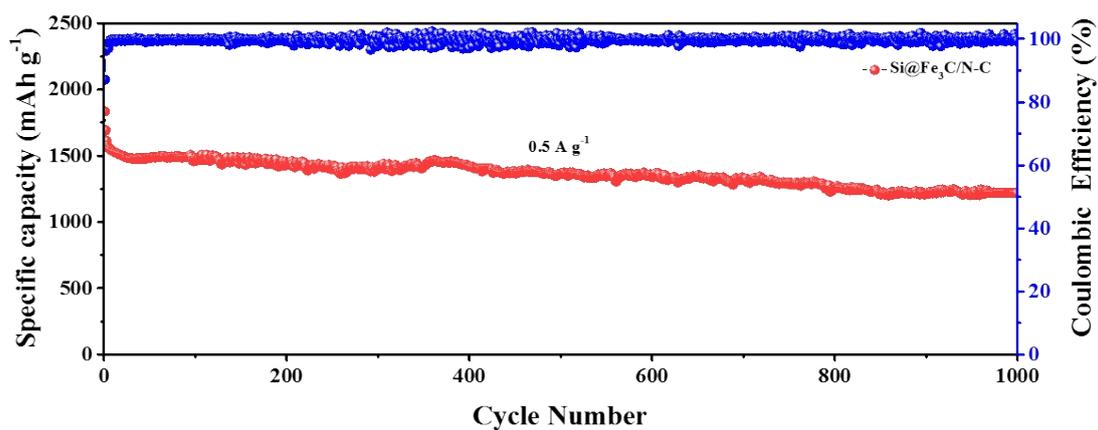


Fig. S9. The electrochemical performance of Si@Fe₃C/N-C cycled 1000 cycles at a current density of 0.5A g⁻¹.

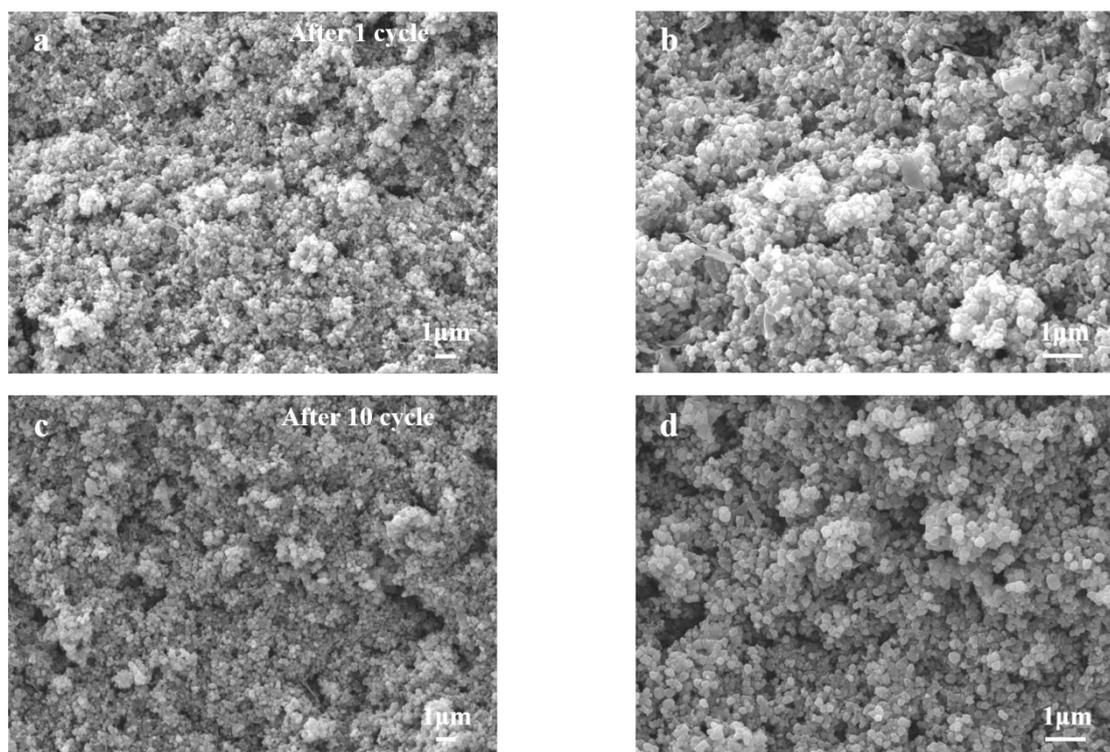


Fig. S10. SEM images of the surface of the Si@Fe₃C/N-C electrode after 1 cycle and 10 cycles under different magnifications. (a, b) after 1 cycle, (c, d) after 10 cycles. The results show that there is no obvious SEI formation on the surface, and the Si@Fe₃C/N-C particles are cross-linked without cracking.

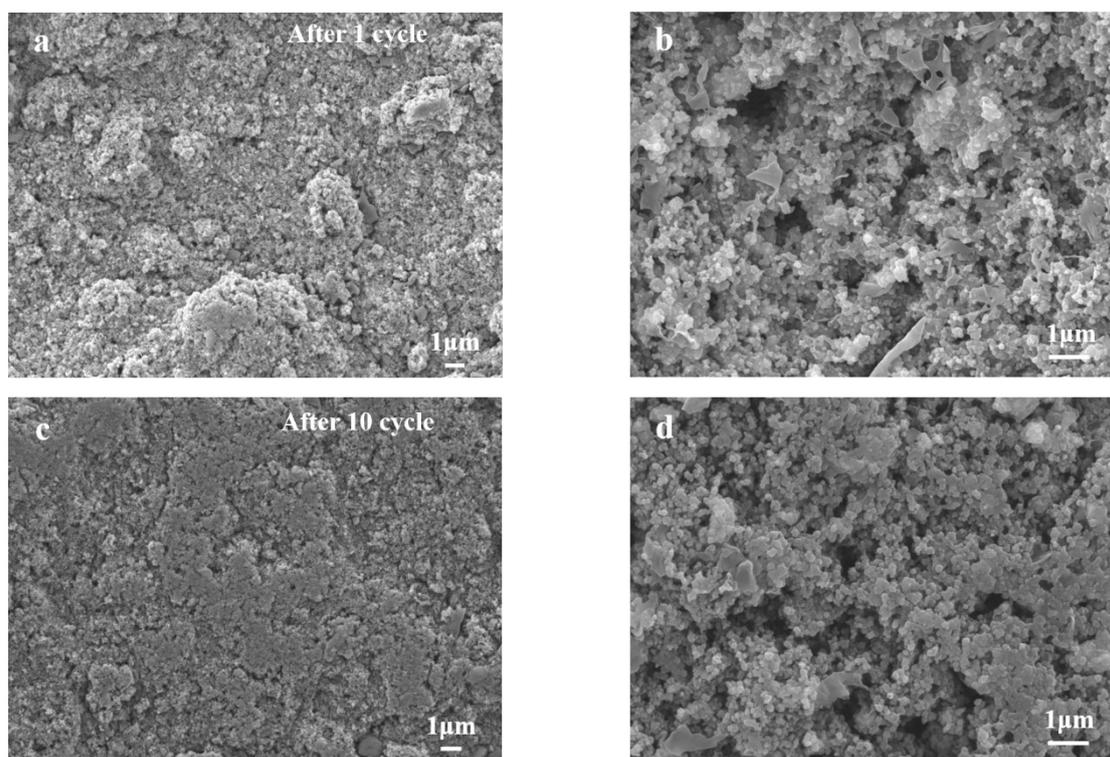


Fig. S11. SEM images of the electrode surface of Si@N-C electrode after 1 cycle and 10 cycles under different magnifications. (a, b) after 1 cycle, (c, d) after 10 cycles. The results showed that a distinct dark brown component (SEI) on the electrode surface was generated after 10 cycles.

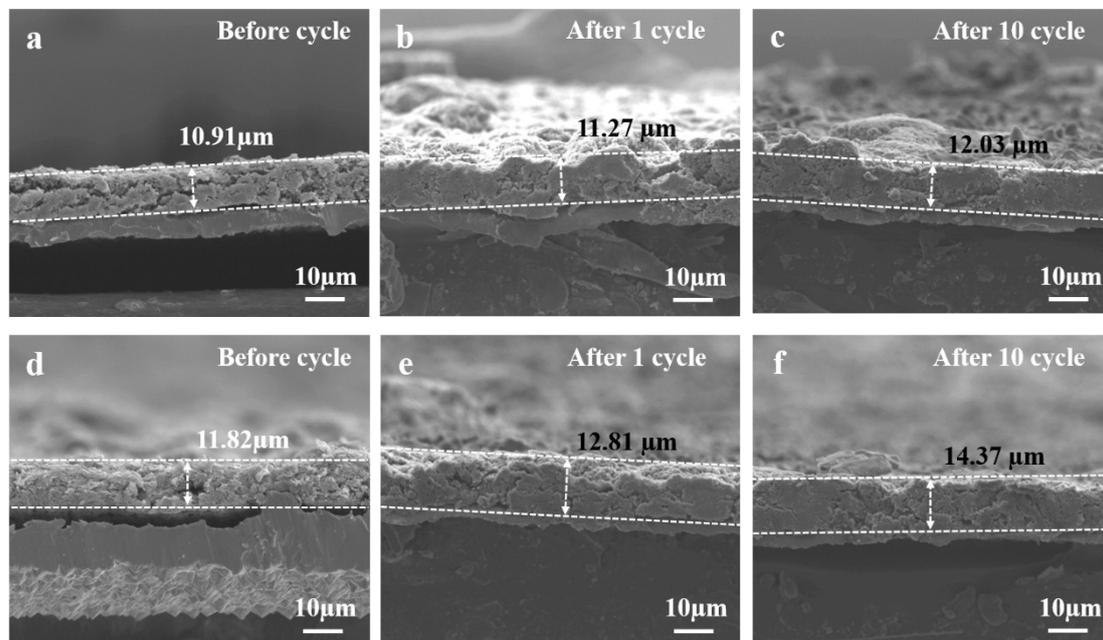


Fig. S12. SEM images of the electrode cross-sections of Si@Fe₃C/N-C and Si@N-C electrodes before, after 1 circle, and after 10 cycles. (a-c) Si@Fe₃C/N-C electrode thickness changes, (d-f) Si@N-C electrode thickness changes. The results show that the thickness of Si@N-C electrode changes more obviously after 10 cycles.

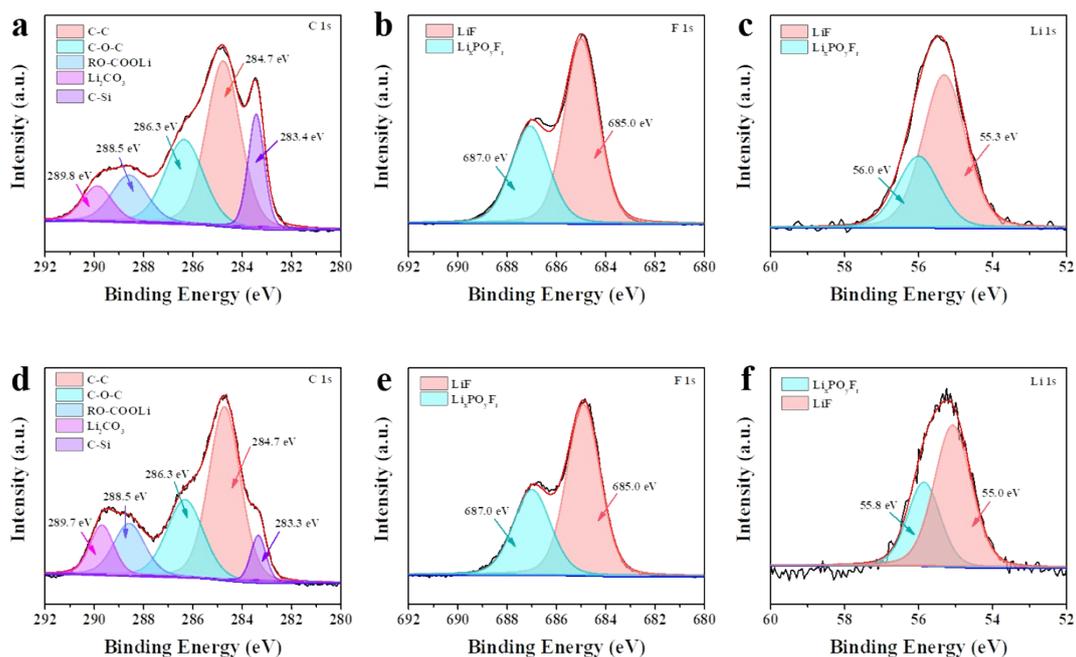


Fig. S13. XPS spectrum analysis of Si@Fe₃C/N-C and Si@N-C electrodes after 10 cycles. (a-c) C 1s, F 1s, Li 1s XPS spectrum of Si@Fe₃C/N-C electrode, (d-f) C 1s, F 1s, Li 1s XPS spectrum of Si@N-C electrode. The C 1s spectrum shown in Fig S11a shows that Strong C-Si bond peak. The C-Si peak in the spectrum shown in Fig S11d is weak, which is due to the thick SEI formed on the surface. Compared with the results of XPS analysis of the electrode after 1 cycle, the LiF peak in the Si@N-C electrode strengthen with the increase of the number of cycles, while the Si@Fe₃C/N-C electrode has no obvious change, indicating that the Si@N-C electrode is in the process of cycling SEI is constantly being produced. In summary, the surface of Si@Fe₃C/N-C electrode tends to generate thin and stable SEI after 10 cycles.

Reference:

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