

Supporting information

Silica Restricting the Sulfur Volatilization of Nickel Sulfide for High-Performance Lithium-Ion Batteries

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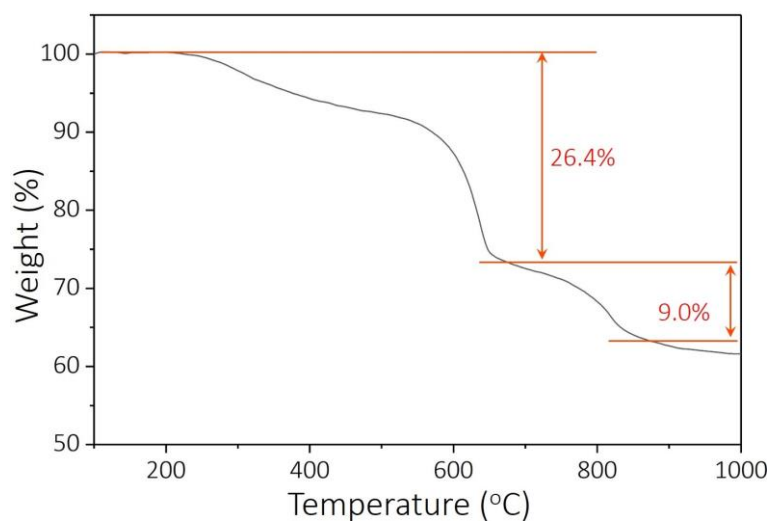


Figure S1. TGA curves of NiS₂.

Table S1. Elementary analysis with Inductive Coupled Plasma Emission Spectrometer (ICP) for Ni and S contents in the NiS_x@C sample.

| | Concentration | Unit | wt% | Mole ratio (S/Ni) |
|--------------|---------------|--------------------|---------|-------------------|
| Ni 231.604 r | 210.9626 | mg L ⁻¹ | 43.9645 | 1.23 |
| S 180.731 r | 142.4983 | mg L ⁻¹ | 29.6966 | |

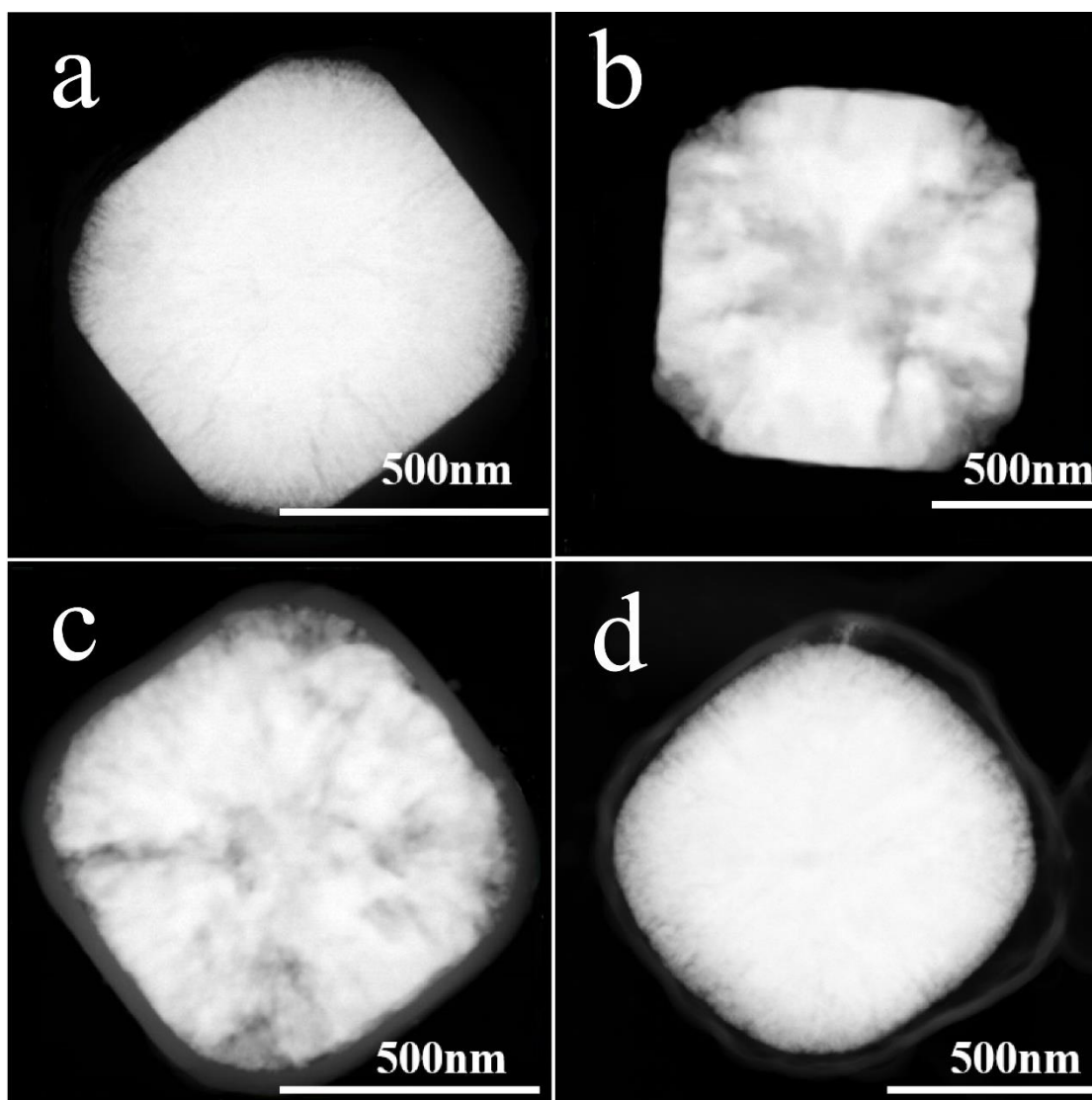


Figure S2. HAADF images of (a) NiS_2 , (b) NiS-600 , (c) NiS/C-600 and (d) $\text{NiS}_x\text{@C}$ yolk-shell microboxes.

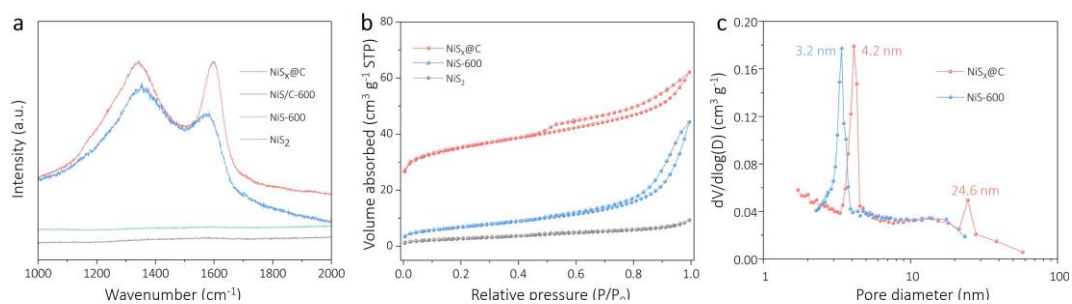


Figure S3. a) Raman spectra of NiS₂, NiS-600, NiS/C-600 and NiS_x@C. b) N₂ adsorption/desorption isotherm of NiS₂, NiS-600 and NiS_x@C. c) Pore size distribution curves NiS-600 and NiS_x@C.

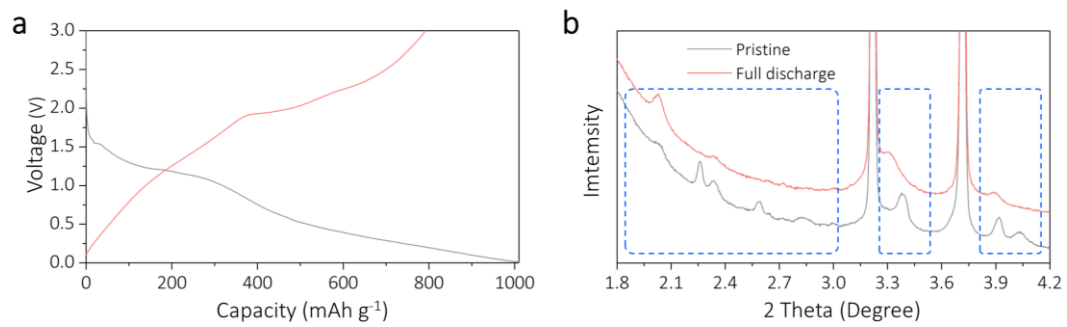


Figure S4. a) Initial discharge/charge curve of NiS_x@C electrode. b) *In-situ* synchrotron HEXRD of NiS_x@C electrode at pristine and full discharge state.

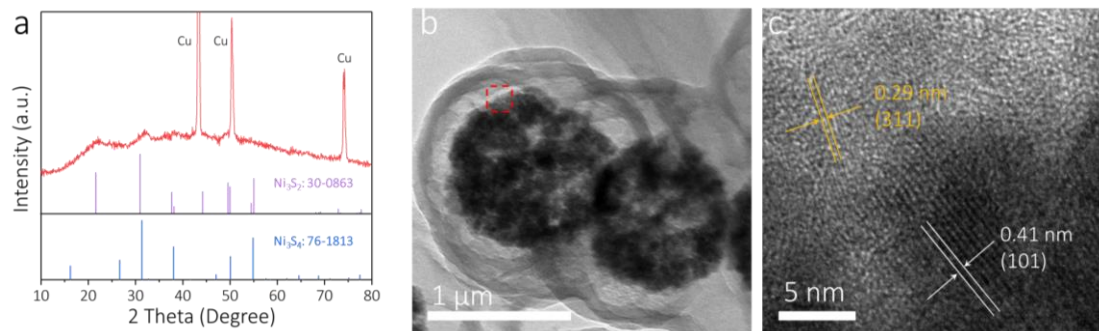


Figure S5. a) XRD pattern, b) TEM image, and c) HRTEM image of NiS_x@C electrode after first charge process.

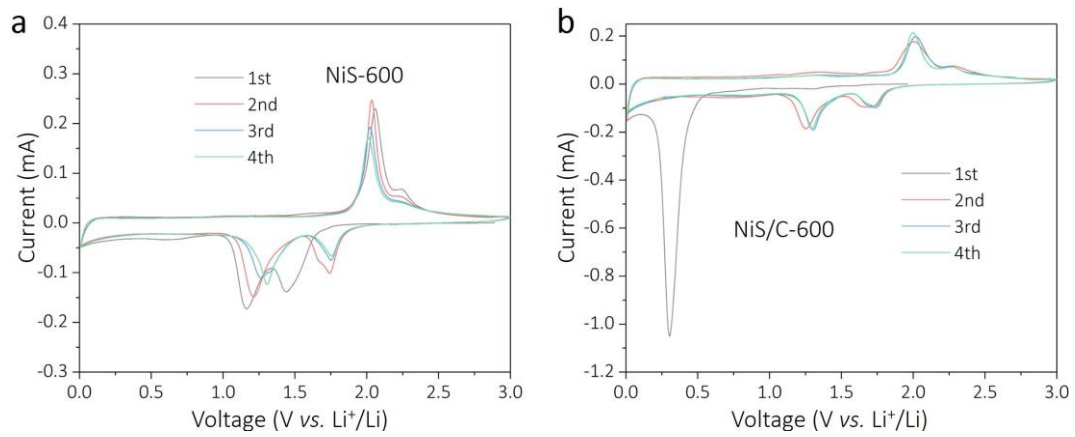


Figure S6. a) Cyclic voltammograms of NiS-600 and b) NiS/C-600 at a scan rate of 0.1 mV s⁻¹.

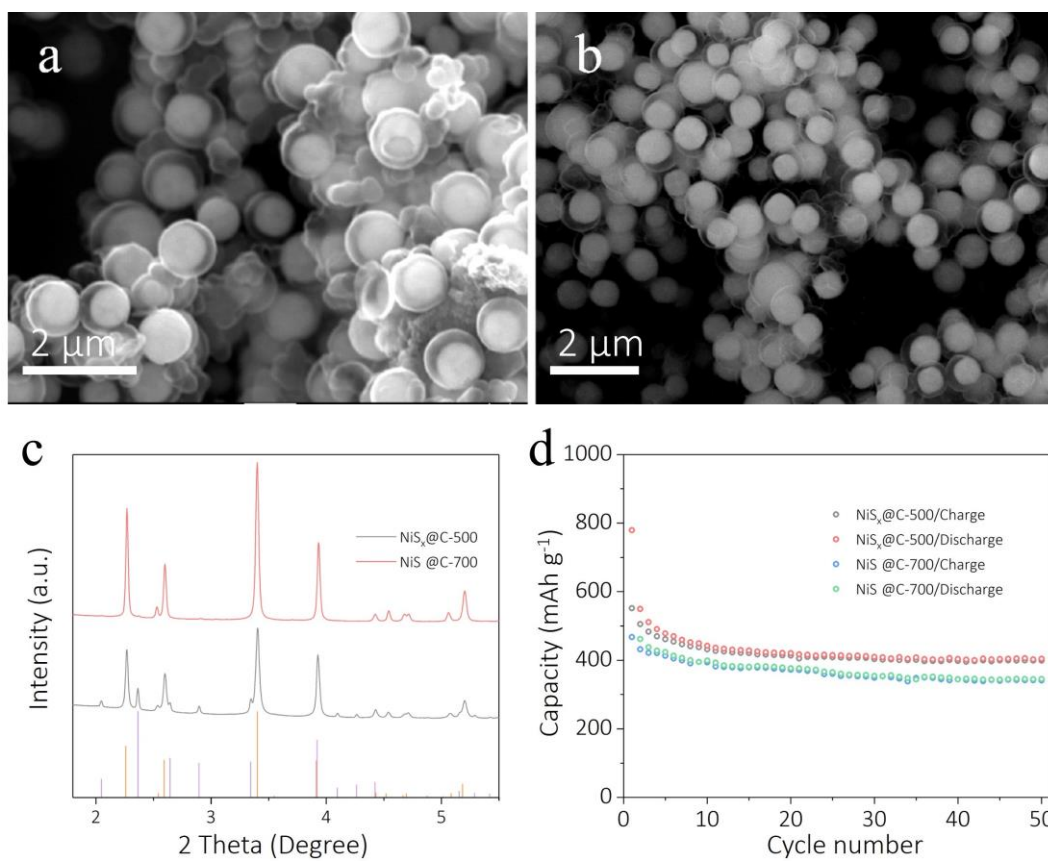


Figure S7. SEM images of NiS_x@C-500 (a) and NiS@C-700 (b). c) HEXRD of NiS_x@C-500 and NiS@C-700. d) Cycling performance of NiS_x@C-500 and NiS@C-700 at 1 A g⁻¹.

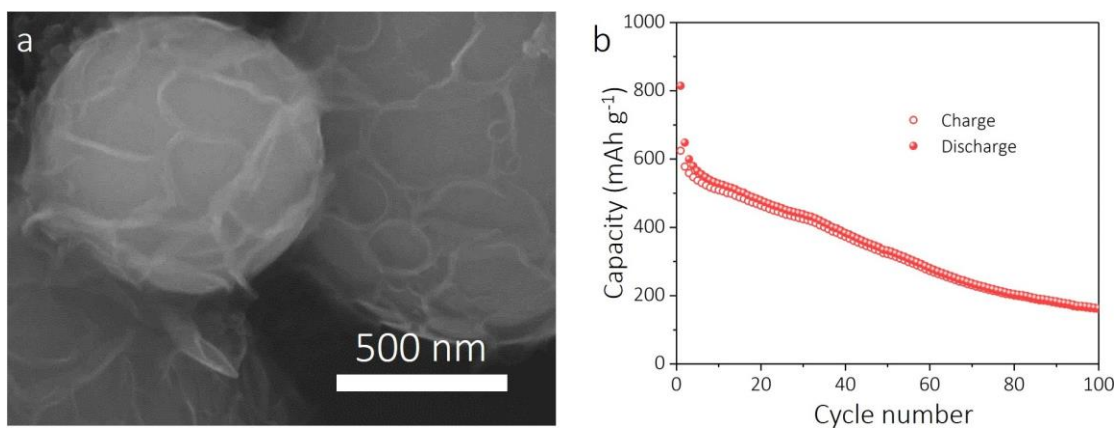


Figure S8. a) SEM images of NiS_x@C-T. b) Cycling performance of NiS_x@C-T at 1 A g⁻¹.

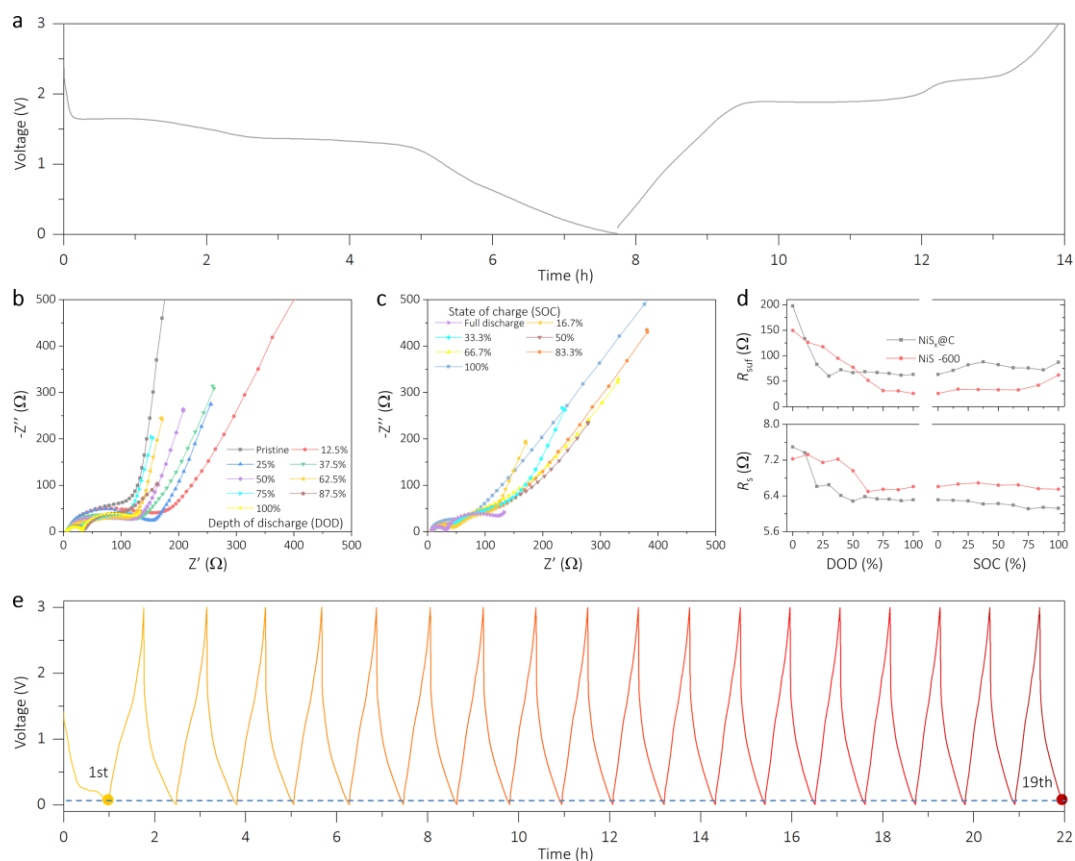


Figure S9. a) Initial discharge/charge curve of NiS-600 electrode for *in-situ* EIS tests. *In-situ* time-lapse EIS profiles of NiS-600 electrode at different depths of discharge (DOD) (b) and different states of charge (SOC) (c) during the initial discharge/charge. d) Plots of electrolyte solution resistance (R_s) and R_{surf} against SOC and DOD. e) Discharge/charge curve of NiS_x@C electrode for *in-situ* EIS tests at 1 A g⁻¹.

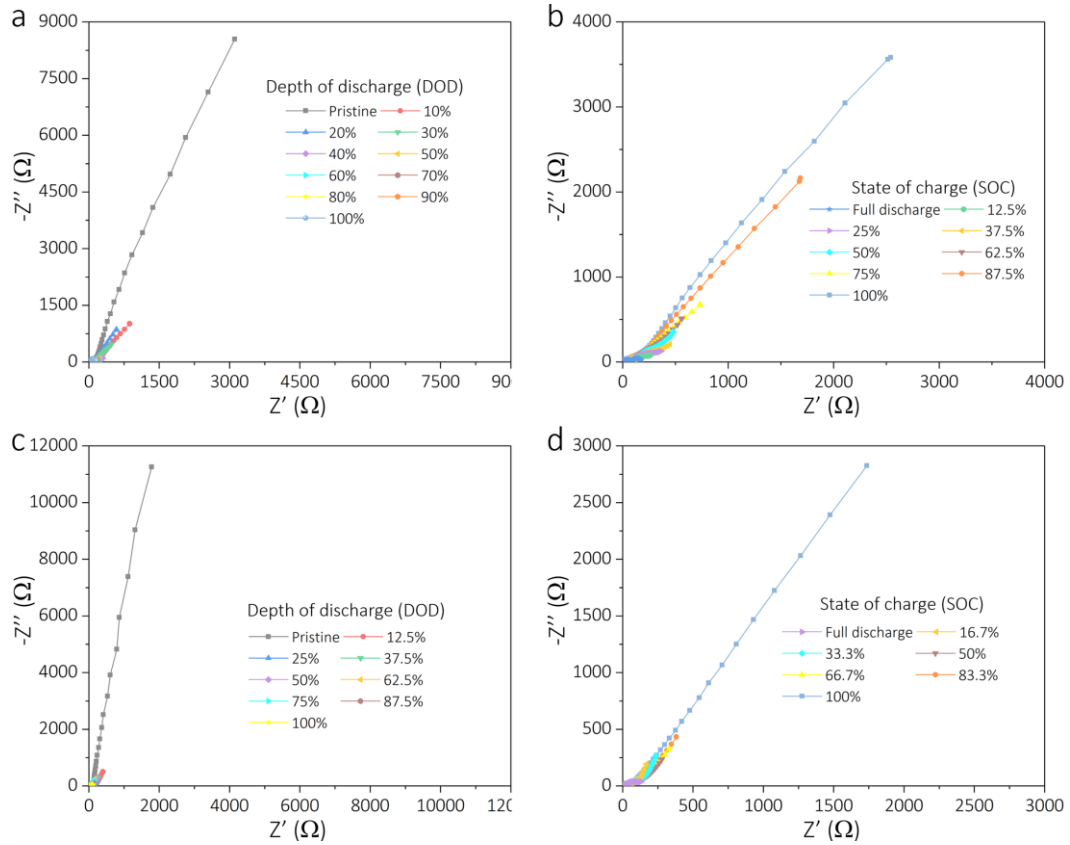


Figure S10. (a-b) Full *in-situ* EIS profiles of NiS_x@C electrode at first discharge/charge process. (c-d) Full *in-situ* EIS profiles of NiS-600 electrode at first discharge/charge process.

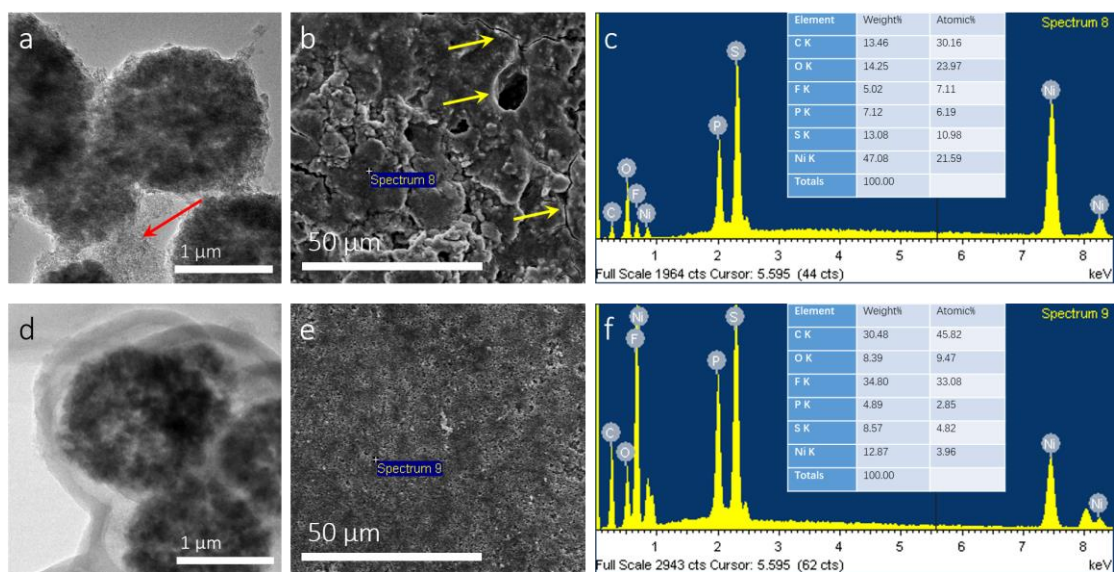


Figure S11. (a-c) TEM and EDS analysis of NiS-600 electrode after 30 cycles at full charge state. (d-f) TEM and EDS analysis of NiS_x@C electrode after 30 cycles at full charge state.

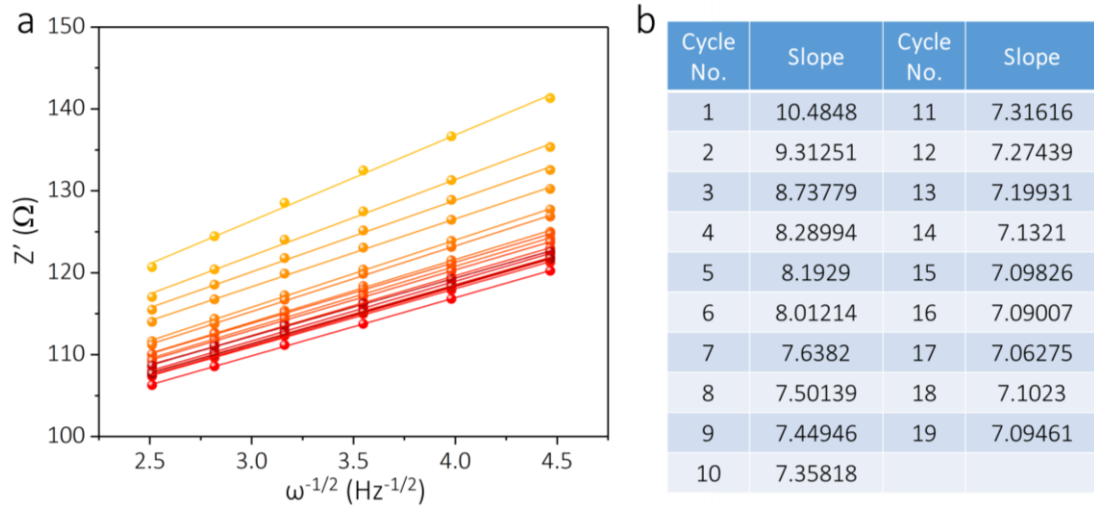


Figure S12. (a) Relationship between Z_{re} and $\omega^{-1/2}$ in the low frequency region for the $NiS_x@C$ electrode. (b) Fitting slope of different cycles.

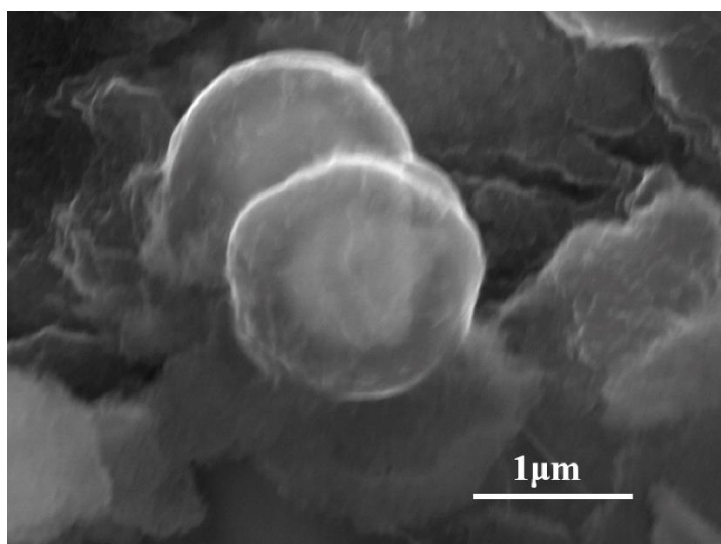


Figure S13. SEM image of $\text{NiS}_x@C$ yolk-shell microboxes electrode after 2000 cycles at 1 A g^{-1} .

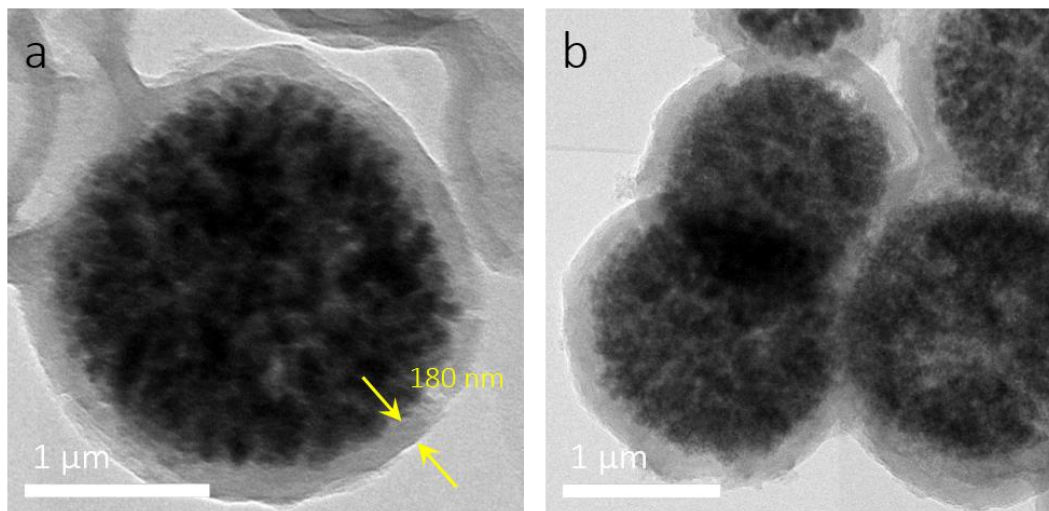


Figure S14. a) TEM image of NiS_x@C electrode after 3 cycles at full discharge state. b) TEM image of NiS_x@C electrode after 30 cycles at full discharge state.

Table S2. Elementary analysis of N, C, H, and S contents in the NiS_x@C and NiS/C-600.

| Sample | N(%) | C(%) | H(%) | S(%) |
|---------------------|------|-------|-------|--------|
| NiS _x @C | 0.59 | 29.91 | 0.133 | 30.488 |
| NiS/C-600 | 0.6 | 29.31 | 0.031 | 25.745 |