

Supporting Information

Zero-strain strategy incorporating TaC with Ta₂O₅ to enhance its rate capacity for long-term lithium storage

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Li⁺ Diffusion coefficient (D_{2Li}) calculated by EIS:

$$D_{2Li} = R^2 T^2 / 2 A^2 n^4 F^4 C^2 \sigma^2$$

where R is the gas constant, T is the absolute temperature, A is the surface area of the anode electrode, n is the number of electrons per molecule during oxidization, F is the Faraday constant, C is the ion concentration, σ is Warburg parameter.

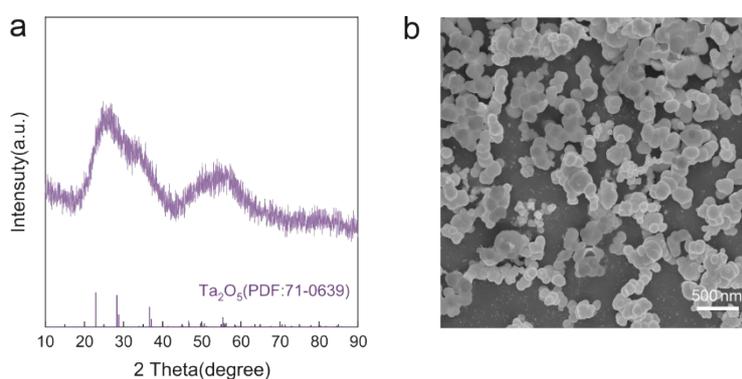


Fig. S1 (a) XRD pattern, and (b) SEM images of amorphous Ta₂O₅@PF hybrid nanospheres.

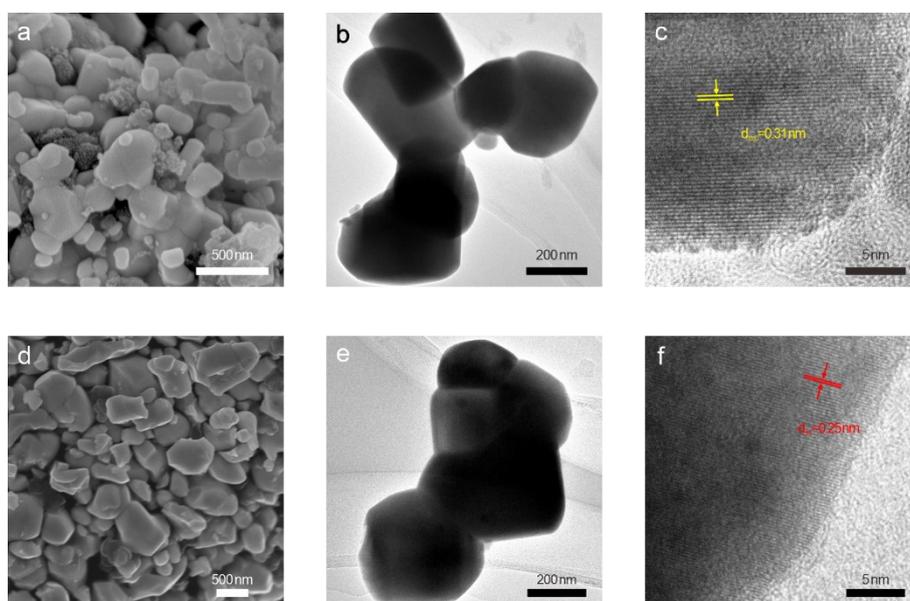


Fig. S2 (a) SEM, (b) TEM, and (c) HRTEM images of Ta₂O₅. (d) SEM, (e) TEM, and (f) HRTEM images of TaC.

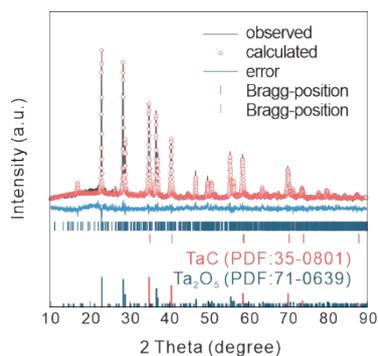


Fig. S3 a) XRD patterns of Ta₂O₅/TaC.

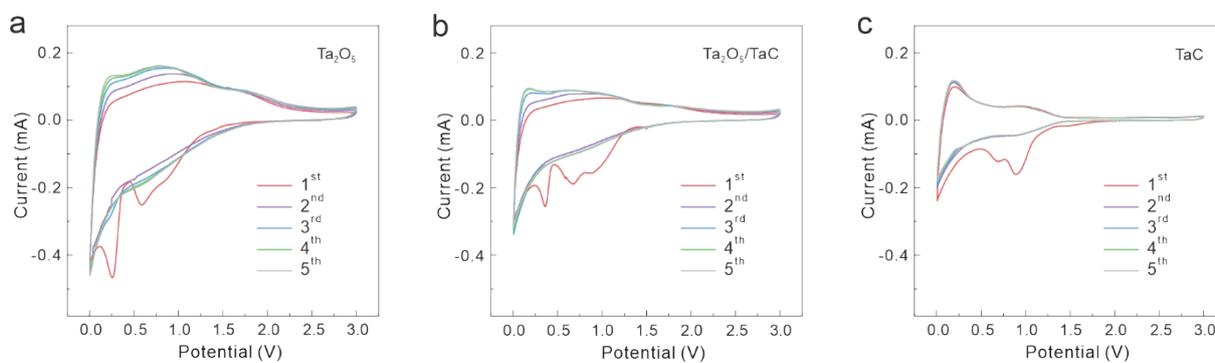


Fig. S4 CV curves of the a) Ta₂O₅, b) Ta₂O₅/TaC, and c) TaC anode at a scan speed of 0.2 mV s⁻¹ for 5 consecutive cycles.

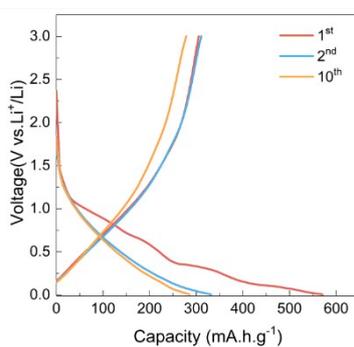


Fig. S5 The discharge/charge profiles of Ta₂O₅/TaC during the first ten cycles.

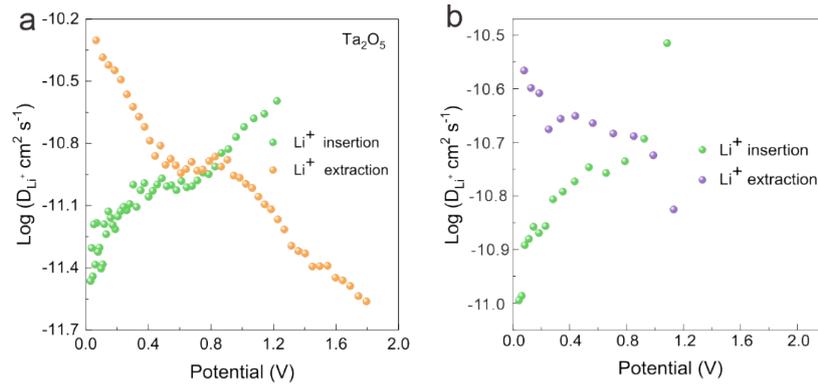


Fig. S6 The calculated D_{Li^+} from GITT curves of a) Ta_2O_5 , b) TaC

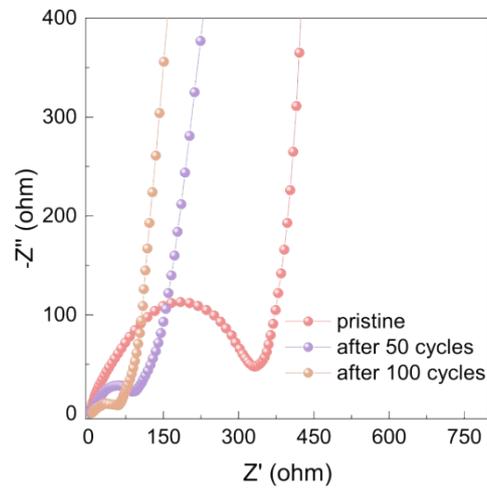


Fig. S7 Nyquist plots of Ta_2O_5/TaC anode in charging state for 50th and 100th cycles as well as before cycling.

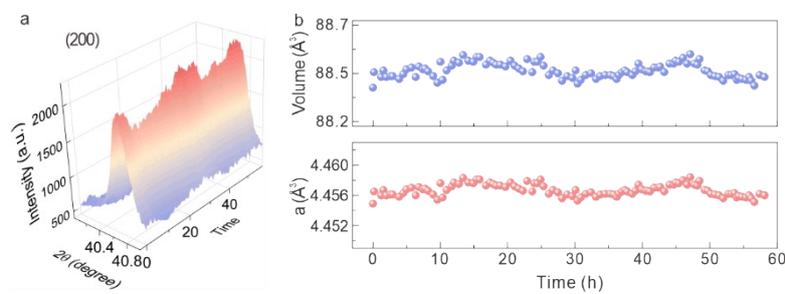


Fig. S8 a) 3D plot of selected in situ XRD patterns in the 2-theta range of $40.01 \sim 40.98^\circ$. b) The change of lattice parameters for TaC during the initial two cycles.

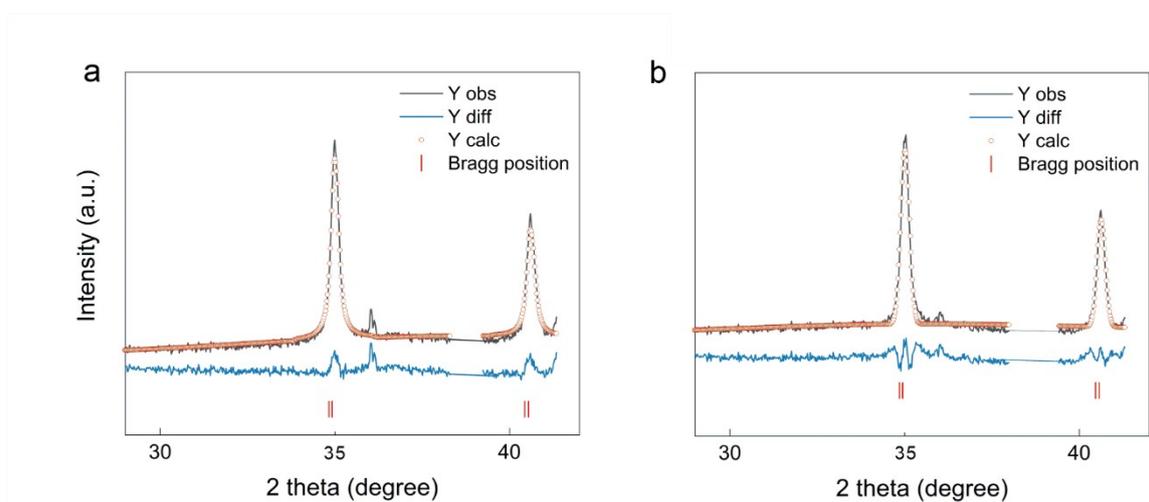


Fig. S9 Representative *in-situ* XRD patterns of Ta₂O₅/TaC in situ cell with Rietveld refinements at (a) 0.01 V (the end of second discharge) and (b) 3.0 V (the end of second charge). The peak at $\sim 38.7^\circ$ originates from the Be window (see Fig. 5a), and was deleted during the refinement process.

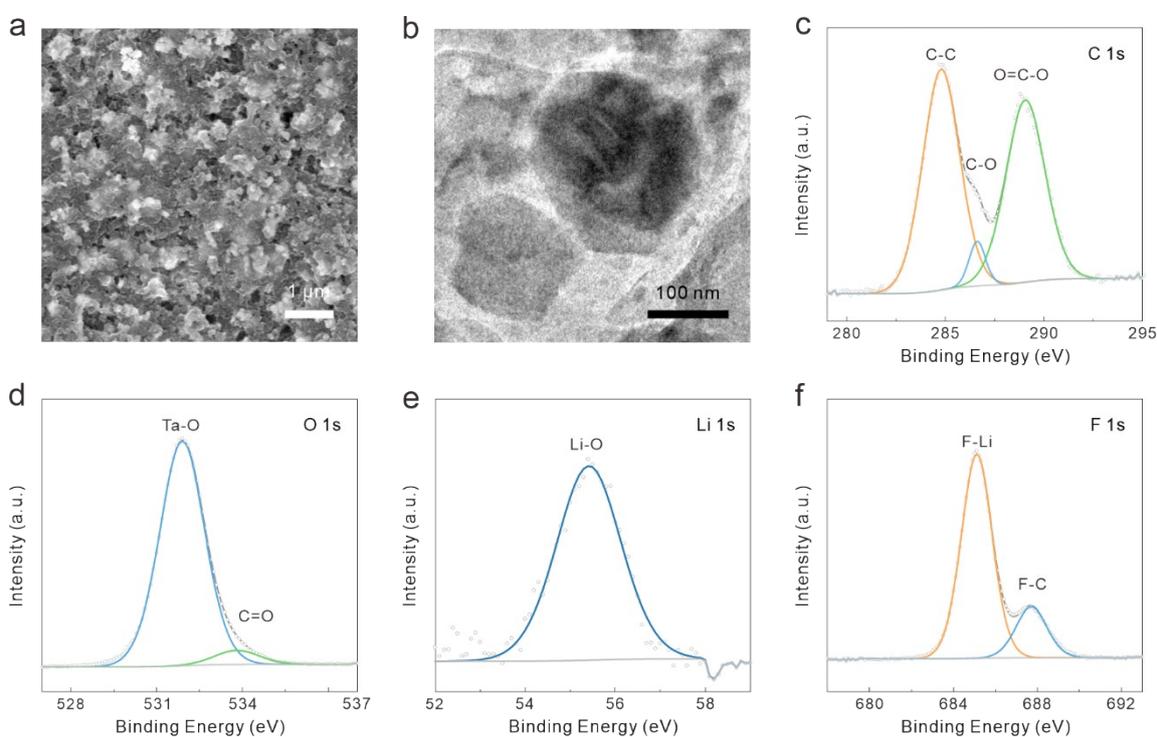


Fig. S10 (a) Low magnification FESEM image, and (b) TEM image of the Ta₂O₅/TaC electrode after 50 cycles. High-resolution XPS spectra of (c) C 1s, (d) O 1s (e) Li 1s, and (f) F 1s for Ta₂O₅/TaC electrode after being charged to 3 V.

Table. S1 The calculated average D_{1Li} values

	Ta ₂ O ₅	Ta ₂ O ₅ /TaC	TaC
Charge D_{1Li}	1.38×10^{-11}	2.26×10^{-11}	2.05×10^{-11}
Discharge D_{1Li}	9.54×10^{-12}	1.64×10^{-11}	1.61×10^{-11}

Table. S2 Summary of R_s and R_{ct} calculated from EIS of Ta₂O₅, Ta₂O₅/TaC, and TaC anode.

	Ta ₂ O ₅	Ta ₂ O ₅ /TaC	TaC
R_s (Ω)	8.2	3.7	7.2
R_{ct} (Ω)	400.0	351.8	255.4