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Electronic Supplementary Information (ESI)

Controllable Synthesis of Few-layer Ammoniated 1T'-phase WS_2 as Anode Material for Lithium-ion Batteries

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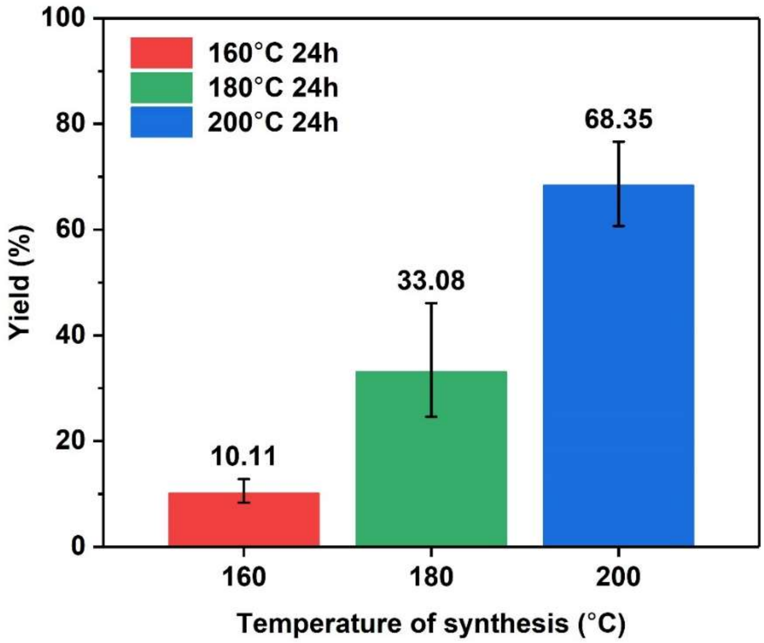

Fig. S1 The yield of as-prepared WS_2 synthesized at different reduction temperatures.

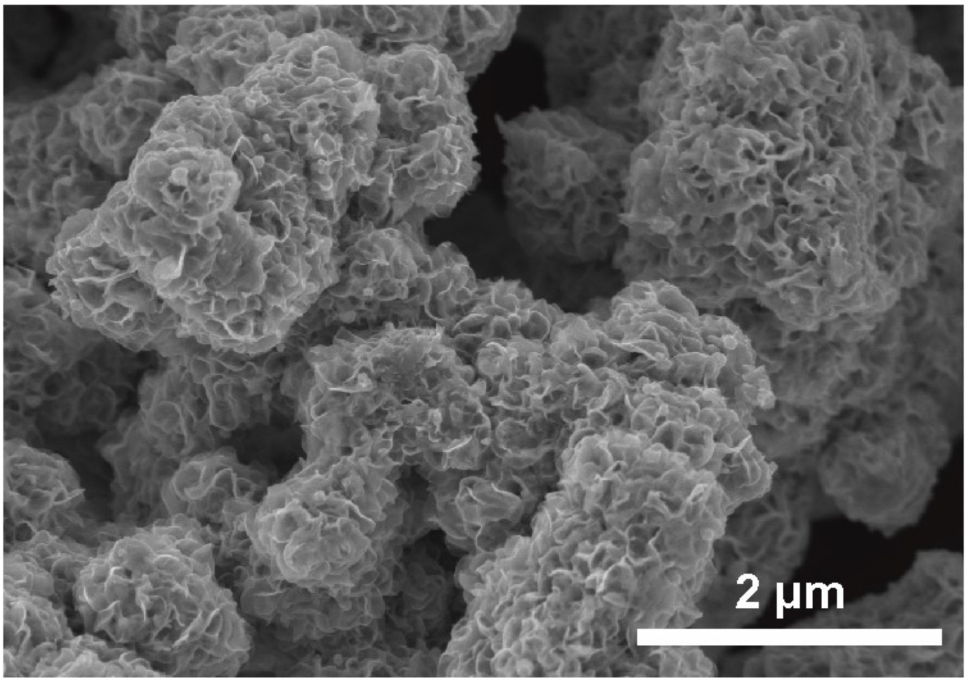

Fig. S2 SEM image of sample 2H-180. The morphology is similar to that of sample 1T'-180 in Fig. 1e.

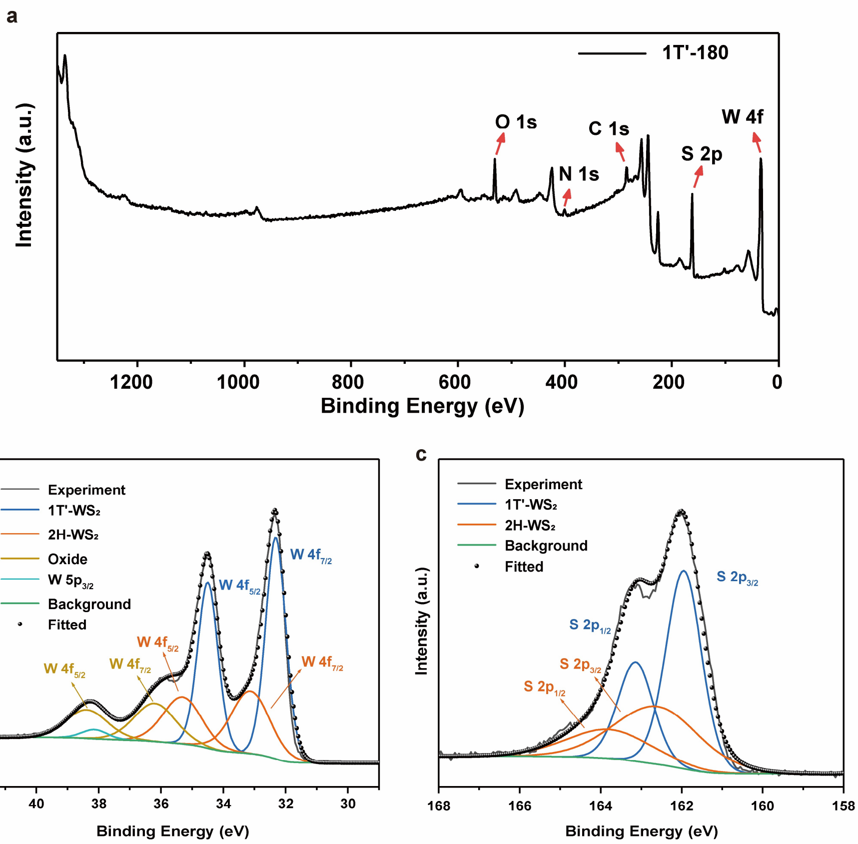

Fig. S3 XPS spectra of 1T'-180: (a) full survey, (b) W 4f and (c) S 2p core level.

Based on the full survey in Fig. S3a, the atomic concentrations for S, O, W, C and N elements are 40.06%, 17.18%, 18.12%, 18.94% and 5.70%, respectively. The C signal in 1T'-180 is attributed to the carbon contamination during the XPS test. The O signal probably origins from surface oxidation of nanostructure WS_2 or absorbed water from air during the sample transfer process. W 4f and S 2p core level peaks are deconvoluted to distinguish the 2H and 1T' phase of WS_2.[1] As shown in Fig. S3b, the spectrum of W 4f core level can ben deconvoluted into four components, three W $4f_{7/2}$ and W $4f_{5/2}$ doublets with the intensity ration of 4:3 and a gap of 2.18eV, and one W $5p_{3/2}$ peak located at a binding energy of 38.21 eV.[2] The W 4f doublet for 1T'-phase WS_2 locates at 32.33 and 34.51 eV (blue curves). The W 4f doublet for 2H-phase WS_2 locates at 33.19 and 35.37 eV (orange curves), which is also observed in sample 2H-180 (Fig. S4a). The W 4f doublet locating at 36.27 and 38.45 eV (yellow curves) is assigned to the oxide state of W. The doublet of 1T'-phase exhibits a shift of ~0.86 eV towards lower binding energy, compared with 2H-phase WS_2.[3] The spectrum of S 2p core level can also be deconvoluted into two doublets, see Fig. S3c. The S 2p doublet is composed of the S $2p_{3/2}$ and the S $2p_{1/2}$ peaks with an intensity ration of 2:1 and a gap of 1.19 eV.[2] The doublet for 1T'-WS_2 locates at 161.95 and 163.14 eV (blue curves) and the one for 2H-phase locates at 162.60 and 163.79 eV (orange curves). The XPS deconvolutions of W 4f and S 2p peaks indicate that the atom ratio of W:S is ~ 1:2 and concentration of 1T' phase is ~59% for sample 1T'-180. The phase concentration of 1T' and 2H is shown in Table S1.

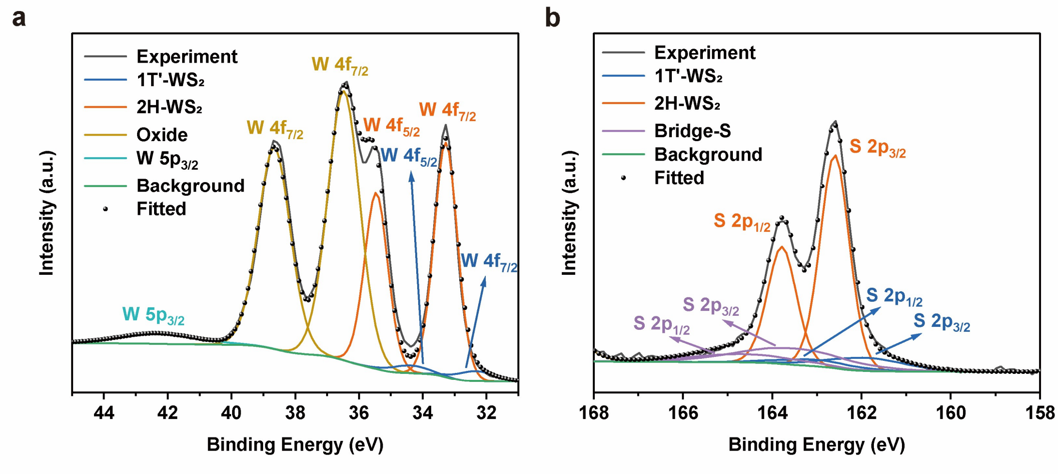

Fig. S4 XPS spectra of sample 2H-180: (a) W 4f, (b) S 2p.

Table. S1 The concentration of 1T'-phase and 2H-phase in different 1T'-WS_2 samples based on the S 2p XPS spectra in Fig. S3 and S5.

Sample	Concentration (%)		Layer numbers
	1T'-phase	2H-phase	
1T'-160	62.8	37.2	4 ~ 6
1T'-180	58.9	41.1	9 ~ 10
1T'-200	55.3	44.7	~ 20

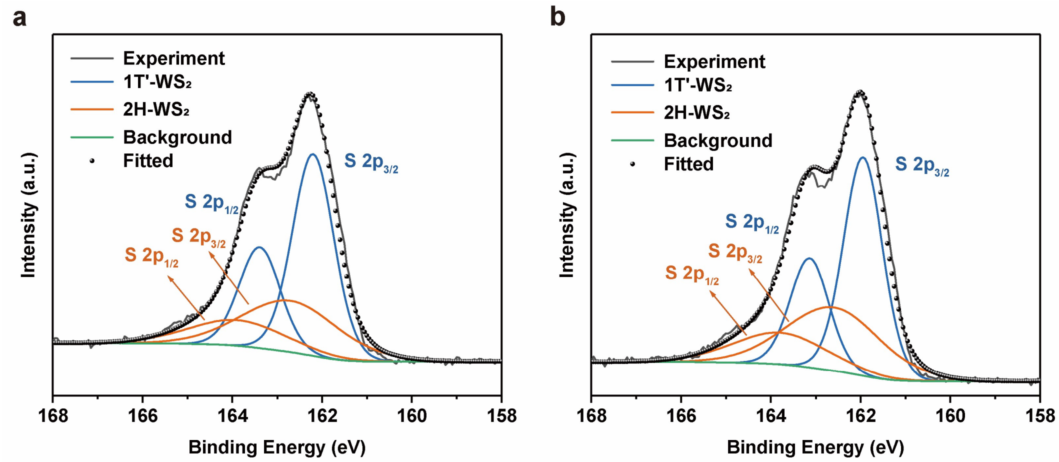

Fig. S5 S 2p XPS spectra of sample (a) 1T'-160 and (b) 1T'-200.

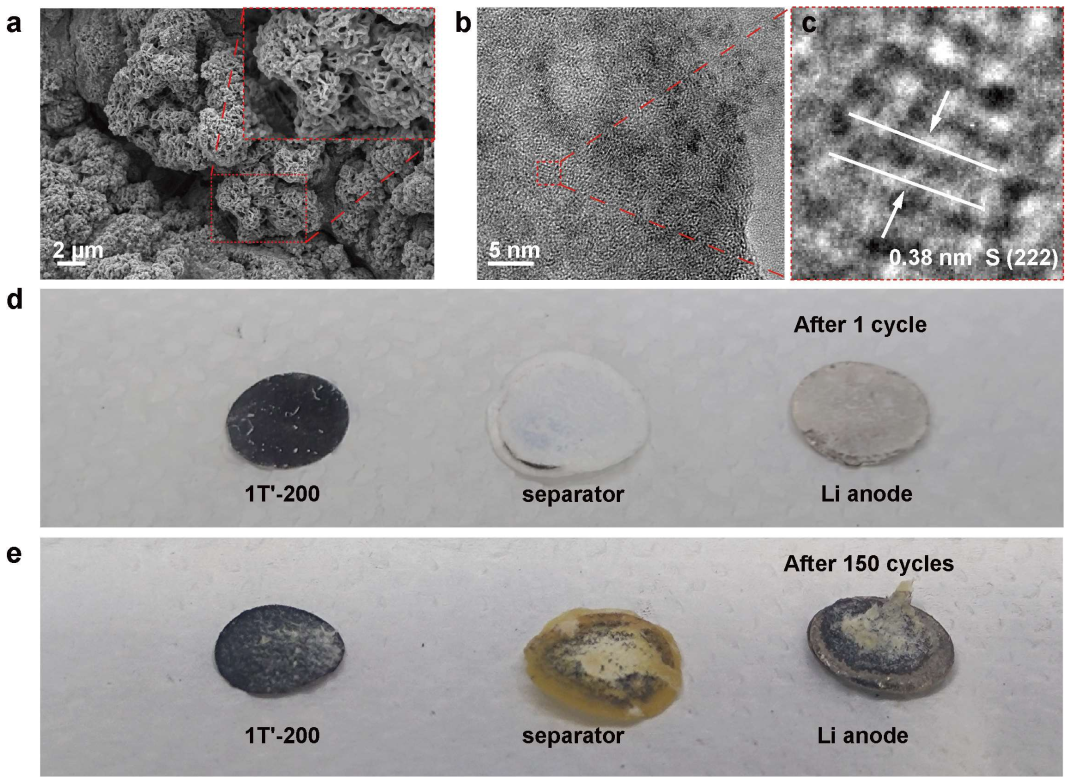

Fig. S6 (a) SEM and (b,c) TEM images of 1T'-200 after 150 cycles at full charge state. (d, e) Photographs of the disassembled batteries of 1T'-200 after different cycles.

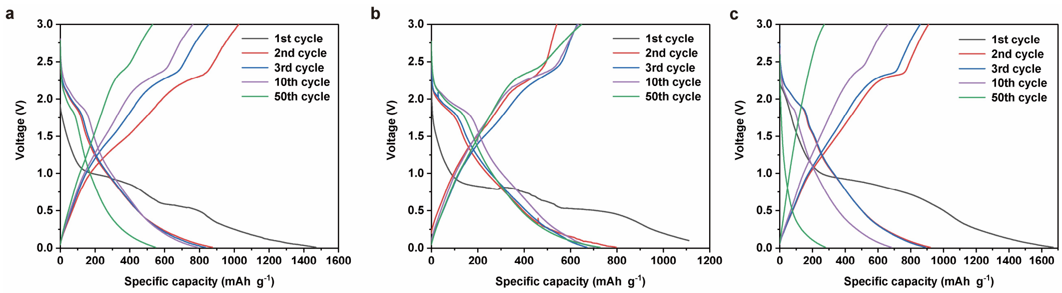

Fig. S7 Galvanometric charge/discharge curves of the (a) 1T'-160 electrode, (b) 1T'-200 electrode and (c) 2H-180 electrode.

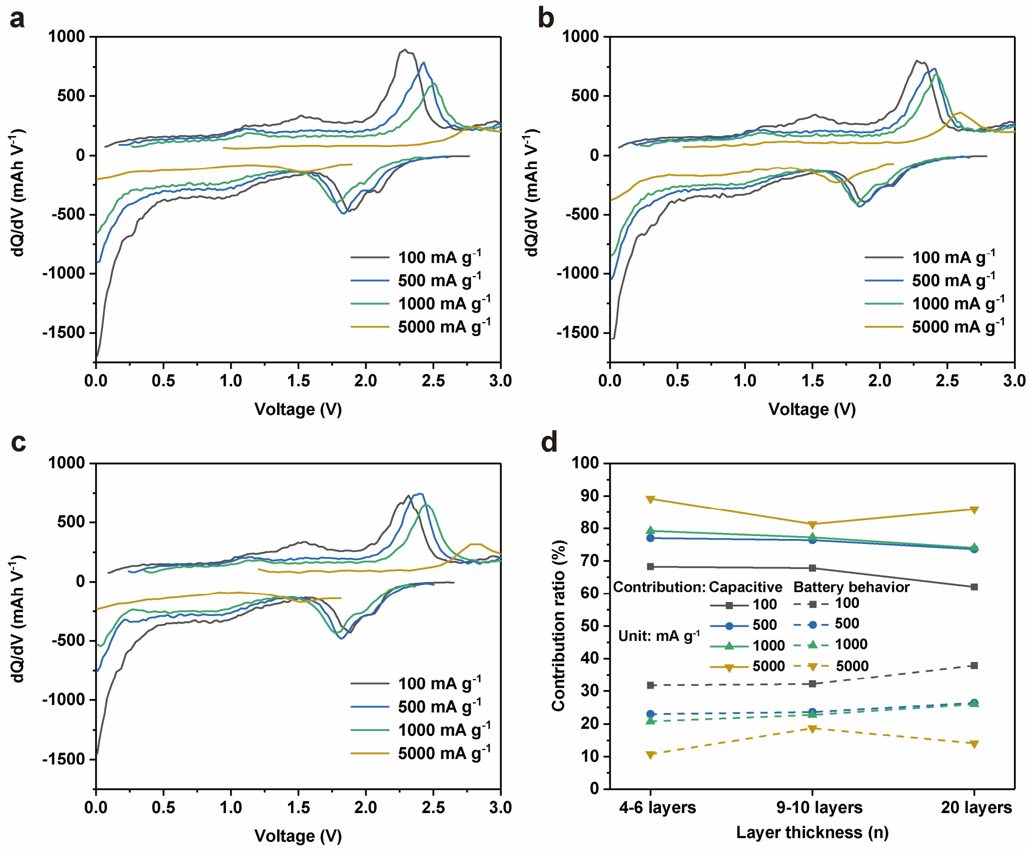

Fig. S8 Differential capacity dQ/dV curves of the (a) 1T'-160 electrode, (b) 1T'-180 electrode, (c) 1T'-200 electrode and (d) corresponding surface controlled and battery behavior controlled contributions.

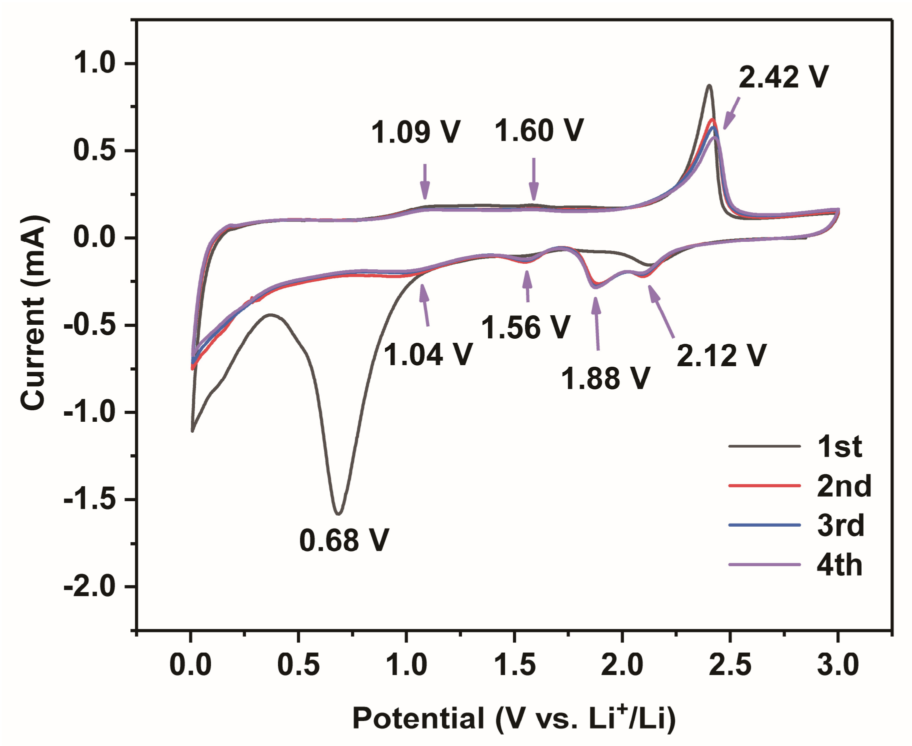

Fig. S9 Cyclic voltammograms of 2H-180 electrode over a potential window of 0.01-3.0 V (vs. Li^+/Li) at a scan rate of 0.1 mV s^{-1}.

References

1 A. Anto Jeffery, C. Nethravathi and M. Rajamathi, *The Journal of Physical Chemistry C*, 2013, **118**, 1386-1396.
2 D. Pierucci, J. Zribi, C. Livache, C. Gréboval, M. G. Silly, J. Chaste, G. Patriarche, D. Montarnal, E. Lhuillier, A. Ouerghi and B. Mahler, *Appl. Phys. Lett.*, 2019, **115**, 32102.
3 Z. Lai, Q. He, T. H. Tran, D. V. M. Repaka, D. Zhou, Y. Sun, S. Xi, Y. Li, A. Chaturvedi, C. Tan, B. Chen, G. Nam, B. Li, C. Ling, W. Zhai, Z. Shi, D. Hu, V. Sharma, Z. Hu, Y. Chen, Z. Zhang, Y. Yu, X. Renshaw Wang, R. V. Ramanujan, Y. Ma, K. Hippalgaonkar and H. Zhang, *Nat. Mater.*, 2021, **20**, 1113-1120.