Electronic Supplementary Information (ESI)

Controllable Synthesis of Few-layer Ammoniated 1T'-phase WS₂ 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.
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 originates 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 be deconvoluted into four components, three W 4f$_{7/2}$ and W 4f$_{5/2}$ doublets with the intensity ratio of 4:3 and a gap of 2.18 eV, 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 ratio 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.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Concentration (%)</th>
<th>Layer numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1T'-phase</td>
<td>2H-phase</td>
</tr>
<tr>
<td>1T'-160</td>
<td>62.8</td>
<td>37.2</td>
</tr>
<tr>
<td>1T'-180</td>
<td>58.9</td>
<td>41.1</td>
</tr>
<tr>
<td>1T'-200</td>
<td>55.3</td>
<td>44.7</td>
</tr>
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</table>
Fig. S5 S 2p XPS spectra of sample (a) 1T'\textsuperscript{-}160 and (b) 1T'\textsuperscript{-}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