Supporting Information

$V_2CT_x$ Catalyzes Polysulfide Conversion to Enhance Redox Kinetics of Li–S Batteries

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Fig. S1. Nitrogen adsorption/desorption isotherm curve of V$_2$CT$_{X}$ nanobelts.
Fig. S2. HRTEM image of a $V_2CT_X$ nanobelt.
**Fig. S3.** SEM images of (a) PP and (b) KB/V<sub>2</sub>CT<sub>X</sub>-PP separators. (c) Cross-sectional SEM image of KB/V<sub>2</sub>CT<sub>X</sub> interlayer.
Fig. S4. Digital photographs of Li$_2$S$_6$ solution and after the addition of KB/V$_2$CT$_X$. 
Fig. S5. (a, b) Magnified cathodic peaks and (c) anode peaks of the two cells.
Fig. S6. CV profiles of (a) PP and (b) KB/V$_2$CT$_X$-PP cells for consecutive cycles.
Fig. S7. CV curves of (a) PP and (b) KB/V$_2$CT$_X$-PP cells at different scan rates.
Fig. S8. LSV analyses of KB/V$_2$CT$_X$-CP and CP cells with Li$_2$S$_6$ catholyte.
Fig. S9. EIS curves of PP and KB/V₂CTₓ-PP cells.
Fig. S10. GCD curves of PP cells at 0.2 C.
**Fig. S11.** GITT curves of cathodes with PP and KB/V$_2$CTx-PP separators during discharge process.
Fig. S12. Photographs for (a) PP and (b) KB/V\textsubscript{2}CT\textsubscript{X}-PP separators toward Li metal anode after 150 cycles at 0.2 C.
Fig. S13. Rate performance of KB/V$_2$CT$_X$-PP cells (1 C = 1675 mA g$^{-1}$)
Fig. S14. GCD curves of a PP cells at different rates.
**Table S1.** Comparison of the cycle performance between this work and other previously reported similar materials

<table>
<thead>
<tr>
<th>Materials</th>
<th>S loading (mg cm⁻²)</th>
<th>Rate (C)</th>
<th>Initial capacity (mAh g⁻¹)</th>
<th>Cycle Number</th>
<th>Capacity decay (% per cycle)</th>
<th>Ref.</th>
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<tbody>
<tr>
<td>d-Ti₃C₂</td>
<td>0.7-1</td>
<td>0.5</td>
<td>899</td>
<td>50</td>
<td>0.64</td>
<td>[1]</td>
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<tr>
<td>Ti₃C₂/T₅V₉ aerogel</td>
<td>1.2</td>
<td>1</td>
<td>980</td>
<td>1500</td>
<td>0.037</td>
<td>[2]</td>
</tr>
<tr>
<td>CNTs/Ti₃C₂Tₓ</td>
<td>0.8</td>
<td>1</td>
<td>987</td>
<td>600</td>
<td>0.063</td>
<td>[3]</td>
</tr>
<tr>
<td>Ti₃C₂Tₓ@Nafion</td>
<td>2</td>
<td>1</td>
<td>920</td>
<td>1000</td>
<td>0.03</td>
<td>[4]</td>
</tr>
<tr>
<td>Nb₂O₃-CNT</td>
<td>1.3-1.5</td>
<td>0.2</td>
<td>1286</td>
<td>100</td>
<td>0.23</td>
<td>[5]</td>
</tr>
<tr>
<td>S@V₂C-Li/C</td>
<td>3.0</td>
<td>0.1</td>
<td>1140</td>
<td>100</td>
<td>0.096</td>
<td>[6]</td>
</tr>
<tr>
<td>V₂C/V₂O₅-CNTs</td>
<td>2.0</td>
<td>1</td>
<td>1055.2</td>
<td>500</td>
<td>0.034</td>
<td>[7]</td>
</tr>
<tr>
<td>KB/V₂CTₓ</td>
<td>1.2</td>
<td>1</td>
<td>1069</td>
<td>1000</td>
<td>0.049</td>
<td>This work</td>
</tr>
</tbody>
</table>
Note 1. The detail calculation scheme of relative activation energy.

CV tests were performed under a scan rate (0.1 mV s\(^{-1}\)) at 298 K as shown in Figure 2a.

Correspondingly, the relationship between electrode potential and activation energy over the Catalyzed-free and In-based batteries could be calculated according to the equation (1):

\[
E_a = E_{a0} + \alpha z F \phi_{\text{cathode}}(Ox|Red)_{IR}
\]

where \(E_a\) is the activation energy of reduction process, \(E_{a0}\) is the intrinsic activation energy, \(\alpha\) is the symmetry coefficient, \(z\) is the number of charge transfer, \(F\) is the Faraday’s constant, \(\phi_{\text{cathode}}(Ox|Red)_{IR}\) is the irreversible potential during cycling.

The Tafel curve calculation formula (2):

\[
\eta_{\text{cathode}} = \frac{RT}{zF} \ln j_0 - \frac{RT}{zF} \ln j_{\text{cathode}}
\]

where \(\eta_{\text{cathode}}\) is the overpotential of the cathode, \(j_0\) is the exchange current density, \(j_{\text{cathode}}\) is the current of the cathode. The equation can be written in a more concise form:

\[
\eta_{\text{cathode}} = a + b \ln j_{\text{cathode}}
\]

\[
b = -\frac{RT}{zF}
\]

where \(a\) is the intercept of Tafel curve, \(b\) is the slop of Tafel curve. Therefore, the equation (1) can be written in a more concise form:

\[
E_a = E_{a0} - \frac{RT}{b} \phi_{\text{cathode}}(Ox|Red)_{IR}
\]

Based on the intercept and slop of the Tafel curve as shown in Figure. 3b, c the
activation energy during the discharge and charge process can be calculated.

The activation energy corresponding to the reduction of $S_8$ to the long-chain Li$_2$S$_n$:

PP cells: $E_{a1} = E_{a1}^0 – 115.77$ kJ mol$^{-1}$

KB/V$_2$CT$_X$-PPcells: $E_{a1}' = E_{a1}^0 – 144.4$ kJ mol$^{-1}$

The difference in activation energy could be calculated by subtracting the activation energy of In-free electrode from that of In-based electrode.

$$E_{a1}' - E_{a1} = (E_{a1}^0 – 144.4) \text{ kJ mol}^{-1} – (E_{a1}^0 – 115.77) \text{ kJ mol}^{-1} = -28.63 \text{ kJ mol}^{-1}$$

The activation energy of long-chain Li$_2$S$_n$ to Li$_2$S:

PP cells: $E_{a2} = E_{a2}^0 – 112.32$ kJ mol$^{-1}$

KB/V$_2$CT$_X$-PP cells: $E_{a2}' = E_{a2}^0 – 137.14$ kJ mol$^{-1}$

$$E_{a2}' - E_{a2} = (E_{a2}^0 – 137.14) \text{ kJ mol}^{-1} – (E_{a2}^0 – 112.32) \text{ k J mol}^{-1} = -24.82 \text{ kJ mol}^{-1}$$

References


