Supporting Information

Conductive and Catalytic VTe$_2$@MgO Heterostructure as Effective Polysulfide Promotor for Lithium–Sulfur Batteries

Menglei Wang$^\dagger$, Yingze Song$^\dagger$, Zhongti Sun$^\dagger$, Yuanlong Shao$^2$, Chaohui Wei$^1$, Zhou Xia$^1$, Zhengnan Tian$^1$, Zhongfan Liu$^{1,3,4}$*, and Jingyu Sun$^{1,3}$*

$^1$College of Energy, Soochow Institute for Energy and Materials InnovationS (SIEMIS), Jiangsu Provincial Key Laboratory for Advanced Carbon Materials and Wearable Energy Technologies, Soochow University, Suzhou 215006, P. R. China
$^2$Physical Sciences and Engineering Division, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia
$^3$Beijing Graphene Institute (BGI), Beijing 100095, P. R. China
$^4$Center for Nanochemistry (CNC), Beijing Science and Engineering Center for Nanocarbons, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China

*Corresponding authors: sunjy86@suda.edu.cn (J. Y. Sun); zfliu@pku.edu.cn (Z. F. Liu).
$\dagger$These authors contributed equally to this work.
Supporting Figures

(a) Schematic set-up of CVD apparatus for the synthesis of $\text{VTe}_2@\text{MgO}$. (b) Experimental procedure for heating and cooling down the CVD furnace.

Figure S1
**Figure S2.** Digital photographs of VTe$_2$/MgO films obtained at different growth temperatures for carrying out conductivity measurements.
**Figure S3.** Photograph of a working light emitting diode connecting a VTe$_2$@MgO-based film, showing favorable conductivity of VTe$_2$@MgO material.
Figure S4. Survey XPS spectrum of VTe$_2$@MgO, indicating the co-existence of Mg, O, Te and V elements.
Figure S5. N$_2$ adsorption/desorption isotherm of VTe$_2$@MgO heterostructure.
Figure S6. CV curves of S/VTe$_2$@MgO (a), S/MgO (b) and bare S (c) cathodes under various scan rates.
Figure S7. Optimized structure of VTe$_2$ (011) surface with side (a) and top (b) view. V and Te atoms are in grey and orange colors, respectively. Mark ‘1’ and ‘2’ are the possible adsorption sites.
**Figure S8.** Possible adsorption configurations of Li atom on the VTe$_2$ (011) surface, namely, li-1 (a) and li-2 (b). V, Te, and Li atoms are in grey, orange and purple colors, respectively. li-1 model is the stable configuration with the adsorption energy of -3.45 eV, lower than li-2 with -2.71 eV.
Figure S9. Visualized adsorption tests of VTe$_2$@MgO and MgO (40 mg) with Li$_2$S$_4$ solution (3.5 mmol L$^{-1}$).
Figure S10. Potentiostatic discharge curves of Li$_2$S$_8$/tetralyme solution on CP-VTe$_2$@MgO and CP-MgO at 2.05 V.
Figure S11. Galvanostatic charge/discharge profiles of S/VTex@MgO and S/MgO cathodes at 0.5 C.
Figure S12. Galvonostatic charge/discharge profiles of S/MgO cathode at various current density from 0.2 to 3.0 C.
Figure S13. Cycling performance of S/VTe$_2$@MgO cathode at 2.0 C.
Figure S14. Cycling performances of VTe$_2$@MgO material at 0.2 C and 1.0 C.
Figure S15. (a) Photograph showing the cathodes from disassembled batteries after 500 cycles at 1.0 C by immersing in 4 mL DME solution for 2 h. (b) Photograph showing the separators from disassembled batteries after 200 cycles at 1.0 C.
Figure S16. SEM inspections of the cathodes from disassembled batteries before and after 200 cycles at 1.0 C.
Figure S17. Galvonostatic charge/discharge profiles of S/VTe$_2$@MgO cathode with the sulfur loading of 4.5 mg cm$^{-2}$ at 0.1 C.
Figure S18. Cycling performance of S/VTe$_2$@MgO cathode with the sulfur loadings of 6.9 mg cm$^{-2}$ (a) and 6.0 mg cm$^{-2}$ (b) at 0.1 C.
Figure S19. Nyquist plots of S/VTe$_2$@MgO cathodes with high sulfur loadings before cycle (a) and after 50 cycles (b).
Figure S20. Galvanostatic charge/discharge profiles of S/VTee@MgO cathode with the sulfur loading of 3.2 mg cm$^{-2}$ at different rates.
Figure S21. Cross-sectional SEM image and corresponding element maps of S/VTe₂@MgO cathode with the sulfur loading of 6.9 mg cm⁻².
Table S1. Comparison of battery performances based on sulfur hosts between this work and other reported studies.

<table>
<thead>
<tr>
<th>Host</th>
<th>Mass loading of S (mg cm(^{-2}))</th>
<th>S content (wt%)</th>
<th>Rate (C)</th>
<th>Cycles</th>
<th>Initial capacity (mAh g(^{-1}))</th>
<th>Capacity decay (% per cycle)</th>
<th>Ref.</th>
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<tbody>
<tr>
<td>VTe(_2)@MgO</td>
<td>1.4-1.6</td>
<td>60</td>
<td>1</td>
<td>1000</td>
<td>972</td>
<td>0.055</td>
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<tr>
<td></td>
<td>1.4-1.6</td>
<td>60</td>
<td>0.5</td>
<td>120</td>
<td>1006</td>
<td>0.13</td>
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<tr>
<td></td>
<td>1.4-1.6</td>
<td>60</td>
<td>0.2</td>
<td>50</td>
<td>1148</td>
<td>0.17</td>
<td></td>
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<tr>
<td></td>
<td>4.5</td>
<td>60</td>
<td>0.1</td>
<td>50</td>
<td>912</td>
<td>0.19</td>
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<td>TiO(_2)/G</td>
<td>3.5</td>
<td>61</td>
<td>0.2</td>
<td>100</td>
<td>~1030</td>
<td>0.44</td>
<td>1</td>
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<tr>
<td>TiC/G</td>
<td>3.5</td>
<td>61</td>
<td>0.2</td>
<td>100</td>
<td>1032</td>
<td>0.35</td>
<td>1</td>
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<td>Co-N-GC</td>
<td>2.0-2.5</td>
<td>49</td>
<td>0.2</td>
<td>100</td>
<td>1440</td>
<td>0.40</td>
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<td>G-V(_2)O(_3)</td>
<td>3.6</td>
<td>63</td>
<td>0.2</td>
<td>70</td>
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<td>0.26</td>
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<td>VS(_2)/G</td>
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<td>61</td>
<td>1</td>
<td>150</td>
<td>520</td>
<td>0.17</td>
<td>4</td>
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<td>PPy-MnO(_2)</td>
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<td>-</td>
<td>1</td>
<td>500</td>
<td>850</td>
<td>0.07</td>
<td>5</td>
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<td>SiO(_2)/TiO(_2)</td>
<td>1.6-2.0</td>
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<td>1</td>
<td>1000</td>
<td>793</td>
<td>0.067</td>
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<tr>
<td>CNTs/Co(_3)(_4)-NBs</td>
<td>1.2</td>
<td>56</td>
<td>2</td>
<td>500</td>
<td>858</td>
<td>0.07</td>
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<td>MoS(_2)</td>
<td>~1.5</td>
<td>60</td>
<td>0.5</td>
<td>100</td>
<td>1033</td>
<td>0.44</td>
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<tr>
<td>Co(_3)O(_4)</td>
<td>1.5-2.0</td>
<td>49</td>
<td>1</td>
<td>100</td>
<td>~1580</td>
<td>0.59</td>
<td>9</td>
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<tr>
<td>Co(_4)N</td>
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<td>49</td>
<td>1</td>
<td>100</td>
<td>~1640</td>
<td>0.39</td>
<td>9</td>
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Supporting References


