Supporting Information

Hierarchical Architecture of Metallic VTe$_2$/Ti$_3$C$_2$T$_x$ MXene Heterostructure for Supercapacitor Applications

Sree Raj K A, ¹ Narad Barman,² Sithara Radhakrishnan,¹ Ranjit Thapa,² and Chandra Sekhar Rout*,¹

¹ Centre for Nano and Material Science, Jain University, Jain global campus, Jakkasandra, Ramanagaram, Bangalore - 562112, India.

² Department of Physics, SRM University – AP, Amaravati 522 240, Andhra Pradesh, India.

*Corresponding author: csrou@gmail.com, r.chandrasekhar@jainuniversity.ac.in (CSR);

Electrochemical Calculations

Three electrode configuration-

**Specific capacitance (C$_{sp}$) from cyclic voltammetry:**

\[
C_{sp} = \frac{\text{Area of CV curve}}{2 \times m \times \theta \times \Delta V}
\]  
(S1)

Where, \(m\) is the mass of active material, \(\nu\) is the scan rate and \(\Delta V\) is the potential window.

**Specific capacitance (C$_{sp}$) from galvanostatic charge discharge:**

\[
C_{sp} = \frac{i \times \Delta t}{m \times \Delta V}
\]  
(S2)

Where, \(i\) is the applied current, \(\Delta t\) is the discharge time.

**Charge balance equation:**¹

\[
\frac{m_+}{m_-} = \frac{C_- \times \Delta V_-}{C_+ \times \Delta V_+}
\]  
(S3)

**Specific capacitance (C$_{sp}$) of ASC from galvanostatic charge discharge:**

\[
C_{sp} = \frac{i \times \Delta t}{m \times \Delta V}
\]  
(S4)
Energy density of ASC;

\[ E_D = \frac{1}{2}CV^2 \]  

(S5)

Where, C is specific capacitance of ASC, V is the working window of ASC.

Power density of ASC;

\[ P_D = \frac{E_D}{\Delta t} \]  

(S6)

Supporting Figures

Figure S1: Low (a) and high (b) resolution FESEM images of etched MXene showing the accordion like morphology.
Figure S2: EDS element mapping of VTX80 sample showing the uniform distribution of V, Te, Ti, and C.
**Figure S3**: (a) TEM image of VTX 80, (b, c) HRTEM images of VTX 80 showing lattice fringes of (004) plane of Ti$_3$C$_2$ MXene and (002) plane of VTe$_2$ and (d) corresponding SAED pattern.
Figure S4: XPS survey spectrum of VTX80 showing the presence of V 2p, Te 3d, C 1s and Ti 2p species.
Figure S5: Cyclic voltammograms of (a) VTe₂, (b) VTX40, (c) VTX120 in varying scan rates, GCD curves of (d) VTe₂, (e) VTX40 and (f) VTX120 in different specific currents ranging from 0.25 to 4 A/g.

Figure S6: (a) Cyclic voltammogram and (b) GCD profile of MXene.
Figure S7: Comparison of the CV curves of VTX80 electrode in 0.5M K₂SO₄ and 0.5M KCl (analysed using a conventional glassy carbo electrode).
**Figure S8:** (a) Comparative CV profile of VTe$_2$, MXene and VTX80 at 100 mV/s, (b) Cyclic stability of VTe$_2$, MXene and VTX80. VTe$_2$ and MXene have a cyclic stability of 71.3% and 66.6% respectively, VTX80 on the other hand showed an improved cyclic stability of 83.3%.

<table>
<thead>
<tr>
<th>Scan Rate (mV/s)</th>
<th>Capacitive Contribution (%)</th>
<th>Diffusive Contribution (%)</th>
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<tbody>
<tr>
<td>10</td>
<td>81.8</td>
<td>18.2</td>
</tr>
<tr>
<td>20</td>
<td>82.9</td>
<td>17.1</td>
</tr>
<tr>
<td>40</td>
<td>83.6</td>
<td>16.4</td>
</tr>
<tr>
<td>60</td>
<td>85.8</td>
<td>14.2</td>
</tr>
<tr>
<td>80</td>
<td>89.2</td>
<td>10.8</td>
</tr>
<tr>
<td>100</td>
<td>90.1</td>
<td>9.9</td>
</tr>
<tr>
<td>200</td>
<td>97.2</td>
<td>2.8</td>
</tr>
</tbody>
</table>

**Table S1:** The segregated capacitive and diffusive contributions obtained by deconvoluting CV using Dunn method.

**Figure S9:** (a-b) Trasatti plots.
<table>
<thead>
<tr>
<th>Sample</th>
<th>$R_s$ ($\Omega$)</th>
<th>$R_{ct}$ ($\Omega$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>VTe$_2$</td>
<td>8.07</td>
<td>9.43</td>
</tr>
<tr>
<td>VTX40</td>
<td>5.5</td>
<td>18.51</td>
</tr>
<tr>
<td>VTX80</td>
<td>2.62</td>
<td>5.48</td>
</tr>
<tr>
<td>VTX120</td>
<td>5.11</td>
<td>9.44</td>
</tr>
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</table>

**Table S2**: The $R_s$ and $R_{ct}$ values of all the samples obtained from Nyquist plot.

**Figure S10**: Characterization of VTX80 electrode after electrochemical analysis. (a) XRD pattern of VTX80 electrode before and after. A notable peak $\sim31^\circ$ which can be assigned to the (101) plane of VTe (JCPDS: 89-7104). XRD pattern of VTX80 electrode shows sharp intense doublet of Ni foam which has been used as the current collector.² (a) low and (b) high resolution FESEM images of VTX80 electrode after the electrochemical analysis. The 3D interconnected structure of VTe$_2$ and MXene is intact after the electrochemical analyses.
Figure S11: Plot of total density of states of VTe$_2$ bulk.

(a) VTe$_2$/FG-MXene

(b) Density of States D(E)

(c) Quantum Capacitance (µF/cm$^2$) vs. Electrode Potential (eV)
Figure S12: (a) Optimized structure of VT$_2$/FG-MXene, (b) total DOS for the proposed model heterostructure and (c) Variation of quantum capacitance against applied electrode potential. Blue, green and pink spheres denote the oxygen, hydrogen and fluorine atoms respectively.

Figure S13: Characterization of the synthesized MoS$_2$/MXene heterostructure used as the negative electrode. (a) The XRD pattern of MoS$_2$/MXene heterostructure showed XRD reflections corresponds to the JCPDS card 37-1492 of MoS$_2$. The (002) peak of Ti$_3$C$_2$ MXene has shifted from 8.8° to 6.4° indicating an increment in the interlayer spacing for the heterostructure similar to VT$_2$/MXene heterostructure. The presence of TiO$_2$ is observed in the heterostructure is due to the surface oxidation of MXene. (b, c) FESEM images of MoS$_2$/MXene reveals a 3D interconnected heterostructure similar to VT$_2$/MXene. It clear from the FESEM images that MXene is acting as the growth template for the growth of MoS$_2$ nanosheets.
Figure S14: Three electrode measurements of MoS$_2$/MXene heterostructure (a) cyclic voltammogram of MoS$_2$/MXene performed in a potential window of -0.2 - -1.0 V in different scan rates and (b) GCD curves of MoS$_2$/MXene in varying specific currents.

Figure S15: (a) Specific capacitance vs specific current plot of the ASC and (b) Nyquist plot of the ASC.

References


