Supporting Information

Li$_3$Cr(MoO$_4$)$_3$: A NASICON-type High Specific Capacity Cathode Material for Lithium Ion Batteries†

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The diffusion coefficient of Li ions (D) is calculated according to the following Eq. (1) and Eq. (2)

\[
D = \frac{R^2 T^2}{2 A n^4 F^4 C^2 \sigma^2}
\]  \hspace{1cm} (1)

\[
Z' = R_s + R_{ct} + \sigma \omega^{-1/2}
\]  \hspace{1cm} (2)

where \( R \) is the gas constant, \( T \) is the absolute temperature, \( A \) is the surface area of the cathode, \( n \) is the number of electrons per molecule during oxidization, \( F \) is the Faraday constant, \( C \) is the concentration of lithium-ion, \( \sigma \) is the Warburg factor which has a relationship with \( Z' \) as shown in Eq. (2), \( R_s \) is the resistance between the electrolyte and electrode, \( R_{ct} \) is the charge transfer resistance, and \( \omega \) is angle frequency.

**Table S1** Kinetic parameters of \( \text{Li}_3\text{Cr(MoO}_4\text{)}_3\text{@C.} \)

<table>
<thead>
<tr>
<th>Sample</th>
<th>( R_{ct} ) (Ω)</th>
<th>( \sigma )</th>
<th>( D_{\text{Li}^+} )(cm(^2)s(^{-1}))/EIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Li}_3\text{Cr(MoO}_4\text{)}_3\text{@C} )</td>
<td>45</td>
<td>53</td>
<td>( 3.0 \times 10^{-17} )</td>
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\( R_{ct} \): charge transfer resistance. \( \sigma \): Warburg factor. \( D_{\text{Li}^+} \): diffusion coefficient of Li\(^+\) ion.
Figure S1 (a) Crystal Structure and (b) BVS-DMs of Li₃Cr(MoO₄)₃.