Oxygen redox activity through a reductive coupling mechanism in the P3-type nickel-doped sodium manganese oxide


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Table S1. Rietveld refinement results for as-synthesized Na$_{0.67}$Ni$_{0.2}$Mn$_{0.8}$O$_2$

<table>
<thead>
<tr>
<th>atom</th>
<th>Wyckoff symbol</th>
<th>x/a</th>
<th>y/b</th>
<th>z/c</th>
<th>Occupancy</th>
<th>Biso</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn1/Ni1</td>
<td>3a</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.825/0.175(3)</td>
<td>0.3(2)</td>
</tr>
<tr>
<td>Na1</td>
<td>3a</td>
<td>0</td>
<td>0</td>
<td>0.167(2)</td>
<td>0.51(5)</td>
<td>4.6(7)</td>
</tr>
<tr>
<td>O1</td>
<td>3a</td>
<td>0</td>
<td>0</td>
<td>0.4004(13)</td>
<td>1</td>
<td>0.86(12)</td>
</tr>
<tr>
<td>O2</td>
<td>3a</td>
<td>0</td>
<td>0</td>
<td>0.6141(13)</td>
<td>1</td>
<td>1.5(2)</td>
</tr>
</tbody>
</table>

Space group $R3m$ $a = 2.8650(1)$ Å $c = 16.8159(16)$ Å

Figure S1. PND patterns for Na$_{0.67}$Ni$_{0.2}$Mn$_{0.8}$O$_2$ extracted at different states of charge.
Figure S2. Voltammetric analysis of Na$_{0.67}$Ni$_{0.2}$Mn$_{0.8}$O$_2$ at a scan rate of 30 µV s$^{-1}$.

Figure S3. Variation of Mn oxidation state, calculated from the position of the centroid of the pre-edge for Na$_{0.67}$Ni$_{0.2}$Mn$_{0.8}$O$_2$ extracted at different states of charge.
Figure S4. O K-edge SXAS spectra recorded in TEY mode for Na$_{0.67}$Ni$_{0.2}$Mn$_{0.8}$O$_2$ extracted at different states of charge.
Figure S5. Complete overview of O K-edge RIXS spectra of Na_{0.67}Ni_{0.2}Mn_{0.8}O_2 extracted at different states of charge.