Supporting Information

First-principles and experimental study of nitrogen/sulfur co-doped carbon nanosheets as anode for rechargeable sodium ion batteries

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Figure S1. (a) The configuration and corresponding density of states (DOS) of graphene. (b) Na adsorption and the corresponding deformation charge density (DCD) map of graphene. The Fermi level ($E_F$) is defined at zero with the dot line.
Figure S2. (a, b) SEM images of GT10.
Figure S3. (a, b) TEM images, (c) HRTEM image and (d) SAED pattern of the as-prepared GT12.
Figure S4. (a, b) TEM images, (c) HRTEM image and (d) SAED pattern of the as-prepared GT15.
Figure S5. (a, b) TEM images, (c) HRTEM image and (d) SAED pattern of the as-prepared GT120.
**Figure S6.** Nitrogen adsorption-desorption isotherm of the four samples.
Figure S7. Top and side views of Divacancy 5-8-5 and Stone-Wales 5577 graphene models: (a, b) the pure, (a', b') S doped and (a'', b'') N, S co-doped graphene. The highlight of 5-8-5 and 5577 is marked with red color.
**Figure S8.** The survey XPS spectra for (a) GT12, (b) GT15, (c) GT110 and (d) GT120, respectively.
Figure S9. Rate performance of GT10 in the potential range of 0.0–3.0 V.
Figure S10. Cyclic voltammograms curves in the potential range of 0.0–3.0 V vs. Na+/Na at a scan rate of 0.2 mV s⁻¹, and galvanostatic charge-discharge profiles at 0.2 A g⁻¹ for (a, b) GT12, (c, d) GT15, and (e, f) GT120, respectively.
Figure S11. Ex-situ XRD patterns of GT110 fresh electrode and discharged electrode after one and a half cycles.
Table S1. EDS Elemental Analysis (wt.%)

<table>
<thead>
<tr>
<th>Samples</th>
<th>N (wt %)</th>
<th>S (wt %)</th>
<th>O (wt %)</th>
<th>C (wt %)</th>
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<tr>
<td>GT12</td>
<td>27.7</td>
<td>3.9</td>
<td>5.7</td>
<td>62.7</td>
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<tr>
<td>GT15</td>
<td>35.28</td>
<td>0.95</td>
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<td>GT110</td>
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<td>0.75</td>
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<tr>
<td>GT120</td>
<td>34.94</td>
<td>0.77</td>
<td>10.53</td>
<td>53.76</td>
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