Supporting Information

Porous Graphdiyne Applied for Sodium Ion Storage

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Fig. S1 (a) The structural representation of a GDY sheet, (b) Typical Raman spectrum of GDY, (c) Survey and (d) C 1s binding energy profiles of GDY.

Raman spectra of bulk GDY (Figure S1b) exhibit two prominent peaks at about 1367.4 cm$^{-1}$ and 1567.5 cm$^{-1}$, corresponding to the typical D band and G band for carbon materials. The intensity of the D band is strongly associated with structural defects, including disordered carbon atoms and edges; the G band corresponds to first-order scattering of the E$_{2g}$ stretching vibration mode observed for $sp^2$-hybridized carbon atom domains in aromatic rings. Generally, the intensity ratio of D band and G band ($I_D/I_G$) is used to estimate the disorder and defects of GDY. The $I_D/I_G$ of GDY was 0.71, suggesting bulk GDY powders possess high order and low content of defects. The peaks at 1921.1 and 2171.8 cm$^{-1}$ were contributed by the vibration of acetylenic linkages (–C≡C–C≡C–). As shown in Figure S1c, the survey scan spectra displayed a pronounced XPS C 1s peak at 284.8 eV, and a weaker O 1s peak at 531.6 eV. The presence of a signal for O 1s arose from the adsorption of O$_2$ when GDY was exposed to air. After subtraction of the Shirley background, followed by fitting with a mixture function of Lorentzian and Gaussian, the C 1s peak (Figure S1d) could be divided into four mainly sub-peaks at 284.5, 285.1, 286.7, and 288.3 eV, which could be assigned to orbitals in C–C ($sp^2$), C≡C (sp), C–O, and C=O bonds, respectively. The area ratio of the $sp$- and $sp^2$-hybridized carbon atoms was 2, which confirmed the structure of GDY comprising benzene rings linked together through two acetylenic linkages.
Table S1. Overview of different types of carbon as anodes for sodium ion batteries.

<table>
<thead>
<tr>
<th>Type of Carbon</th>
<th>Potential Range (V vs Na⁺/Na)</th>
<th>Current Densities (mA g⁻¹)</th>
<th>Capacities (mAh g⁻¹)</th>
<th>Surface Area (m² g⁻¹)</th>
<th>Additional Information</th>
<th>Citation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hard carbon</td>
<td>0-3</td>
<td>30</td>
<td>290</td>
<td></td>
<td>100 cycles with 93% of capacity retention at 50 mA g⁻¹ for first 10 cycles and then 100 mA g⁻¹ for next 100 cycles, a reversible capacity of 160 mAh g⁻¹ is stably obtained.</td>
<td>10</td>
</tr>
<tr>
<td>Hollow carbon nanospheres</td>
<td>0-3</td>
<td>50</td>
<td>223</td>
<td>410</td>
<td>82.2% capacity retention over 400 cycles at 50 mA g⁻¹, a reversible capacity of 149 mAh g⁻¹ at 500 mA g⁻¹.</td>
<td>11</td>
</tr>
<tr>
<td>Hollow carbon nanowires</td>
<td>0.01-1.2</td>
<td>50</td>
<td>251</td>
<td>34.1</td>
<td>a reversible capacity of 72 mA h g⁻¹ at 10 A g⁻¹</td>
<td>12</td>
</tr>
<tr>
<td>N-doped porous carbon fibres</td>
<td>0-3</td>
<td>50</td>
<td>296</td>
<td>372.4</td>
<td></td>
<td>13</td>
</tr>
<tr>
<td>Graphite</td>
<td>-0.5-2</td>
<td>37.2</td>
<td>close to 100</td>
<td></td>
<td>1000 cycles with coulombic efficiencies&gt;99.87%</td>
<td>15</td>
</tr>
<tr>
<td>Expanded graphite</td>
<td>0-2</td>
<td>20</td>
<td>284</td>
<td></td>
<td>maintain a capacity of 184 mAh g⁻¹ at 100 mA g⁻¹, retain 73.92% of its capacity after 2000 cycles</td>
<td>17</td>
</tr>
<tr>
<td>Reduced graphene oxide</td>
<td>0.01-2</td>
<td>40</td>
<td>174.3</td>
<td>330.9</td>
<td>a high capacity of 141 mAh g⁻¹ at 40 mA g⁻¹ over 1000 cycles</td>
<td>18</td>
</tr>
<tr>
<td>Carbon black</td>
<td>0-1.5</td>
<td>4.96</td>
<td>~130</td>
<td>22.1</td>
<td>a reversible of capacity of 261 mAh g⁻¹ after 300 cycles at 50 mA g⁻¹, an excellent capacity retention of 98.2 % after 1000 cycles at 100 mA g⁻¹</td>
<td>This work</td>
</tr>
</tbody>
</table>

The citations in this Table are related to the references in the main article.
Fig. S2 UV-Vis spectrum of porous GDY. And plots of $(Ahv)^2$ versus photon energy ($hv$).

Fig. S3 I–V curve of porous GDY.
Fig. S4 Rate performance of super P in a sodium half-cell.

Fig. S5 (a, c) SEM images and (b, d and e) TEM images of porous GDY before and after cycles.
References