Unraveling the water-mediated proton conduction mechanism along the surface of graphene oxide

Supporting Information

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Figure S1 Atomic structure of single cell graphene used to construct the GO sheets.

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Figure S2. Preparation protocol of the atomic structure of GO covered by epoxide functional groups
Figure S3. Preparation protocol of the atomic structure of GO covered by hydroxyl functional groups

Figure S4 Water density distribution as a function of distance to graphene sheet in S3
different water weight ratio conditions

Figure S5 Averaged water density distribution as a function of distance to E10, E20 and E30 GO sheets in different water weight ratio conditions

Figure S6 Averaged water density distribution as a function of distance to H10, H20 and H30 GO sheets in different water weight ratio conditions
Figure S7 Spatial distribution of adsorbed water on E10 GO sheet in different water weight ratio conditions

Figure S8 Spatial distribution of adsorbed water on E20 GO sheet in different water weight ratio conditions
Figure S9 Spatial distribution of adsorbed water on E30 GO sheet in different water weight ratio conditions

Figure S10 Spatial distribution of adsorbed water on H10 GO sheet in different water weight ratio conditions
Figure S11 Spatial distribution of adsorbed water on H20 GO sheet in different water weight ratio conditions

Figure S12 Spatial distribution of adsorbed water on H30 GO sheet in different water weight ratio conditions
Figure S13 Convergence test of energy profiles for proton conduction between adjacent epoxide functional groups

Figure S14 Convergence test of energy profiles for proton conduction between epoxide functional group and adsorbed water molecule

Figure S15 Convergence test of energy profiles for proton conduction between adjacent
hydroxyl functional groups

Figure S16 Convergence test of energy profiles for proton conduction between hydroxyl functional group and adsorbed water molecule.

Table S1 The estimated corresponding relationship between water weight ratio (H₂O/GO) and relative humidity at T = 298 ± 5 K [S1]

<table>
<thead>
<tr>
<th>Water weight ratio</th>
<th>10%</th>
<th>20%</th>
<th>30%</th>
<th>40%</th>
<th>50%</th>
</tr>
</thead>
<tbody>
<tr>
<td>RH</td>
<td>&lt;0.11</td>
<td>0.30–0.58</td>
<td>0.75–0.93</td>
<td>0.93–0.97</td>
<td>&gt;0.97</td>
</tr>
</tbody>
</table>

Reference