Supporting Information

Controlling of the Electronic Properties of WS$_2$ by Graphene Oxide

Substrate from First-principles calculations

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Table S1. Band gaps of pristine WS$_2$ and some GO/WS$_2$ heterostructures with and without considering SOC effect.

<table>
<thead>
<tr>
<th>Band Gap/eV</th>
<th>WS$_2$</th>
<th>WS$_2$/GO-h$_2$e (8%)</th>
<th>WS$_2$/GO-h$_2$e (40%)</th>
<th>WS$_2$/GO-h$_2$e (56%)</th>
<th>WS$_2$/GO-h$_2$e (80%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBE</td>
<td>1.92</td>
<td>0.32</td>
<td>1.29</td>
<td>1.72</td>
<td>1.91</td>
</tr>
<tr>
<td>PBE+SOC</td>
<td>1.58</td>
<td>0.33</td>
<td>1.15</td>
<td>1.48</td>
<td>1.57</td>
</tr>
</tbody>
</table>

Fig. S1. Different stacking patterns and the binding energies per WS$_2$ unit of graphene and WS$_2$ hybrids.
Fig. S2. Binding energies of WS$_2$ and GO with epoxy distributed on single side and on both sides heterostructures.

Fig. S3. The distances between S atoms in WS$_2$ and O atoms in GO as the function of oxygen concentration.
Fig. S4. Band gaps of the free-standing graphene oxide as the oxygen concentration increasing.

Fig. S5. Optimized Structures of GO and WS$_2$ heterostructures. (a) to (d) are the structures of e-GO/WS$_2$ (h$_2$-GO/WS$_2$) at the first peak, the peak valley and the second peak of the band gaps. Their oxygen concentrations are 0.28 (0.32), 0.48 (0.52) and 0.72 (0.72), respectively. (g) to (i) are the heterostructures with the same oxygen concentration of 0.48 but with different hydroxyl to epoxy ratios of 1:1, 2:1 and 4:1, respectively.