Supplementary Information

Efficient Hydrogen Generation from Water using Nanocomposite flakes based on Graphene and Magnesium.

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Supplementary Note 1: S1 Sketch of Deposition of Mg on G by plasma sputtering

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Supplementary Note S10 Energy density of Mg/G and other technologies to store the energy

S1 Sketch of Deposition of Mg on G by plasma sputtering
S2 Hydrogen generation using Mg/Gr exposed to Nitrogen and Air

![Graph showing hydrogen generation over time with different glove bag gases](image-url)
S3 SEM and EDX

The EDX analysis of Mg/G (30 min deposition). The peak of magnesium reveals that the primary material present on the surface of G is magnesium. Carbon peak is the signal due to the G substrate; we detected carbon because the scanning depth of EDX is quite high (> 1 micron) and because the Mg surface is not entirely uniform.
S4 XRD spectra of Mg/G after the reaction with water

X-Ray diffraction pattern of sample holder [a], Graphene/Magnesium samples [b] and subtraction curve [c]
S5 Survey XPS spectra, and Atomic concentration of Mg C and O on Mg/G before and after the immersion in water by XPS
Table 1. The surface chemical composition of Mg/G (60 min) as determined by XPS analysis before and after the reaction of Mg/G with water.

<table>
<thead>
<tr>
<th></th>
<th>Binding Energy eV</th>
<th>At% as-prepared</th>
<th>At% After reaction With Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1s</td>
<td>73.84</td>
<td>61.37</td>
<td></td>
</tr>
<tr>
<td>C-C</td>
<td>284.35</td>
<td>60.44</td>
<td>47.9</td>
</tr>
<tr>
<td>C-O C-OH</td>
<td>286.3</td>
<td>8.75</td>
<td>5.77</td>
</tr>
<tr>
<td>C=O</td>
<td>288.08</td>
<td>1.95</td>
<td>2.49</td>
</tr>
<tr>
<td>π-π*</td>
<td>290.54</td>
<td>5.7</td>
<td>5.21</td>
</tr>
<tr>
<td>O1s</td>
<td>17.61</td>
<td>29.24</td>
<td></td>
</tr>
<tr>
<td>Mg(OH)₂</td>
<td>530.92</td>
<td>6.86</td>
<td>9.38</td>
</tr>
<tr>
<td>CO-Mg(O)</td>
<td>532.34</td>
<td>9.08</td>
<td>13.59</td>
</tr>
<tr>
<td>H₂O</td>
<td>534.19</td>
<td>1.68</td>
<td>6.26</td>
</tr>
<tr>
<td>Mg2p</td>
<td>8.54</td>
<td>9.39</td>
<td></td>
</tr>
<tr>
<td>Mg(OH)₂</td>
<td>50.1</td>
<td>4.38</td>
<td>4.35</td>
</tr>
<tr>
<td>Mg(O)</td>
<td>51.5</td>
<td>3.35</td>
<td>4.60</td>
</tr>
<tr>
<td>-</td>
<td>52.11</td>
<td>0.82</td>
<td>0.44</td>
</tr>
</tbody>
</table>
S6: Video of the H₂ bubbles produced by Mg/G in water

bubble hydrogen generation.avi

S7: Video of H₂ generation and energy production using a Fuel cell

S7 EES (2).avi
S8 Spectra of Air lab as determined by PTRMS
S9 Energy density calculations:

\[ \text{Mg} + 2\text{H}_2\text{O} \rightarrow \text{Mg(OH)}_2 + \text{H}_2 \]
\[ \Delta H_f = -354 \text{ kJ mol}^{-1} \]

The reaction needs for 1 mole H\(_2\) 2 mole of water and produce hydrogen gas and heat

A) Hydrogen production evaluation:

Mass of powder Mg Graphene

\[ m_{\text{powder}} = 0.001 \text{ g} \]

H\(_2\) Gravimetric storage density

\[ \rho_{\text{g/g}} = 3\% \]

Hydrogen evolution from powder

\[ m_{\text{H}_2} = m_{\text{powder}} \times \rho_{\text{g/g}} = 3 \times 10^{-5} \text{ g} \]

Energy Balance:

\[ \text{LHV}_{\text{H}_2} = 119 \text{ kJ/g} \]

Chemical energy in produced hydrogen:

\[ E_{\text{H}_2} = \text{LHV}_{\text{H}_2} \times m_{\text{H}_2} = 3.57 \text{ J} \]

For a energy density based on powder of:

\[ E_{\text{H}_2,\text{powder}} = \frac{E_{\text{H}_2}}{m_{\text{powder}}} = 3.57 \text{ kJ/g} \]

B) Heat production by Gr+Mg powder and water reaction
Based on the number of Mg moles reacted:

\[ \text{Mg} + \text{H}_2\text{O} \rightarrow \text{Mg(OH)}_2 + \text{H}_2 \]

\[ n_{\text{H}_2} = n_{\text{Mg}} \]

So, considering the previous H2 production, \( m_{\text{H}_2} \),

\[ n_{\text{Mg}} = n_{\text{H}_2} = \frac{m_{\text{H}_2}}{\text{PM}_{\text{H}_2}} = 1.5 \times 10^{-5} \text{ moles} \]

Considering, Enthalpy of Mg and water reaction equals to \( \Delta H = 354 \text{ kJ/moles} \), it is possible to evaluate total heat released by chemical reaction of Hydrogen production,

\[ E_{\text{heat}} = n_{\text{Mg}} \times \Delta H = 5.31 \text{ j} \]

So, from previous calculation it is possible to resume total output energy of reaction between Mg(Graphene) powder and water for a unit of mass:

\[ E_{\text{heat powder}} = \frac{E_{\text{heat}}}{m_{\text{powder}}} = 5.31 \text{ kJ/g} \]

With a total energy balance of:

\[ E_{\text{tot}} = E_{\text{heat powder}} + E_{\text{H}_2\text{powder}} = 3.51 \text{ kJ} + 5.31 \text{ KJ} = 8.81 \text{ KJ/gr} \]

C) Estimation of water consumption

The Stoichiometric quantity of consumed water by reaction is:

\[ n_{\text{H}_2\text{O}} = 2 \times n_{\text{H}_2} = 3.2 \times 10^{-5} \text{ moles} \]

For a mass of:

\[ m_{\text{H}_2\text{O}} = n_{\text{H}_2\text{O}} \times \text{PM}_{\text{H}_2\text{O}} = 54.045 \times 10^{-5} \text{ g} \]

And a total consumption for mass unit of powder of,

\[ m_{\text{H}_2\text{O powder}} = \frac{m_{\text{H}_2\text{O}}}{m_{\text{powder}}} = 0.57 \text{ g}_{\text{H}_2\text{O/gpowder}} \]

Finally, considering also the water amount in the total energy balance, the density of energy from the powder (Mg+graphene) and water system is:

\[ m_{\text{tot}} = m_{\text{H}_2\text{O powder}} + m_{\text{powder}} = 1.57 \text{ g} \]
for an energy density of,

\[ \rho_{\text{Energy tot}} = \frac{E_{\text{tot}}}{m_{\text{tot}}} = 5.61 \text{ kJ/g} \]

Or considering only chemical energy released as H\(_2\) gas,

\[ \rho_{\text{H2 tot}} = \frac{E_{\text{heat powder}}}{m_{\text{tot}}} = 2.23 \text{ kJ/g} \]

**S10 Energy density of Mg/G and other technologies to store the energy**

<table>
<thead>
<tr>
<th>Energy density</th>
<th>kJ/gr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressed Hydrogen (700 atm)</td>
<td>150</td>
</tr>
<tr>
<td>Mg/Gr theoretical</td>
<td>14</td>
</tr>
<tr>
<td>Mg/Gr (this work)</td>
<td>3.5 (H(_2)) + 5.3 (Heat)</td>
</tr>
<tr>
<td>Lithium battery</td>
<td>1-2</td>
</tr>
<tr>
<td>Fly wheel</td>
<td>1</td>
</tr>
<tr>
<td>Ni-Cd</td>
<td>1</td>
</tr>
<tr>
<td>Lead acid battery</td>
<td>0.18</td>
</tr>
</tbody>
</table>