Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Information

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

Bartali R.[1*], Speranza G.[1], K.F.Aguey-Zinsou[2], Testi M.[1], Micheli V.[1], Canteri R.[1], Fedrizzi M.[1], Gottardi G.[1], Coser G.[1], Crema L.[1], Pucker G.[1], Setijani E.[1,2], and Laidani N[1].

1) *Fondazione Bruno Kessler, Center Materials and Microsystems Via Sommarive 18, 38100 Italy.*

2) MERLin, School of Chemical Engineering, The University of New South Wales, Sydney, Australia

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

Supplementary Note 2: S2 Hydrogen generation using Mg/G exposed to Nitrogen and Air

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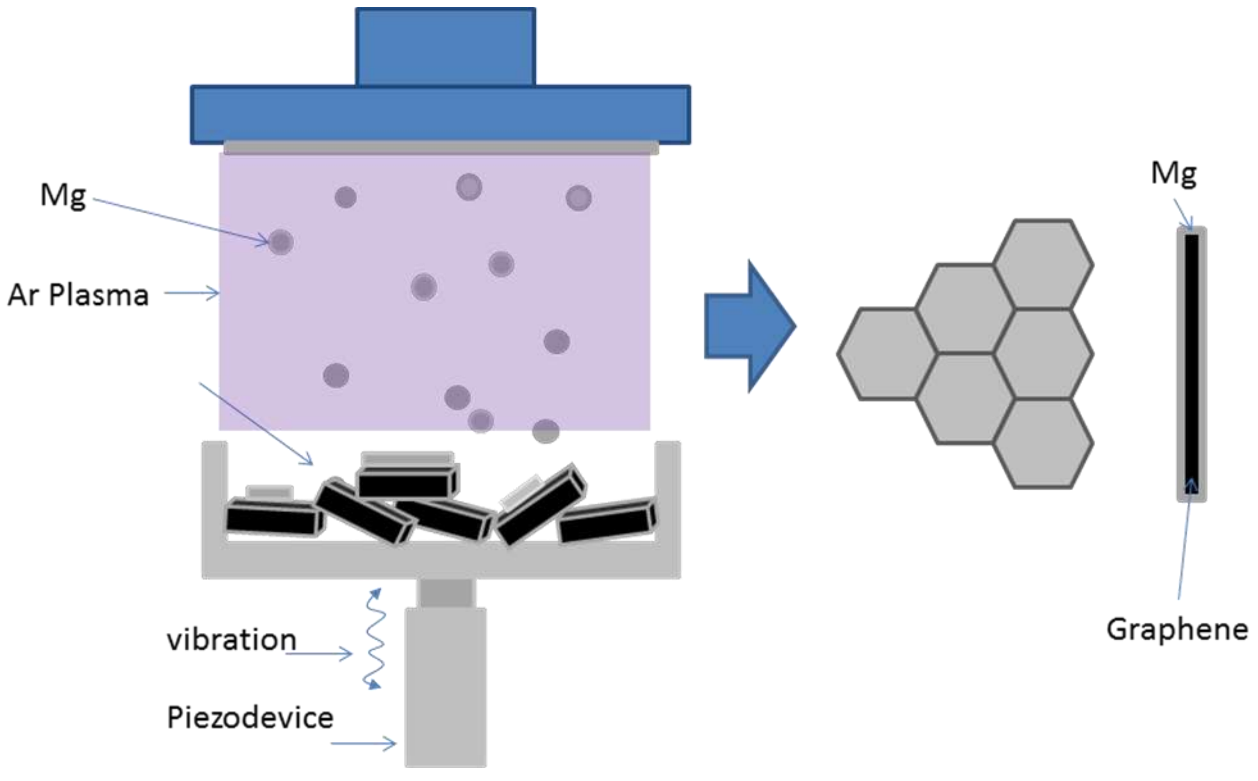
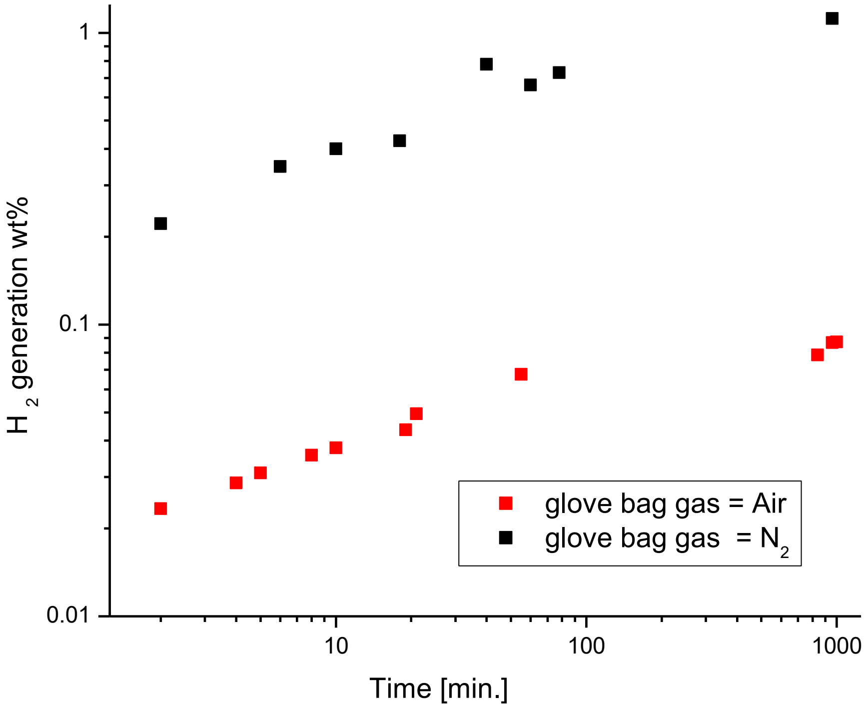
Supplementary Note S10 Energy density of Mg/G and other technologies to store the energy

S1 Sketch of Deposition of Mg on G by plasma sputtering

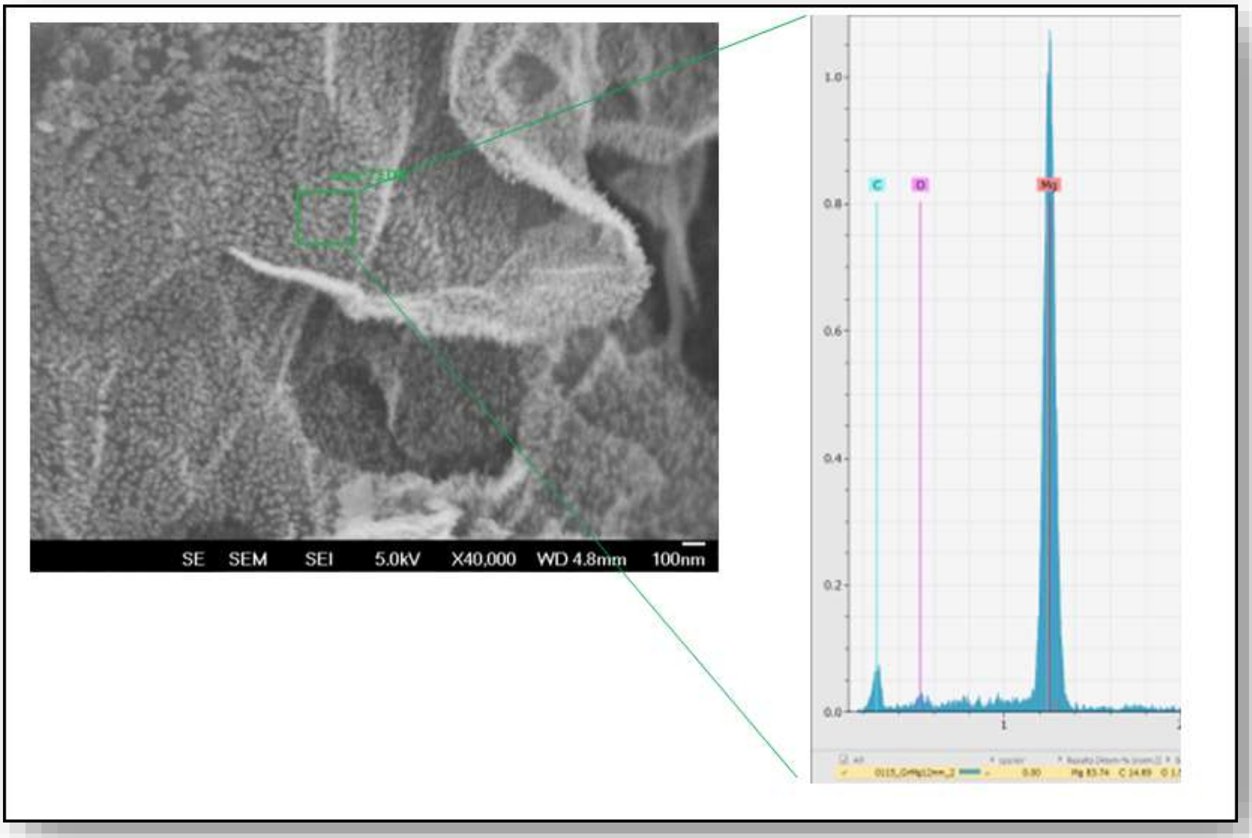


S2 Hydrogen generation using Mg/Gr exposed to Nitrogen and Air

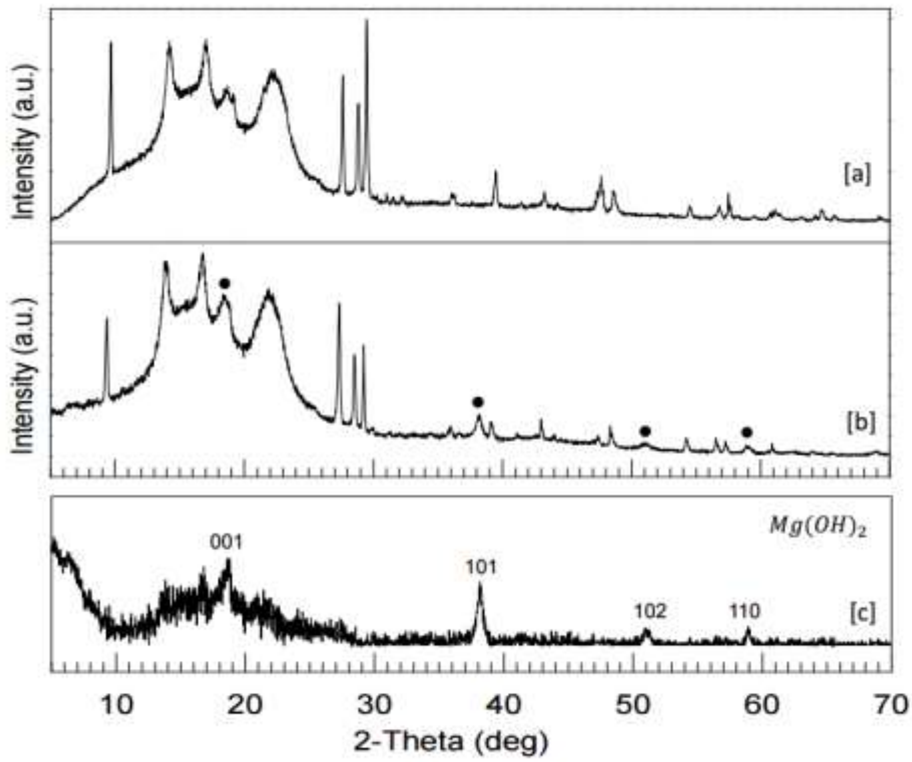


S3 SEM and EDX

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

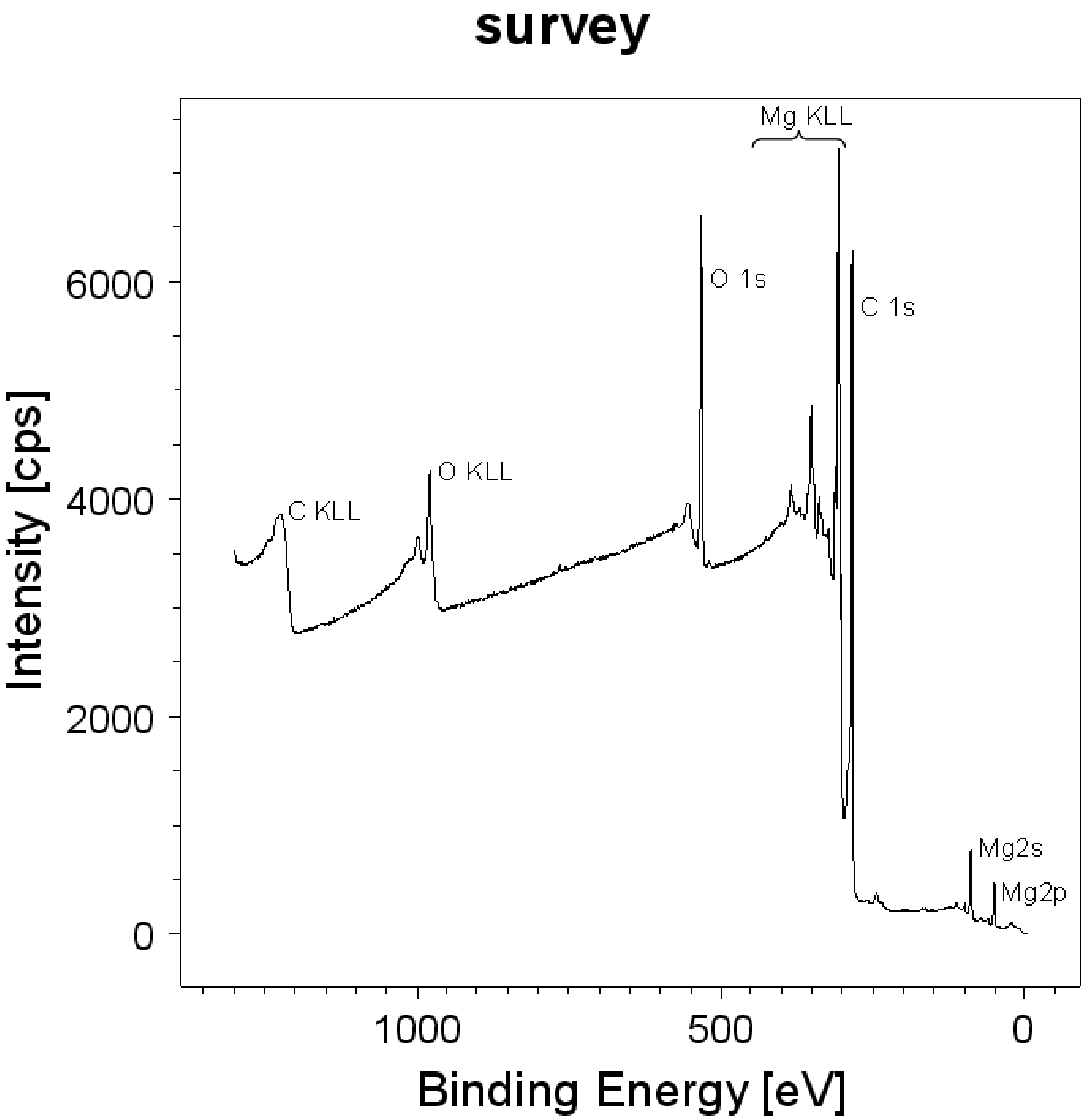


Table 1. The surface chemical composition of Mg/G (60 min) as determined by XPS analysis before and after the reaction of Mg/G with water.

	Binding Energy eV	At% as-prepared	At% After reaction With Water
C1s		73.84	61.37
C-C	284.35	60.44	47.9
C-O C-OH	286.3	8.75	5.77
C=O	288.08	1.95	2.49
π-π*	290.54	5.7	5.21
O1s		17.61	29.24
$Mg(OH)_2$	530.92	6.86	9.38
CO-Mg(O)	532.34	9.08	13.59
H_2O	534.19	1.68	6.26
Mg2p		8.54	9.39
$Mg(OH)_2$	50.1	4.38	4.35
Mg(O)	51.5	3.35	4.60
-	52.11	0.82	0.44

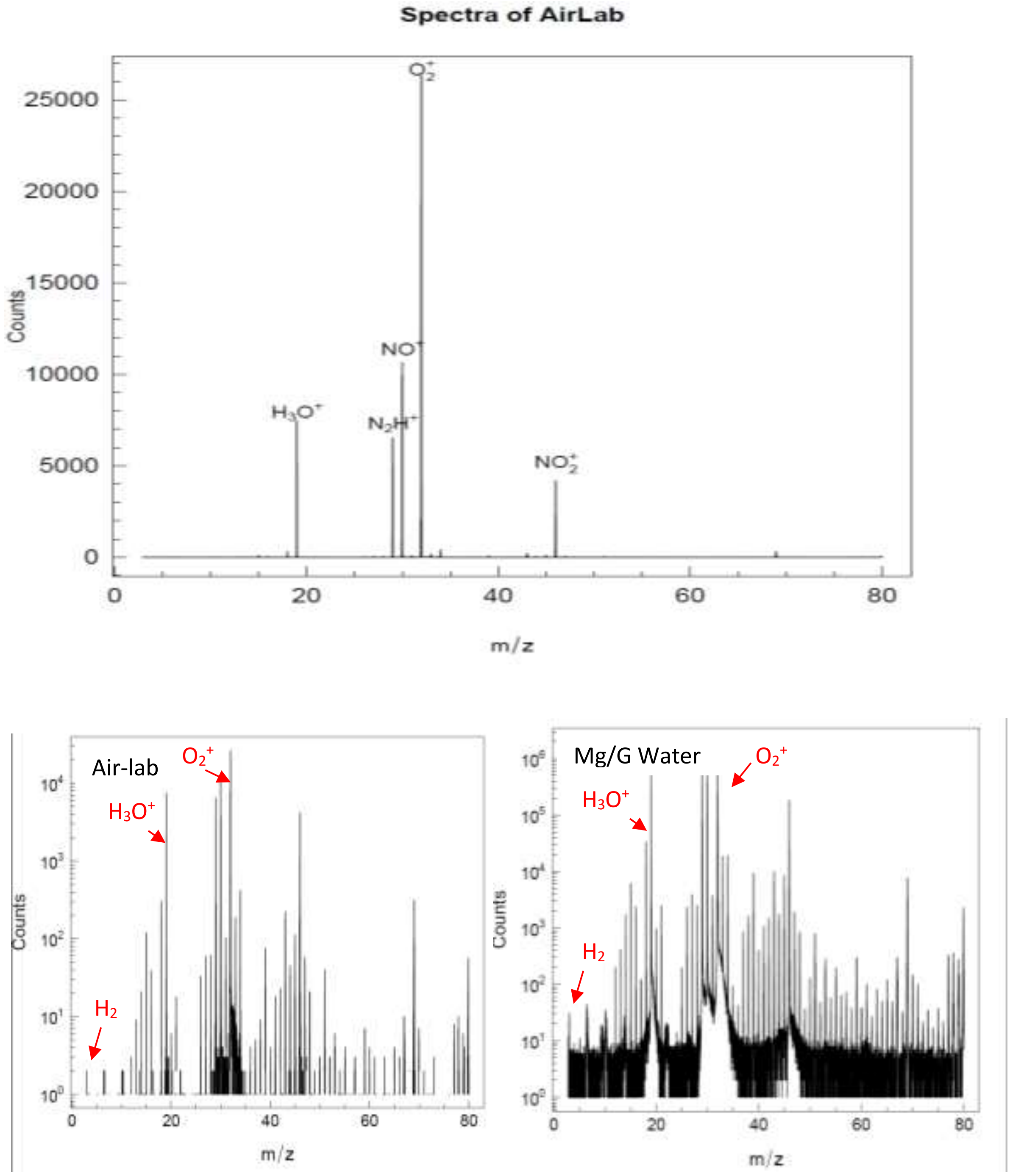
S6: Video of the H_2 bubbles produced by Mg/G in water

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:**

$$Mg + 2H_2O \rightarrow Mg(OH)_2 + H_2$$
$$\Delta H_r = -354\,kJ\,mol^{-1}$$

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_{Powder}= 0.001 g

H_2 Gravimetric storage density

$\rho_{g/g}$=3%

Hydrogen evolution from powder

m_{H2}= m_{Powder} x $\rho_{g/g}$ = 3e-5 g

Energy Balance:

LHV_{H2}=119 k/g

Chemical energy in produced hydrogen:

E_{H2}= LHV_{H2}x m_{H2}=3.57 J

For a energy density based on powder of:

E_{H2}^{powder}= E_{H2}/ m_{Powder}= 3.57 kJ/g

B) Heat production by Gr+Mg powder and water reaction

Based on the number of Mg moles reacted:

$Mg + H_2O \rightarrow Mg(OH)_2 + H_2$

$n_{H2}=n_{Mg}$

So, considering the previous H2 production, m_{H2},

$n_{Mg}= n_{H2}= m_{H2}/PM_{H2}$ = 1.5e-5 moles

Considering, Enthalpy of Mg and water reaction equals to ΔH= 354 kJ/moles, it is possible to evaluate total heat released by chemical reaction of Hydrogen production,

$E_{heat}= n_{Mg} x\ \Delta H$ = 5.31 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: $E_{heat}^{powder}= E_{heat} /m_{Powder}$=5.31 kJ/g

With a total energy balance of:

$E_{tot}= E_{heat}^{powder} + E_{H2}^{powder}$ = 3,51 kJ+5.31 KJ = 8,81KJ/gr

C) Estimation of water consumption

The Stoichiometric quantity of consumed water by reaction is:

$n_{H2O}= 2 \times n_{H2}$ == 3.2e-5moles

For a mass of:

$m_{H2O}= n_{H2O} \times PM_{H2O}$= 54.045e-5 g

And a total consumption for mass unit of powder of,

$m_{H2O}^{powder}= m_{H2O}/ m_{Powder}$= 0.57 g_{H2O}/gp_{owder}

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

$m_{tot}= m_{H2O}^{powder}+ m_{Powder}$= 1.57 g for a energy density of,

$\rho^{Energy}_{tot}= E_{tot}/ m_{tot}= 5.61$ kJ/g

Or considering only chemical energy released as H_2 gas,

$\rho^{H2}_{tot} =E_{heat}^{powder}/ m_{tot} = 2.23$ kJ/g

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

	Energy density kJ/gr
Compressed Hydrogen (700 atm)	150
Mg/Gr theoretical	14
Mg/Gr(this work)	3.5 (H_2)+5.3(Heat)
Lithium battery	1-2
Fly wheel	1
Ni-Cd	1
Lead acid battery	0.18