Supporting information

Belonging to the manuscript

Thermodynamics and stability of the Mg-H-F system for thermochemical energy storage applications

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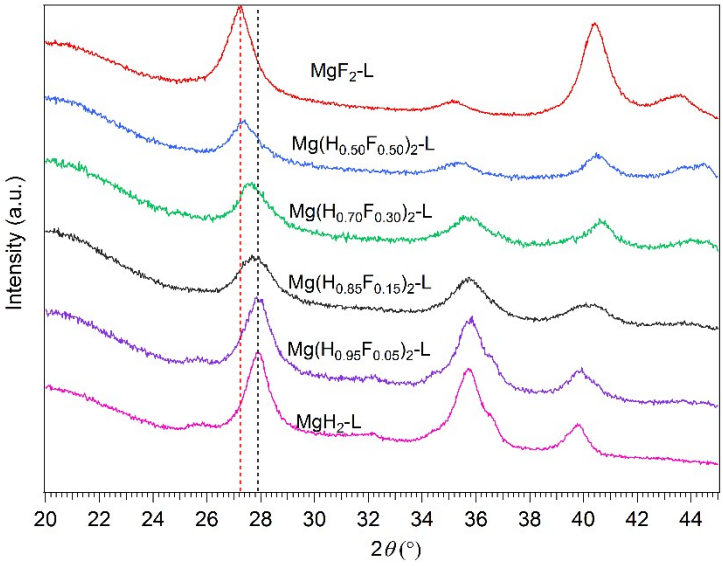

Fig. S1. *Ex-situ* XRD data for samples ball milled for 40 hours (*L*) collected at room temperature. λ =1.5418 Å. Red and black dot line's refers to main peaks of MgF_2 and MgH_2 respectively.

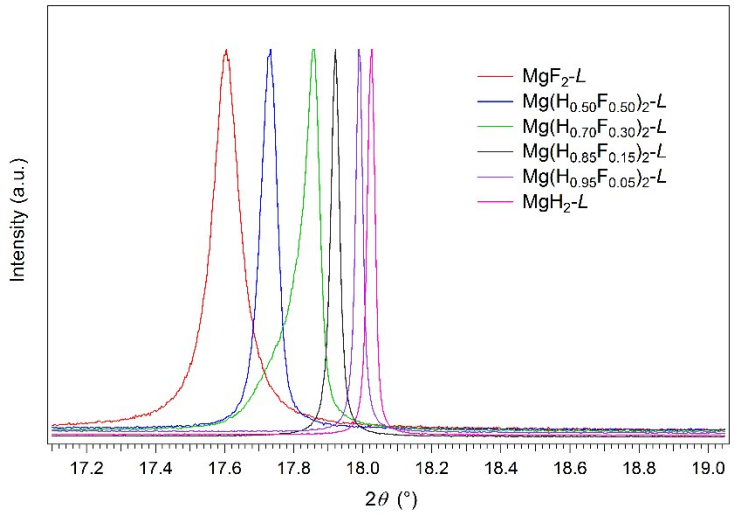

Fig. S2. *In situ* SR-XRD at room temperature of $Mg(H_xF_{1-x})_2$-*L* samples ball milled for 40 hours and annealed. λ = 1.000389(1) Å.

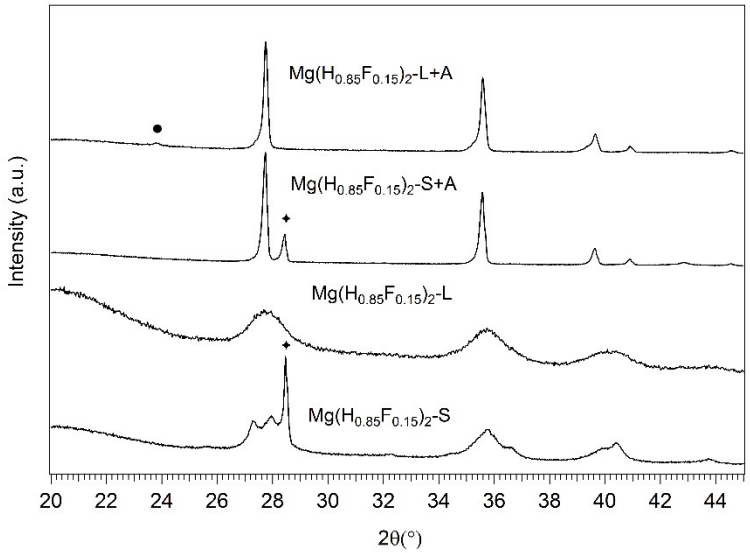

Fig. S3. Comparison between SR-XRD of samples ball milled for 10 and 40 hours and then annealed (A). ●=Mg_2FeH_6, ✦=Si. λ = 1.5418 Å, at room temperature.

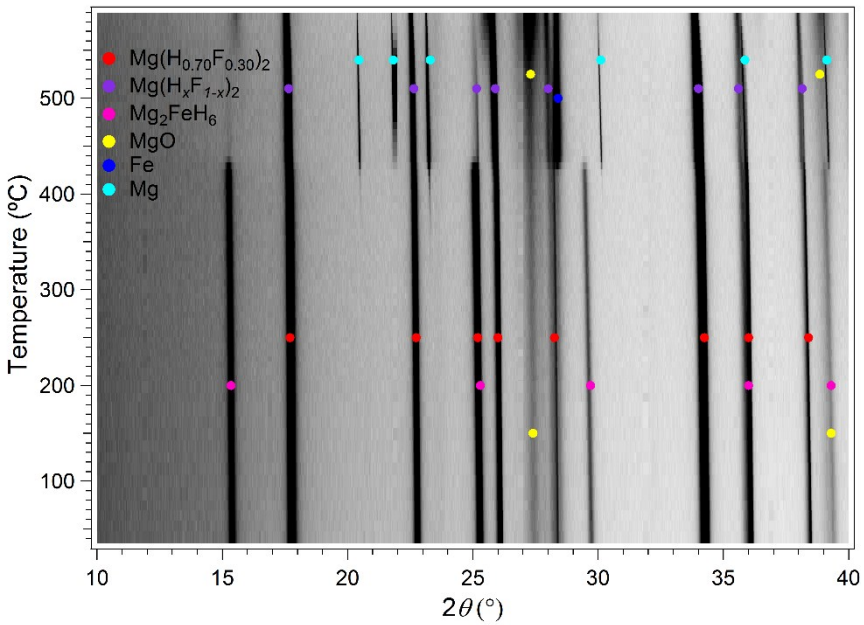

Fig. S4. *In situ* XRD for $Mg(H_{0.70}F_{0.30})$-*L* performed under vacuum using a $\Delta T/\Delta t$ = 10°C/min before 200 °C and 5 °C/min after 200 °C. λ = 1.000389(1) Å.

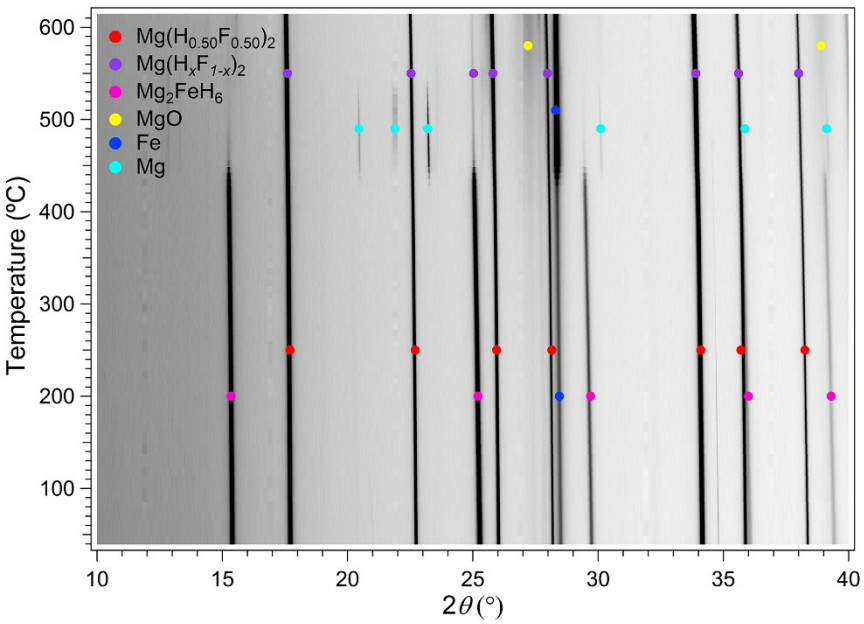

Fig. S5. *In situ* XRD for $Mg(H_{0.50}F_{0.50})$-*L* performed under vacuum using a $\Delta T/\Delta t$ = 10°C/min before 200 °C and 5 °C/min after 200 °C. λ = 1.000389(1) Å.

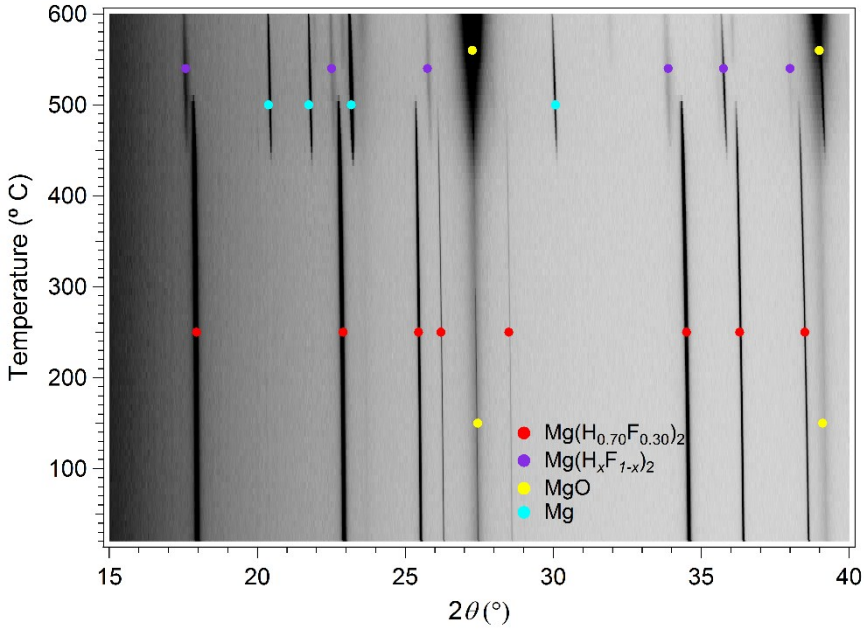

Fig. S6. *In situ* XRD for $Mg(H_{0.95}F_{0.05})$-*L* performed under vacuum using a $\Delta T/\Delta t$ = 10°C/min before 200 °C and 5 °C/min after 200 °C. λ = 1.000389(1) Å .

Table S1. Summary of parameters and data collected from PCT desorption measurements of $Mg(H_{0.85}F_{0.15})_2$-*S* Pressure and H_2 wt% uncertainties

Temperature (°C)	Observed Desorption H_2 (wt%)	Final Pressure (bar)	Theoretical H_2 wt%	Difference between observed vs theoretical H2 wt%
438	4.57 ± 0.14	14.5	5.4	0.83
444	4.37 ± 0.29	24.1	5.4	1.03
450	4.85 ± 0.19	4	5.4	0.55
461	4.61 ± 0.15	19.8	5.4	0.79

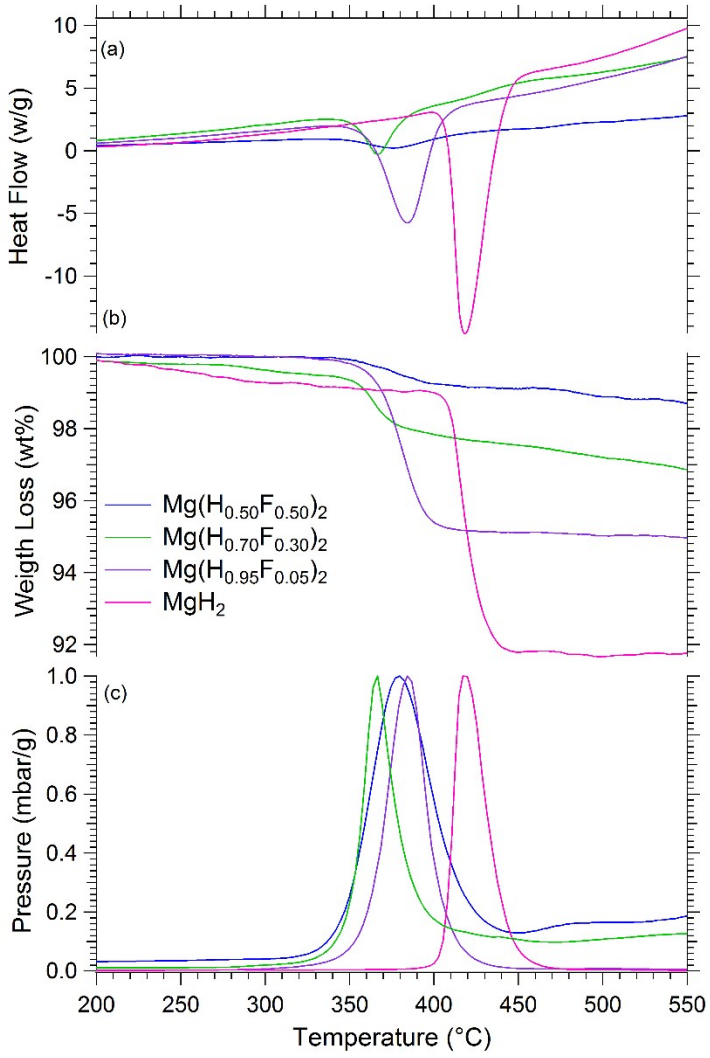

Fig. S7. Simultaneous thermal analysis of $Mg(H_xF_{1-x})_2$-*L* samples by (a) DSC, (b) TGA and (c) MS. $\Delta T/\Delta t$ = 10 °C/min. DSC and MS data are normalised to the mass of the sample.

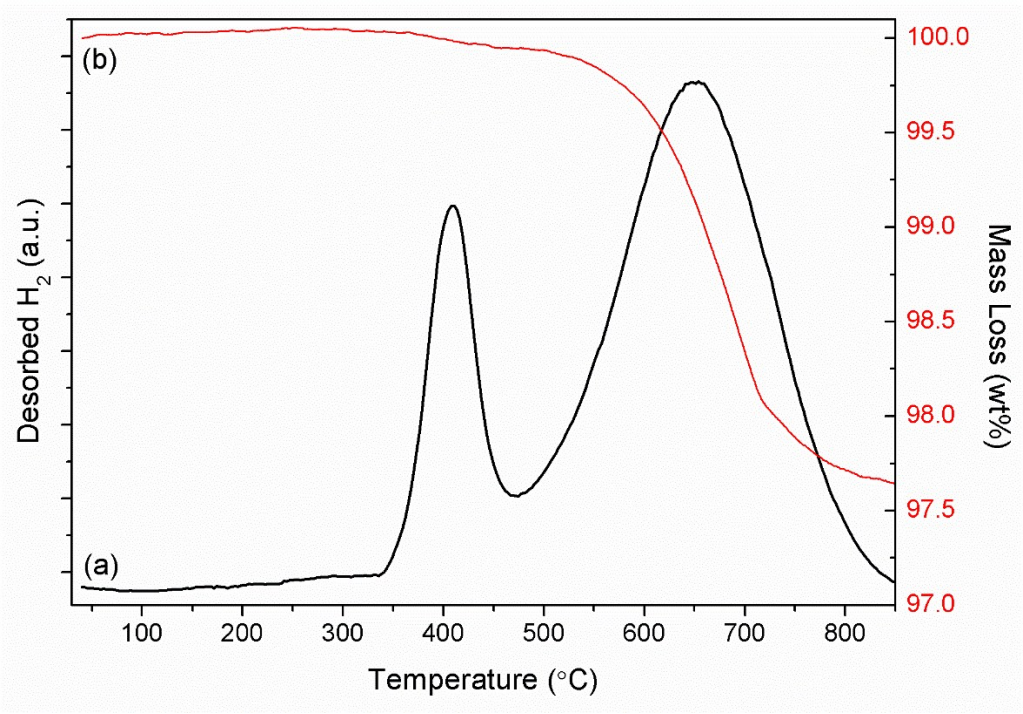

Fig. S8. Simultaneous thermal analysis of $Mg(H_{0.50}F_{0.50})$-*L*. by (a) MS and (b) TGA. $\Delta T/\Delta t$ = 10 °C/min.

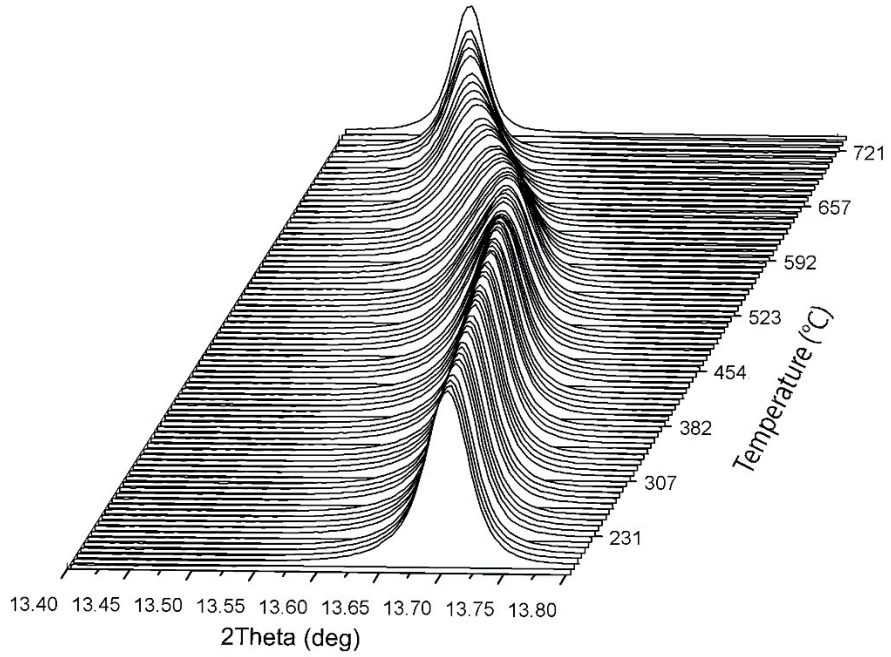

Fig. S9. *In situ* XRD for $Mg(H_{0.50}F_{0.50})$-*L*. λ = 0.774541(1) Å.