Supporting Information

Enhancement of Hydrogen Desorption from Nano-Composite Prepared by Ball-Milling MgH_2 with in-situ Aerosol-Spraying $LiBH_4$

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This Supporting Information contains:

Number of pages: 6 (S1-S6)

Number of figures: 9 (Figure S1-Figure S9)

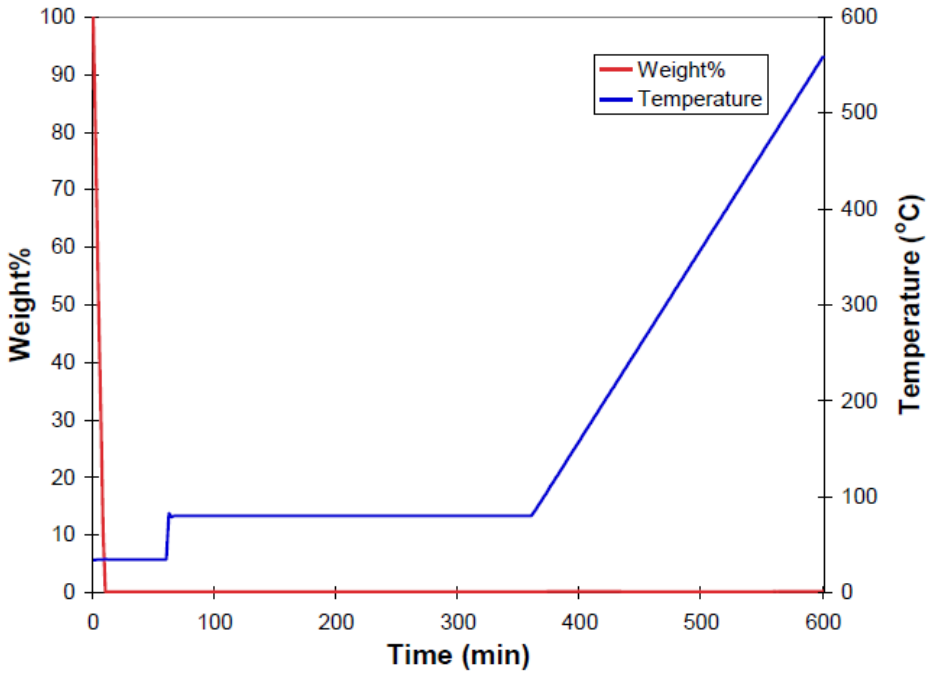

Figure S1. The thermogravimetric analysis of pure tetrahydrofuran (THF). The heating condition is: (i) held at room temperature for 60 min with a flowing argon atmosphere, (ii) jumped to 80℃ and held for 300 min, and (iii) heated at 2 ℃/min to 550℃. Note that all THF vaporizes in the first 20-min holding at room temperature. This is not a surprise at all because the boiling temperature of THF is 66℃.

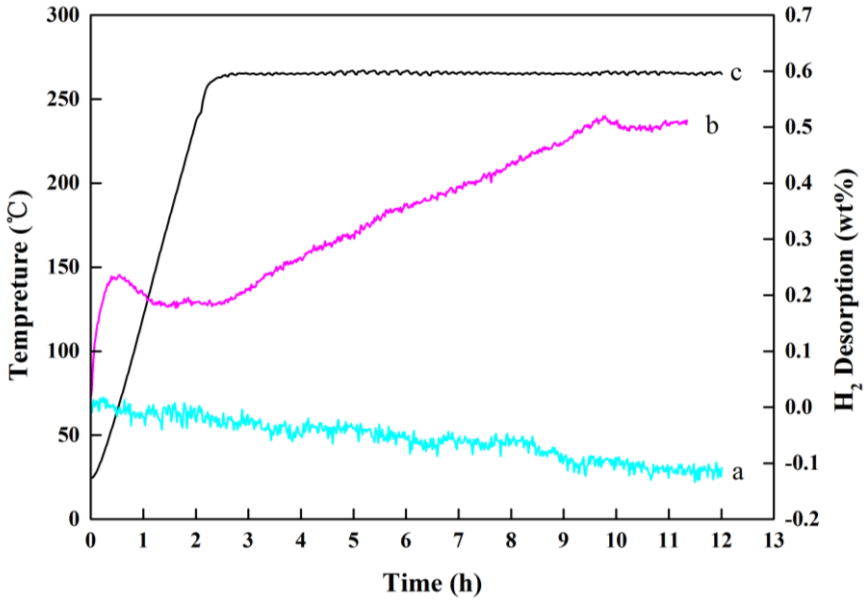

Figure S2. Behaviors of the empty PCT cell (a) under vacuum and (b) under 90 MPa H_2 are also included, (c) is the experimental temperature.

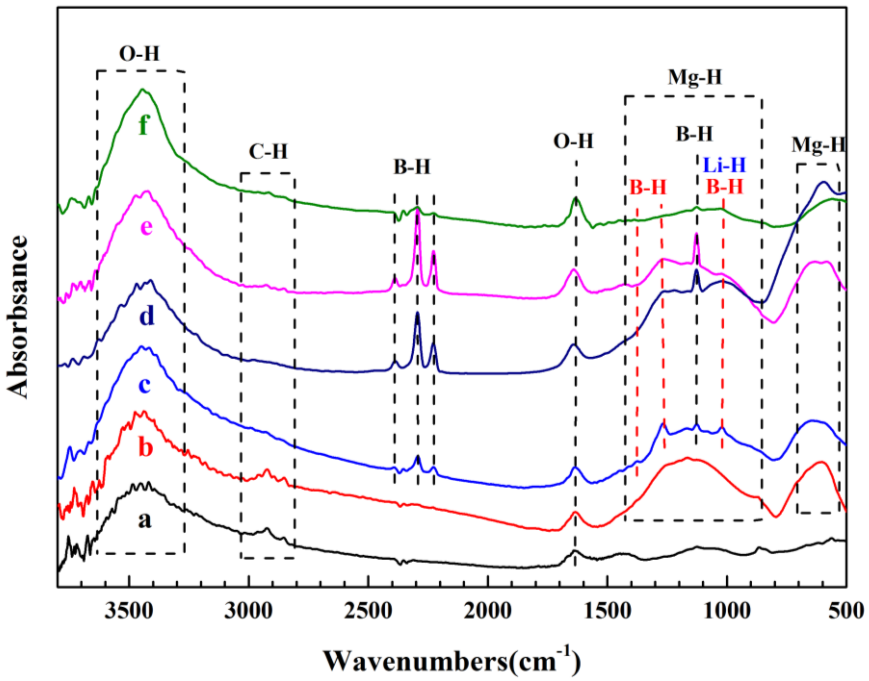

Figure S3. FTIR spectra of: (a) the commercially purchased bulk KBr powder, (b) hand mixed MgH_2 + C mixture, (c) the BMAS powder at the as-synthesized condition, (d) the BMAS powder after one dehydrogenation (1R), (e) the BMAS powder after one dehydrogenation and then one re-hydrogenation (1S), and (f) the BMAS powder after 7 cycles of dehydrogenation and re-hydrogenation and finally dehydrogenation (8R).

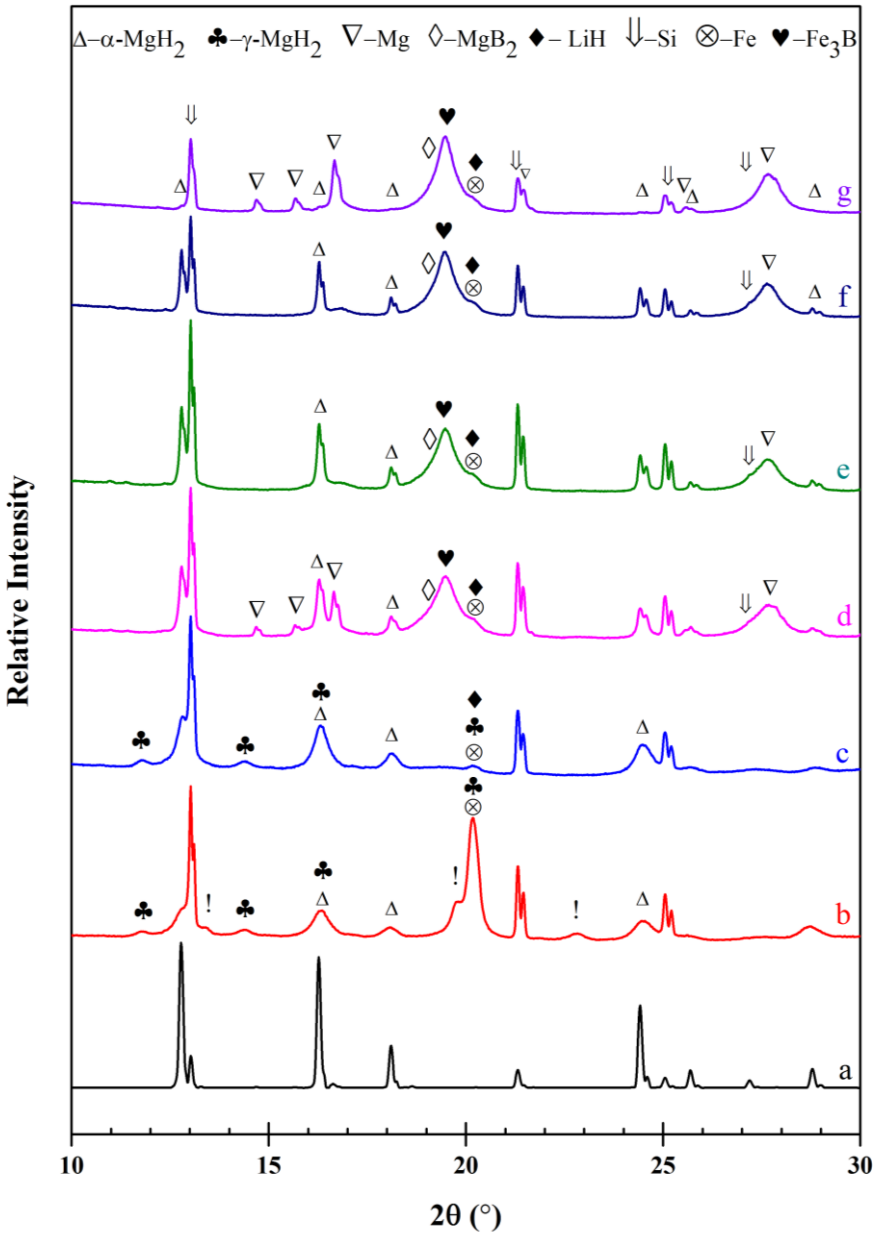

Figure S4. XRD patterns of: (a) hand mixed MgH_2 + C mixture, (b) MgH_2 + C mixture ball milled for 920 min but without aerosol spraying, (c) the BMAS powder at the as-synthesized condition, (d) the BMAS powder after one dehydrogenation (1R), (e) the BMAS powder after one dehydrogenation and then one re-hydrogenation (1S), (f) the BMAS powder after 4 cycles of dehydrogenation and re-hydrogenation (4S), and (g) the BMAS powder after 7 cycles of dehydrogenation and re-hydrogenation and finally dehydrogenation (8R). Note that 10 wt.% coarse-grained Si of 99.9% purity was added as the internal reference in each sample, and "!" stands for unknown compounds.

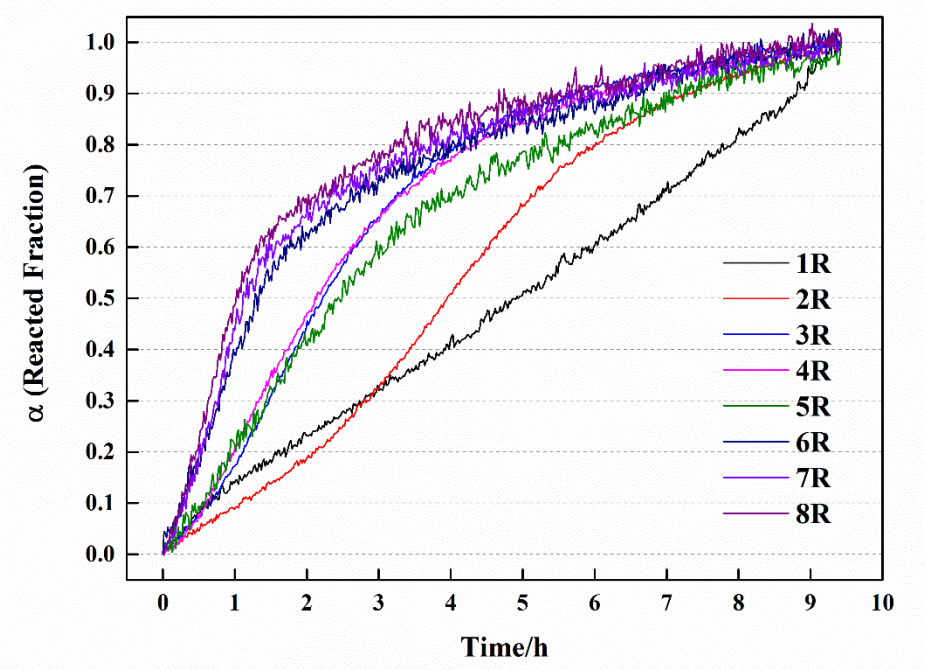

Figure S5. Normalized isothermal dehydrogenation curves of the BMAS powder with 50% $LiBH_4$ at 265 °C.

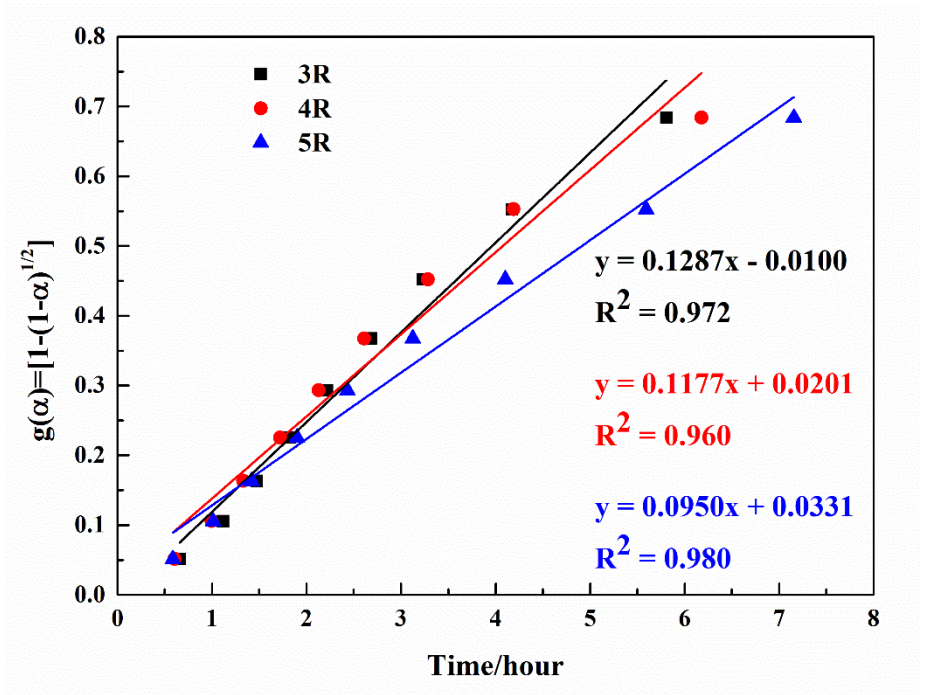

Figure S6. Time dependence of R2 kinetic modeling equations for the third, fourth and fifth dehydrogenation of the BMAS powder with 50% $LiBH_4$ at 265 °C.

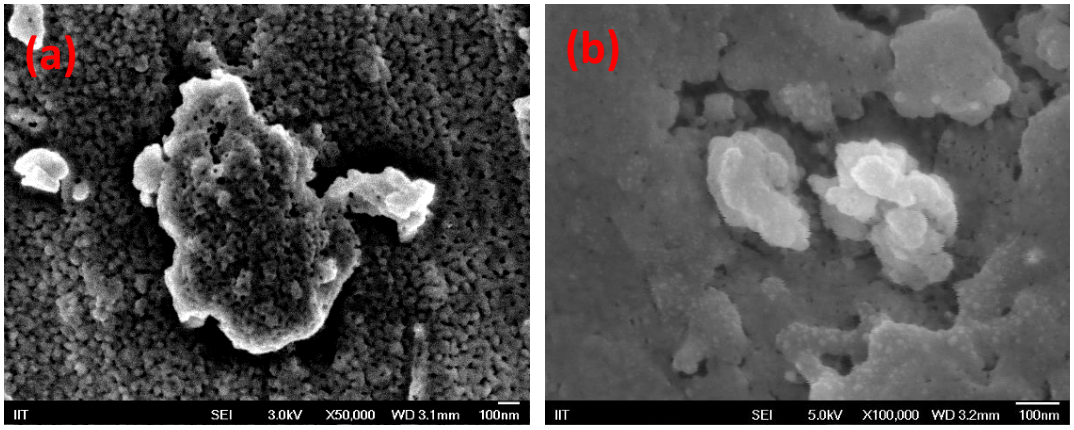

Figure S7. FESEM images of: (a) hand-mixed MgH_2 + 5 vol.% C mixture and (b) BMAS powder with 50% $LiBH_4$.

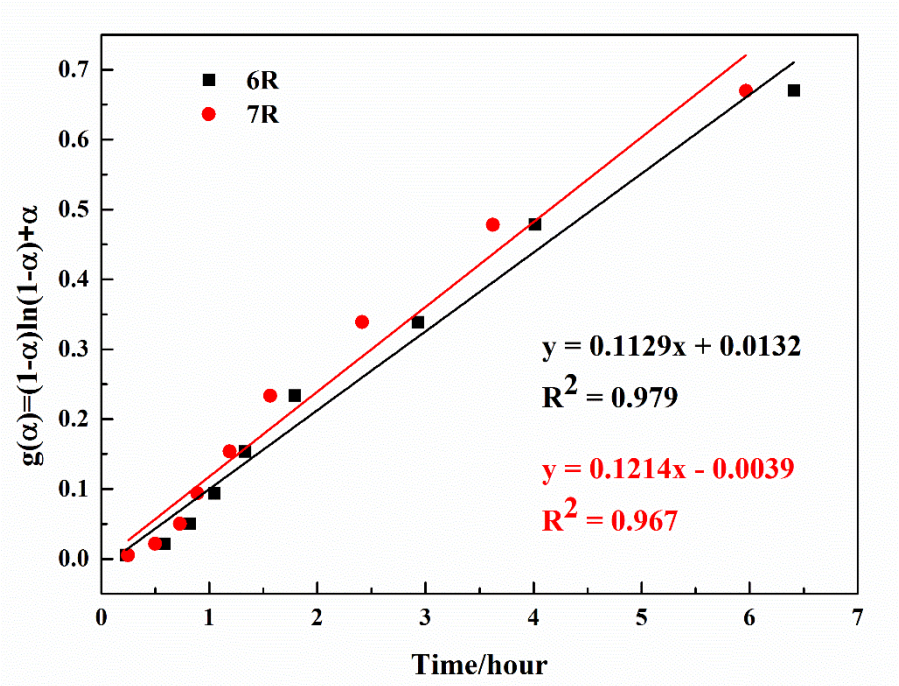

Figure S8. Time dependence of D2 kinetic modeling equations for the sixth and seventh dehydrogenation of the BMAS powder with 50% $LiBH_4$ at 265 ^oC.

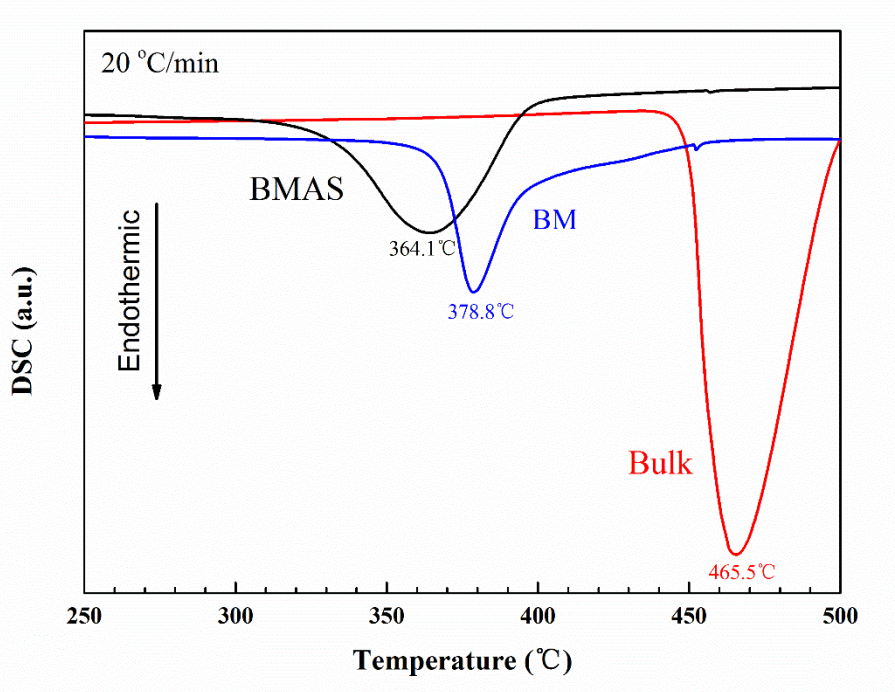

Figure S9. DSC curves of the Bulk (bulk $LiBH_4$), BM (ball-milled MgH_2+C), and BMAS (BMAS powder with 50% $LiBH_4$) at a heating rate of 20 °C/min.