

## Supplementary Information:

### Enhanced hydriding-dehydriding performance of $2\text{LiBH}_4\text{-MgH}_2$ composite by the catalytic effects of transition metal chlorides

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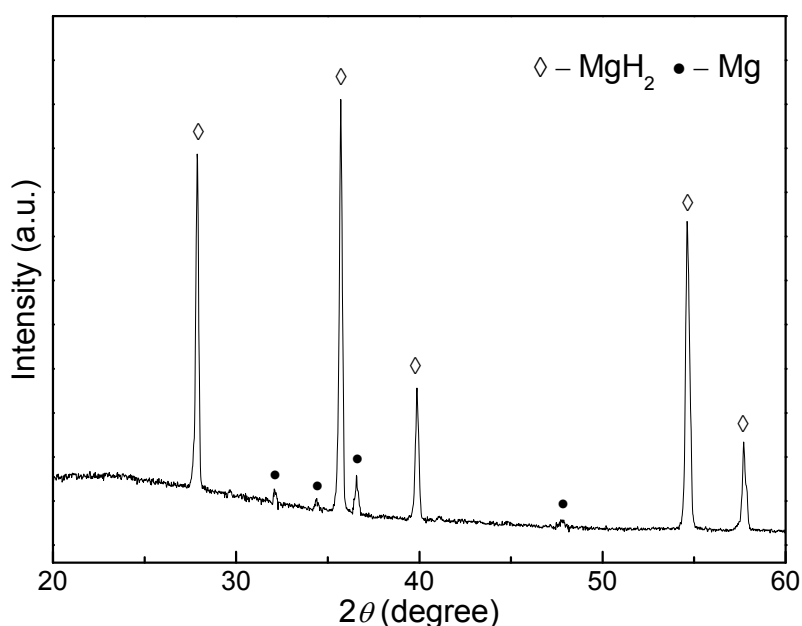


Figure S1. XRD pattern of the as-purchased  $\text{MgH}_2$  from Alfa Aesar.

Table S1. Peak Temperatures for Each Sample in DSC Profiles.

Peak / °C	A	B	C	D
Sample				
undoped	116.5	293.1	371.5	448.3
$2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{FeCl}_2$	103.4	291.9	330.5	434.9
$2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{CoCl}_2$	104.2	287.7	311.2	427.6
$2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{NiCl}_2$	104.9	286.1	297.5	408.4

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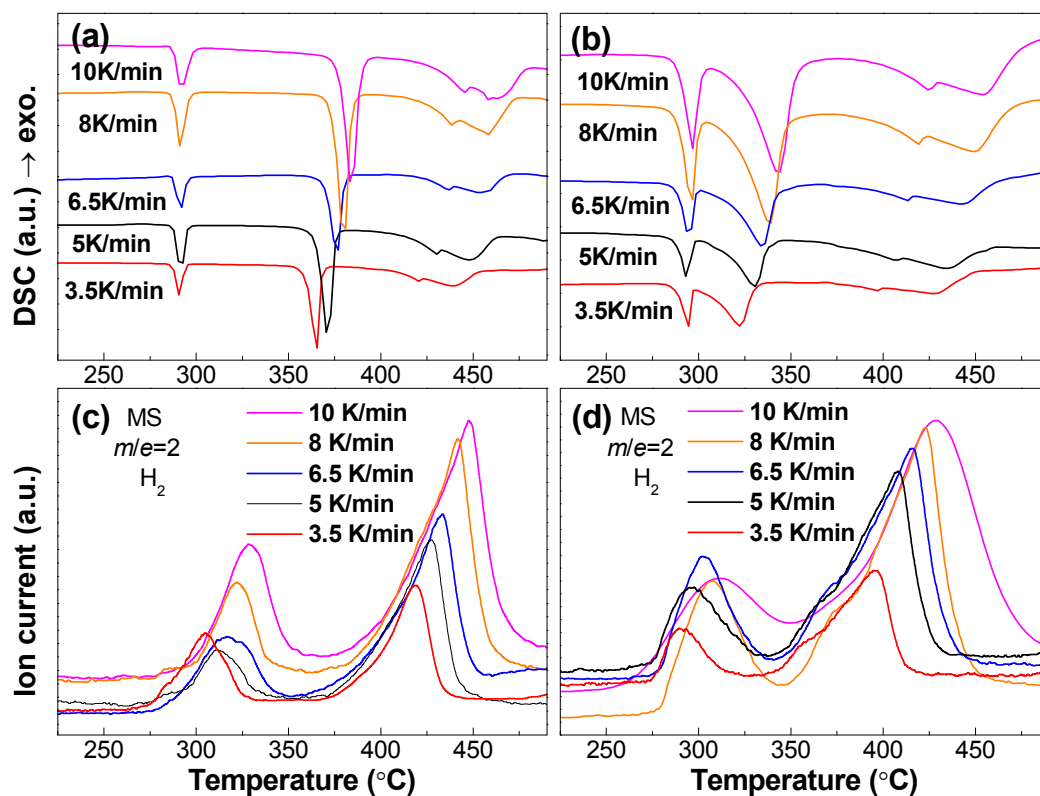


Figure S2. DSC-MS curves of the as-milled  $2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{MCl}_2$  ( $M = \text{Fe}, \text{Co}, \text{Ni}$ ) composites at various heating rates. (a) undoped, (b) doped with  $0.1\text{FeCl}_2$ , (c) doped with  $0.1\text{CoCl}_2$ , (d) doped with  $0.1\text{NiCl}_2$ .

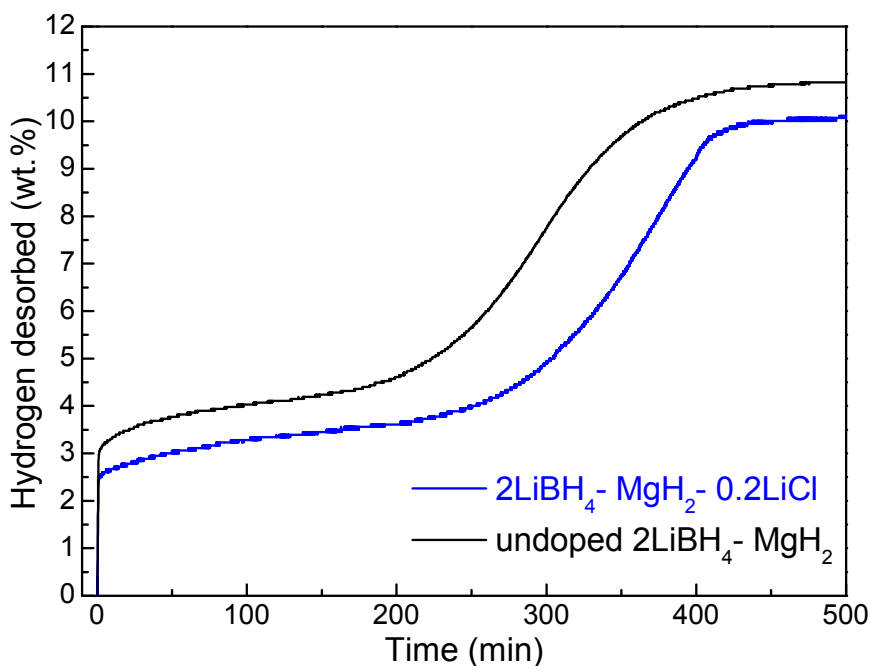


Figure S3. Isothermal dehydrogenation curves of the  $2\text{LiBH}_4\text{-MgH}_2\text{-}0.2\text{LiCl}$  sample under 4 bar  $\text{H}_2$  at  $430^\circ\text{C}$ .

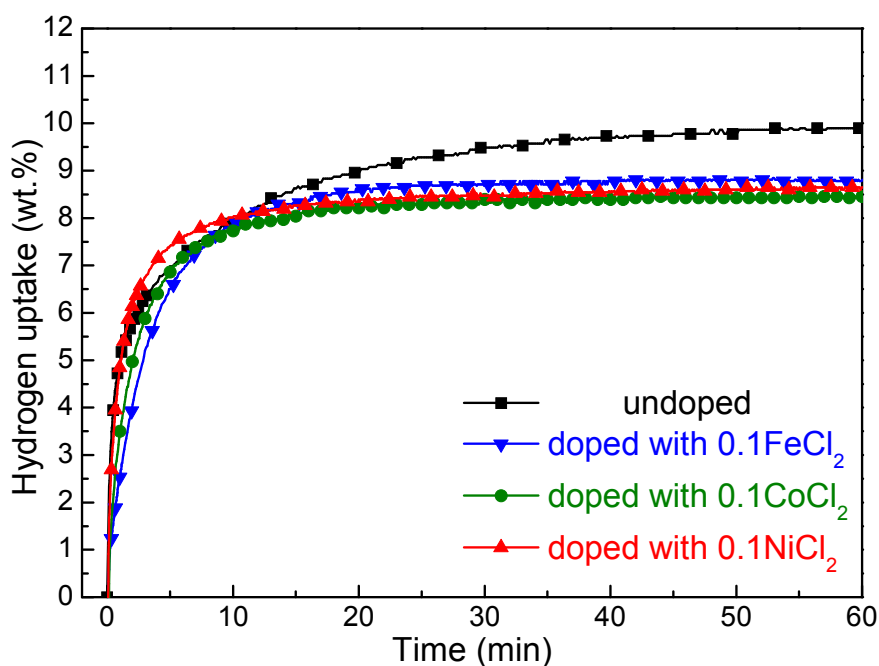


Figure S4. Isothermal rehydrogenation curves of the dehydrogenated  $2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{MCl}_2$  ( $M = \text{Fe}, \text{Co}, \text{Ni}$ ) composites under 80 bar  $\text{H}_2$  at 430 °C.

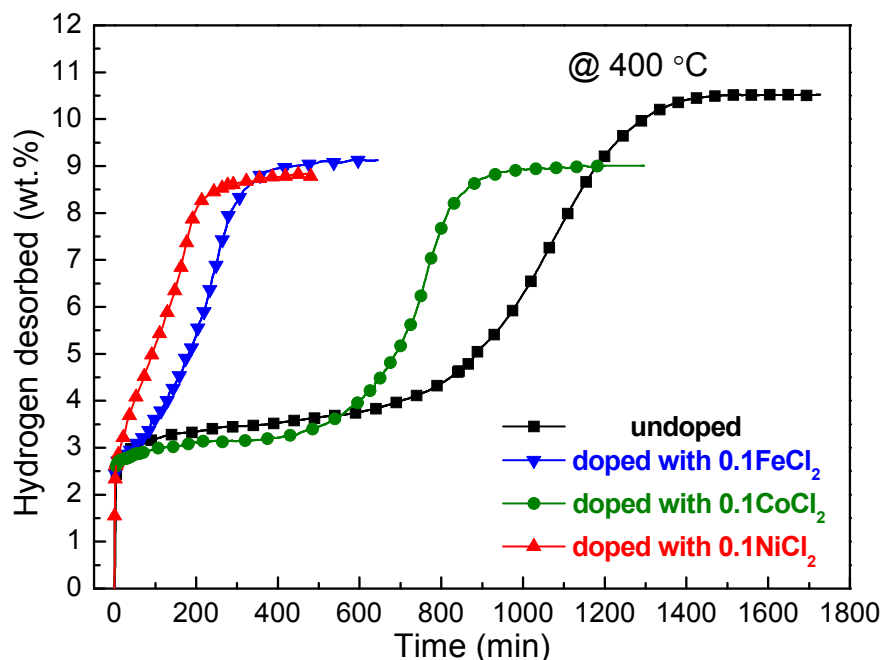


Figure S5. Isothermal dehydrogenation curves of the as-milled  $2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{MCl}_2$  ( $M = \text{Fe}, \text{Co}, \text{Ni}$ ) samples under 4 bar hydrogen back pressure at 400 °C.

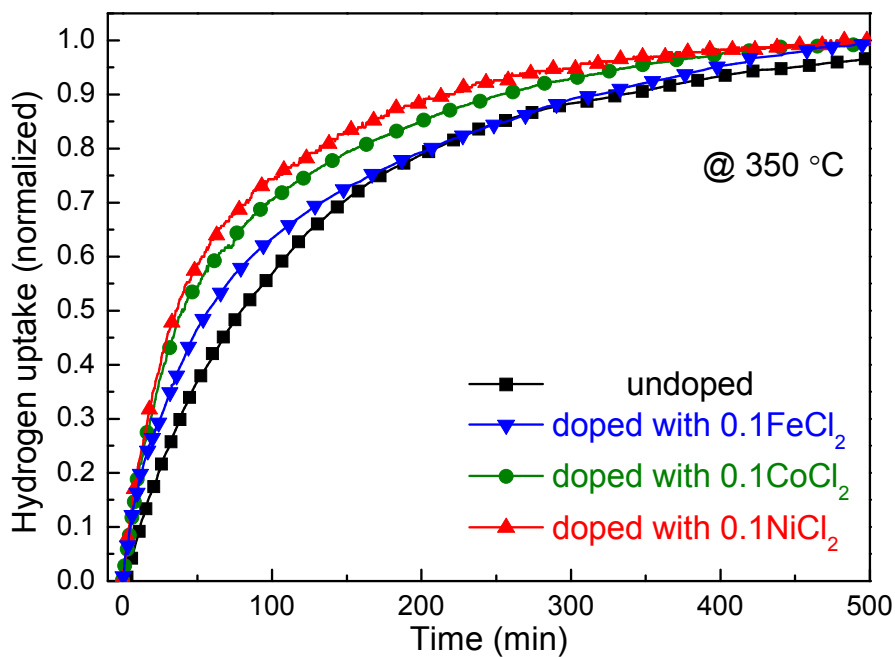


Figure S6. Normalized isothermal rehydrogenation curves of the dehydrogenated  $2\text{LiBH}_4\text{-MgH}_2\text{-}0.1\text{MCl}_2$  ( $M = \text{Fe}, \text{Co}, \text{Ni}$ ) composites under 80 bar  $\text{H}_2$  at 350 °C.

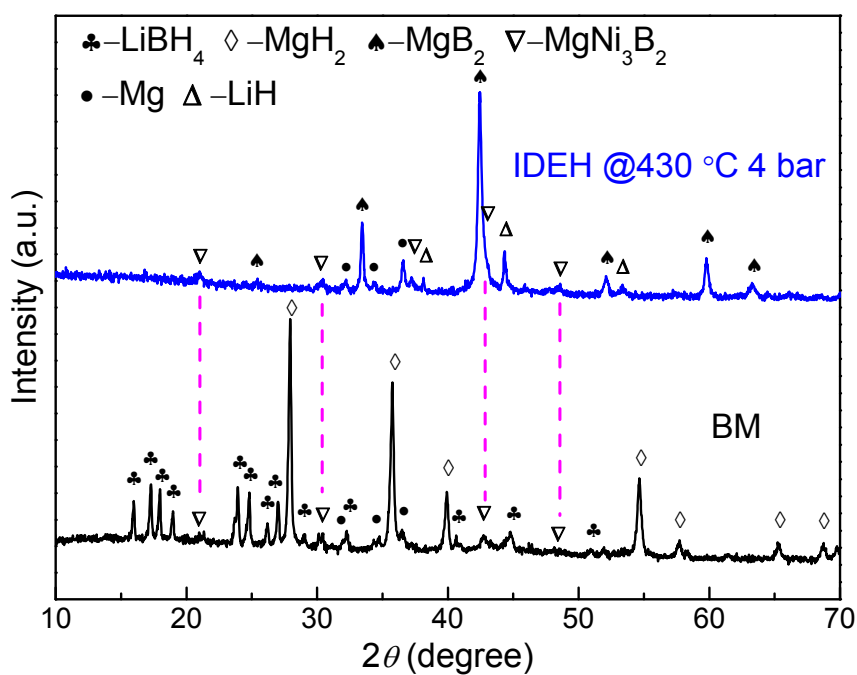


Figure S7. XRD patterns of the as-milled and isothermal dehydrogenated  $2\text{LiBH}_4\text{-MgH}_2\text{-}0.033\text{MgNi}_3\text{B}_2$  sample.