Facile Preparation of β-/γ-MgH$_2$ Nanocomposites under Mild Conditions and Pathways to Rapid Dehydrogenation.

Supplementary Information

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Table S1(a) Refined atomic parameters of γ-MgH$_2$ phase

atom	site	x	y	Z	$U_{\text{iso}} \times 100$ / Å^2
Mg(1)	4c	0	0.3483(11)	¼	7.6(5)
H(1)	8d	0.7710	0.6085	0.4199	3.8

[a] Space group *Pbcn*, a = 4.4399(10) Å, b = 5.4090(13) Å, c = 4.8804(5) Å

Table S1(b) Refined atomic parameters of β-MgH$_2$ Phase

atom	site	x	y	Z	$U_{\text{iso}} \times 100$ / Å^2
Mg(1)	2a	0	0	0	1.79(6)
H(1)	4f	0.3168	0.3168	0	3.4

[a] Space group *P4$_2$*/m n m, a = 4.5111(3) Å, c = 3.0162(6) Å

Table S1(c) Refined atomic parameter of Mg Phase

atom	site	x	y	z	$U_{\text{iso}} \times 100$ / Å^2
Mg(1)	2c	1/3	2/3	1/4	8.1

[a] Space group *P6$_3$*/m m c, a = 3.2073(6) Å, c = 5.2005(17) Å
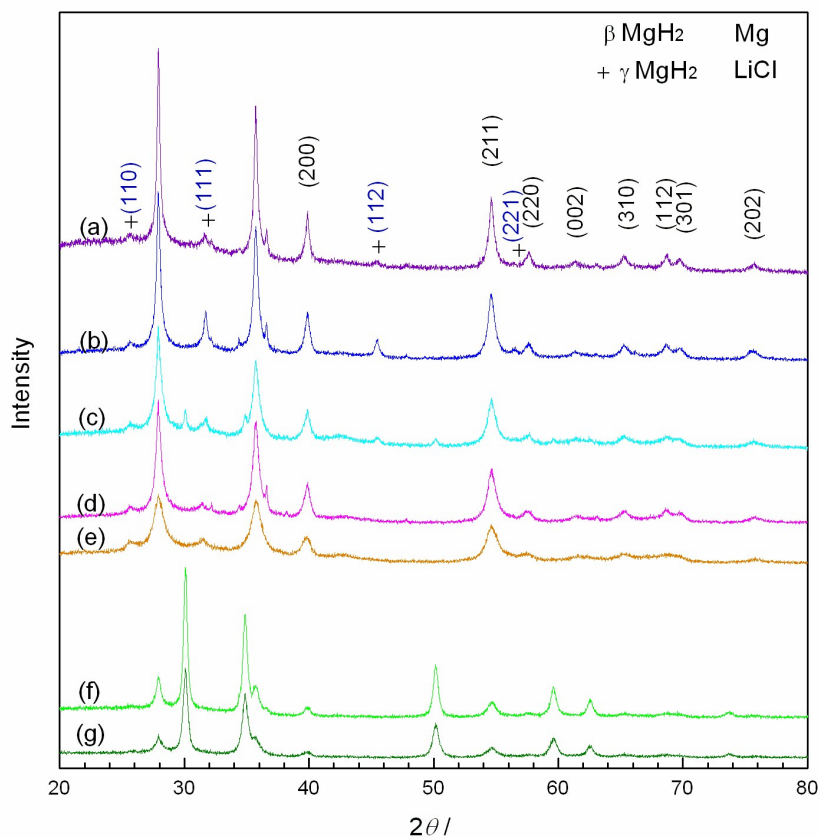
Fig. S1 PXD patterns of β-/γ-MgH$_2$ prepared under different conditions: (a) ball milled for 1 h with LiCl added and washed with THF; (b) ball milled for 4 h with LiCl added and washed with THF; (c) ball milled for 6 h with LiCl added and washed with THF; (d) ball milled for 2 h and washed with THF; (e) ball milled for 4 h and washed with THF; (f) ball milled for 2 h with LiCl added; (g) ball milled for 4 h with LiCl added.