Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Improvement of hydrogen storage property of three-component $Mg(NH_2)_2$-$LiNH_2$-LiH composites by additives

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Table S1 Values of various functions of α in some commonly used reaction equations together with those extracted from $Mg(NH_2)_2$-$LiNH_2$-4LiH and the $Mg(NH_2)_2$-$LiNH_2$-3.9LiH-0.1KH samples.

	Value for $t/t_{0.5}$									$Mg(NH_2)_2$-$LiNH_2$-4LiH		$Mg(NH_2)_2$-$LiNH_2$-3.9LiH-0.1KH	
α	$D_1(\alpha)$	$D_2(\alpha)$	$D_3(\alpha)$	$D_4(\alpha)$	$F_1(\alpha)$	$R_2(\alpha)$	$R_3(\alpha)$	$A_2(\alpha)$	$A_3(\alpha)$	140°C	180°C	140°C	180°C
0.1	0.040	0.033	0.028	0.032	0.152	0.174	0.165	0.390	0.533	0.20	0.24	0.66	0.63
0.2	0.160	0.140	0.121	0.135	0.322	0.362	0.349	0.567	0.685	0.38	0.44	0.76	0.75
0.3	0.360	0.328	0.295	0.324	0.515	0.556	0.544	0.717	0.801	0.58	0.59	0.83	0.84
0.4	0.640	0.609	0.576	0.595	0.737	0.768	0.762	0.858	0.903	0.78	0.79	0.90	0.92
0.5	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.00	1.00	1.00	1.00
0.6	1.440	1.521	1.628	1.541	1.322	1.253	1.277	1.150	1.097	1.22	1.45	1.04	1.07
0.7	1.960	2.207	2.568	2.297	1.737	1.543	1.607	1.318	1.198	1.51	2.31	1.12	1.14
0.8	2.560	3.115	4.051	3.378	2.322	1.887	2.014	1.524	1.322	1.96	4.00	1.35	1.24
0.9	3.240	4.363	6.747	5.028	3.322	2.334	2.602	1.822	1.492	3.28	8.65	1.95	1.49

Table S2 selected compositions of the $Mg(NH_2)_2$-$LiNH_2$-LiH system in this study.

$Mg(NH_2)_2$	$LiNH_2$	LiH	KH
1	1	4	—
1	1	3.9	0.1
2	1	4	—
2	1	3.9	0.1
1	2	4	—
1	2	3.9	0.1
1	1	5	—
1	1	4.9	0.1
2	1	5	—
2	1	4.9	0.1
1	2	5	—
1	2	4.9	0.1
1	1	6	—
1	1	5.9	0.1
2	1	6	—
2	1	5.9	0.1
1	2	6	—
1	2	5.9	0.1

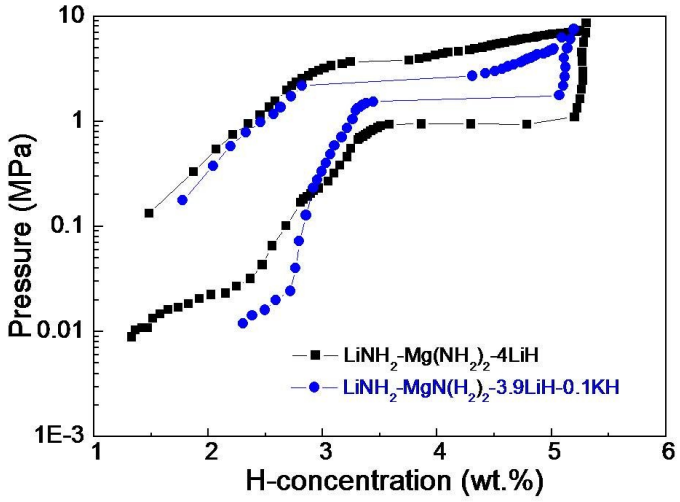

Fig. S1 experimental PCIs of the $Mg(NH_2)_2$-$LiNH_2$-4LiH and $Mg(NH_2)_2$-$LiNH_2$-3.9LiH-0.1KH samples at 180°C. The hysteresis of the PCIs is significantly reduced to 0.82MPa for the $Mg(NH_2)_2$-$LiNH_2$-3.9LiH-0.1KH sample compared with 2.78MPa for the $Mg(NH_2)_2$-$LiNH_2$-4LiH sample.

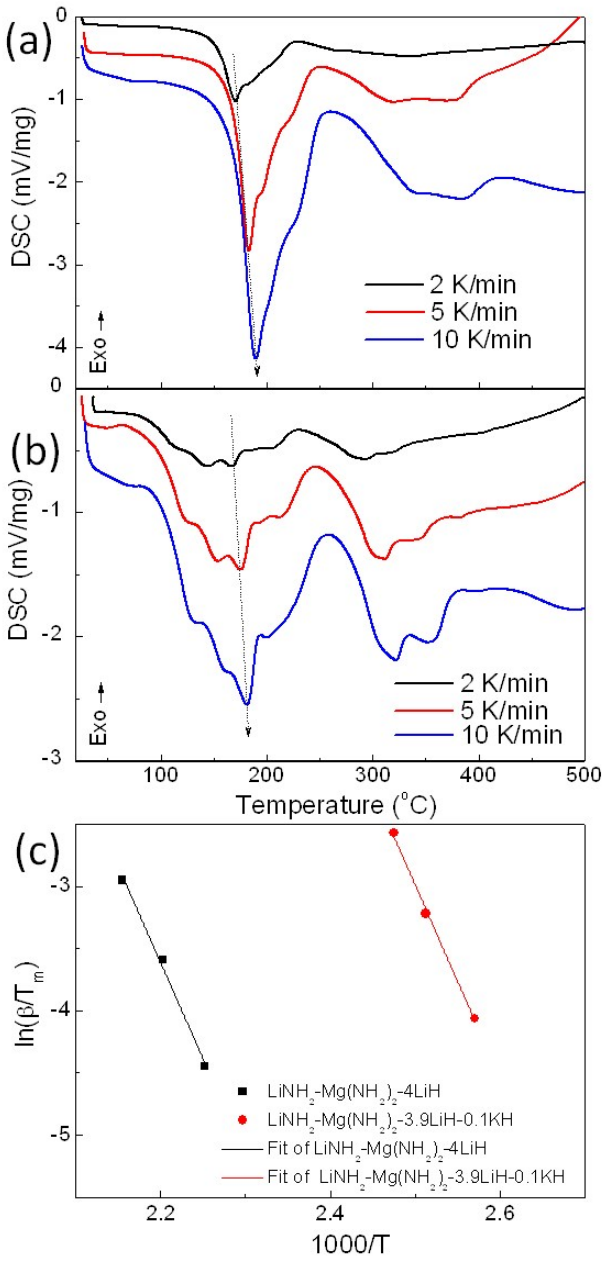

Fig. S2 DSC traces of (a) $Mg(NH_2)_2$-$LiNH_2$-4LiH and (b) $Mg(NH_2)_2$-$LiNH_2$-3.9LiH-0.1KH samples at different heating rates. (c) Kissinger's plots for the above two samples.

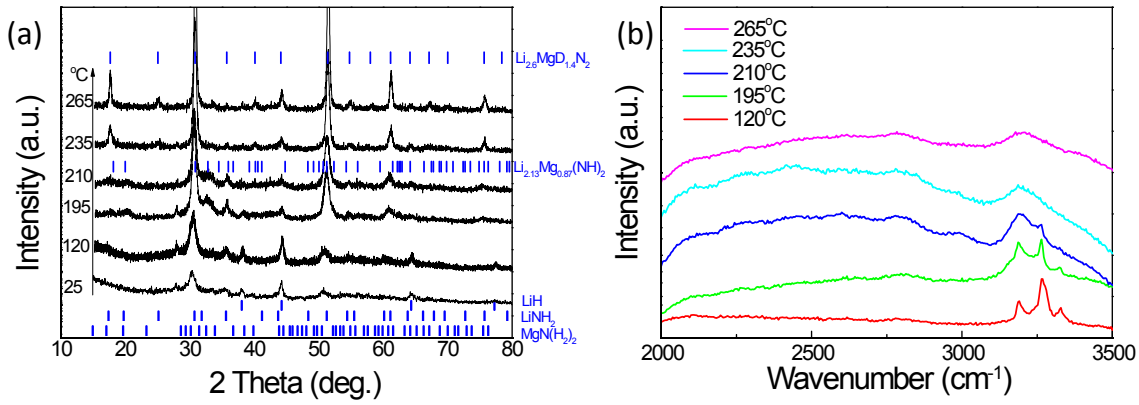

Fig. S3 Evolution of (a) XRD patterns and (b) Raman spectra of the $Mg(NH_2)_2$-$LiNH_2$-4LiH composite during dehydrogenation.

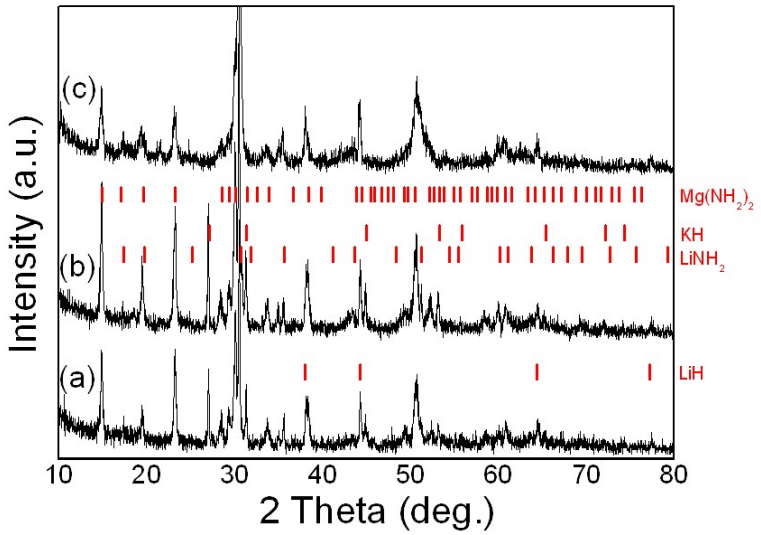

Fig. S4 XRD patterns of (a) 1st cycled and (b) 12th cycled $Mg(NH_2)_2$-$LiNH_2$-3.9LiH-0.1KH, and (c) 12th cycled $Mg(NH_2)_2$-$LiNH_2$-4LiH, all in hydrogenated state.