Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Improvements in the hydrogen storage properties of the $Mg(NH_2)_2$-LiH composite by KOH addition

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Table S1: Composition of sample KOH after thermal treatment. All data have been obtained by Rietveld analysis using MAUD software[30,31] on the patterns reported in Fig. 4.

	$Mg(NH_2)_2$	$LiNH_2$	KH	LiH	MgO	R_{wp}
Space group	I41/acd:2	I-4	Fm-3m	Fm-3m	Fm-3m	8.39
Cellparameters (Å) (±0.005)	a= 10.447 c= 19.962	a= 5.041 c= 10.259	a= 5.715	a= 4.100	a= 4.2096	
Wt%(±5%)	58	18	2	17	4	
Molar %(±5%)	26	17	1	53	2	

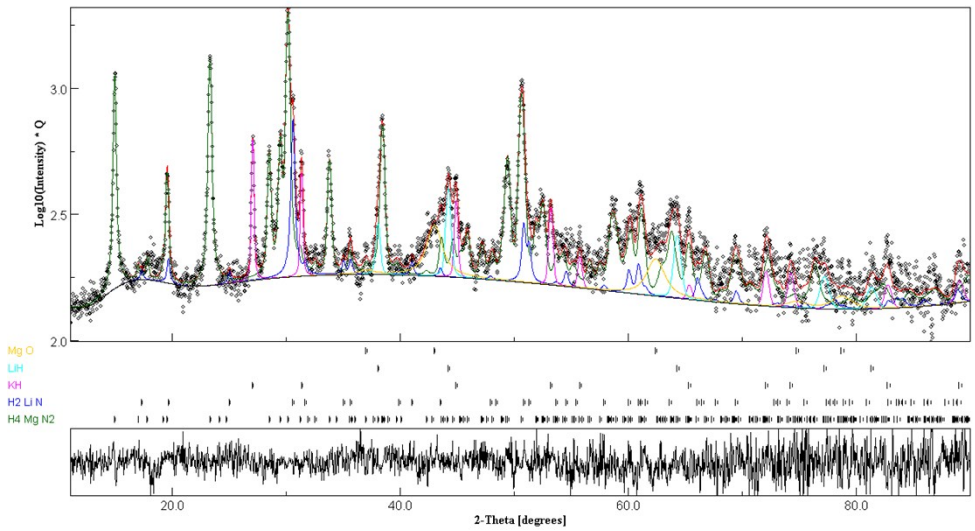

Figure S1: Experimental data XRPD, calculated points and base line for sample KOH after thermal treatment.

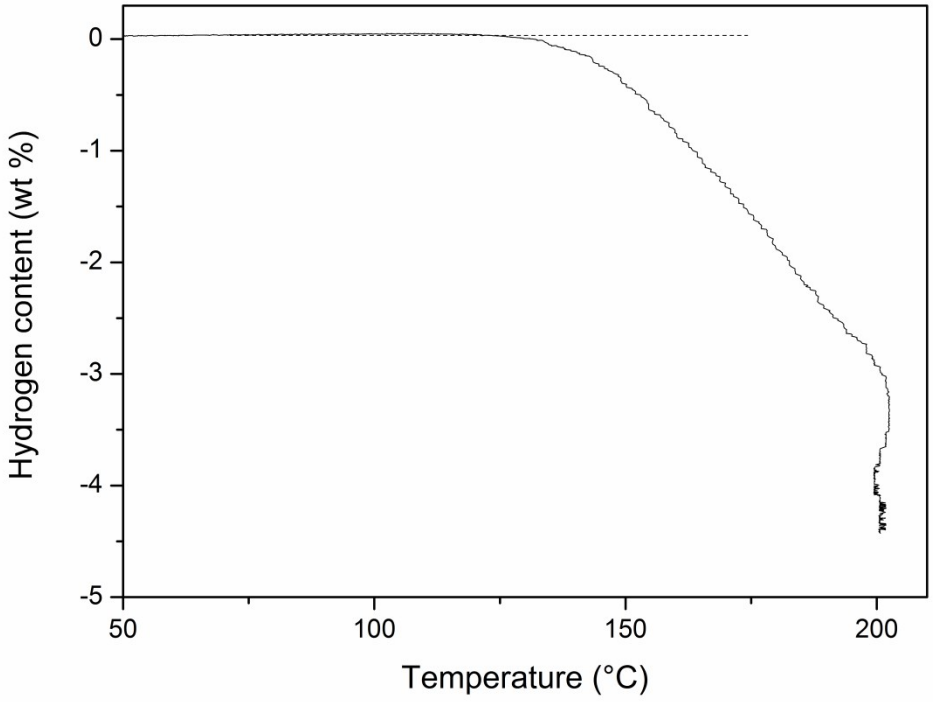

Figure S2: Non isothermal measurement of LMKOH sample.

Table S2: Composition of isothermally dehydrogenated LMKOH sample.

	$Li_2Mg(NH)_2$	$LiNH_2$	KH	MgO	R_{wp}
Space group	Fm-3m	I-4	Fm-3m	Fm-3m	
Cell parameters (Å) (±0.005)	a= 5.031	a= 5.041 c= 10.259	a= 5.715	a= 4.2096	9.1
Wt %	22	66	2	10	
Molar %	17	78	1	4	

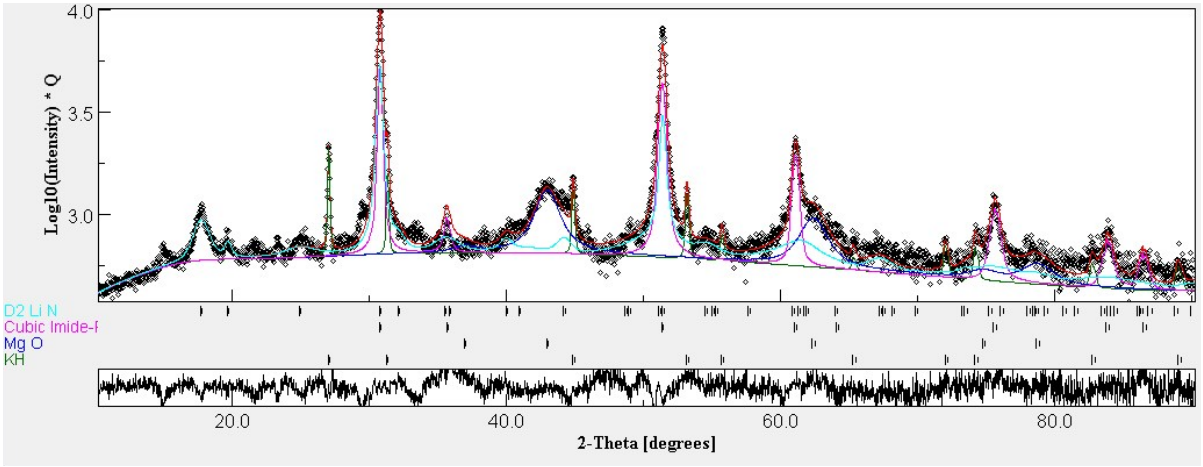

Fig.S3: Experimental data XRPD, calculated points and base line for the isothermally dehydrogenated LMKOH sample.

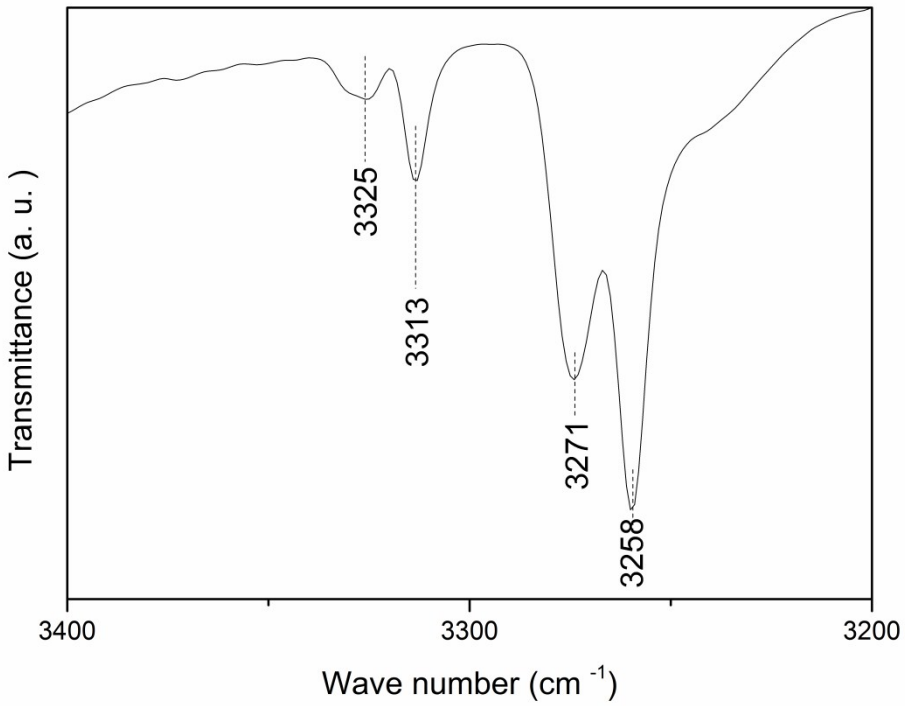

Figure S4: FTIR of sample LMKOH after rehydrogenation at 200°C.

Table S3: Composition of sample KOH after rehydrogenation.

	$Mg(NH_2)_2$	$LiNH_2$	KH	LiH	MgO	Fe	R_{wp}
Space group	I41/acd:2	I-4	Fm-3m	Fm-3m	Fm-3m	Im-3m	
Cell parameters (Å) (±0.005)	a= 10.447 c= 19.962	a= 5.041 c= 10.259	a= 5.715	a= 4.100	a= 4.2096	a= 2.852	5.6
Wt %	58	14	2	18	6.5	0.5	
Molar %	25	13	1	56	4	0	

Figure S5: Experimental XRPD data, calculated points and base line for sample KOH after rehydrogenation.

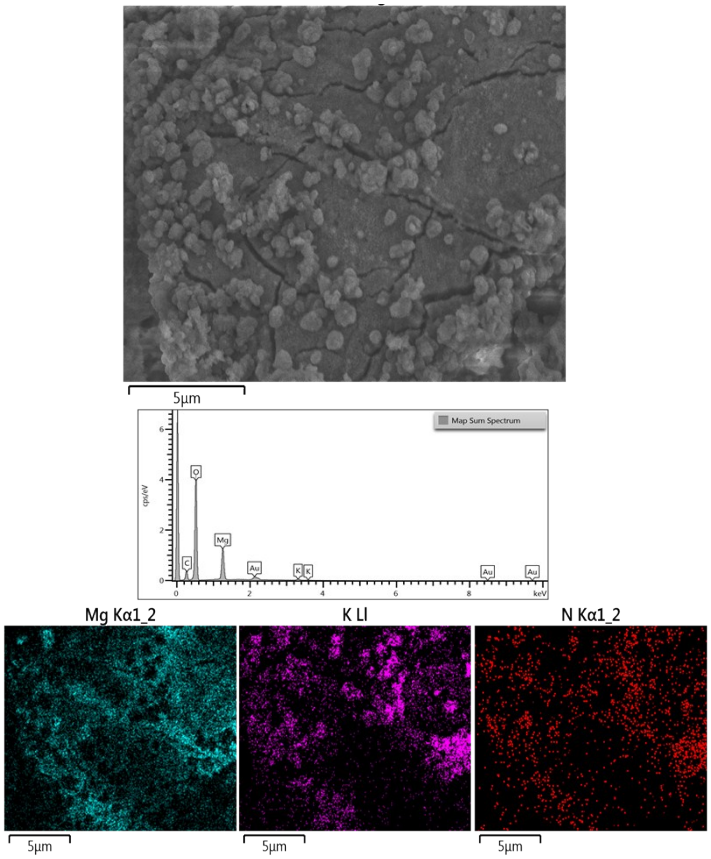

Figure S6: SEM micrograph, EDX spectrum and chemical mapping of the absorbed sample.

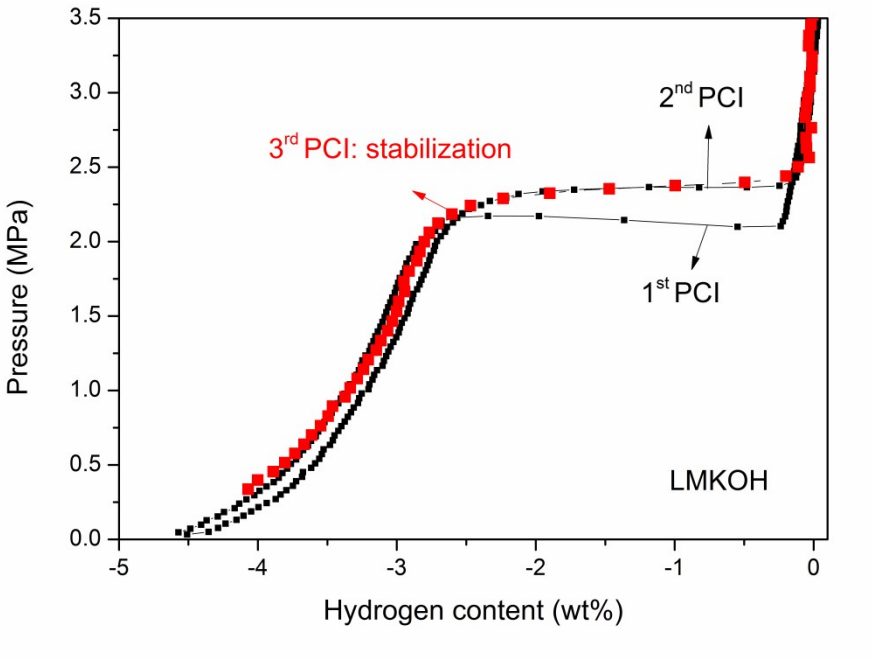

Figure S7: Cycling of PCIs at 200 °C of the LMKOH sample.

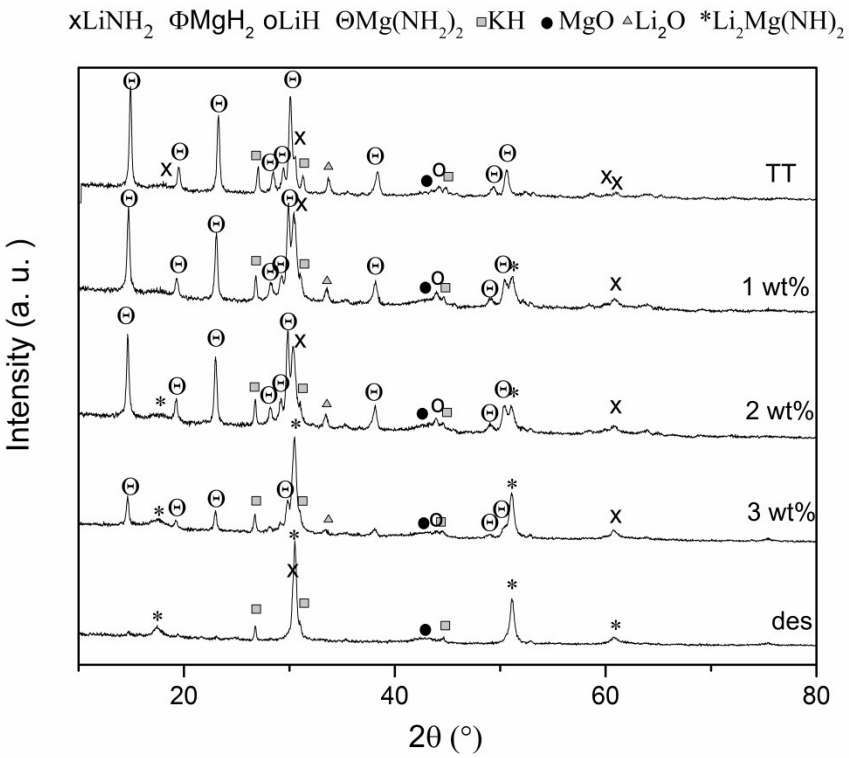

Figure S8: XRPD at different stages of dehydrogenation of the LMKHOH sample.