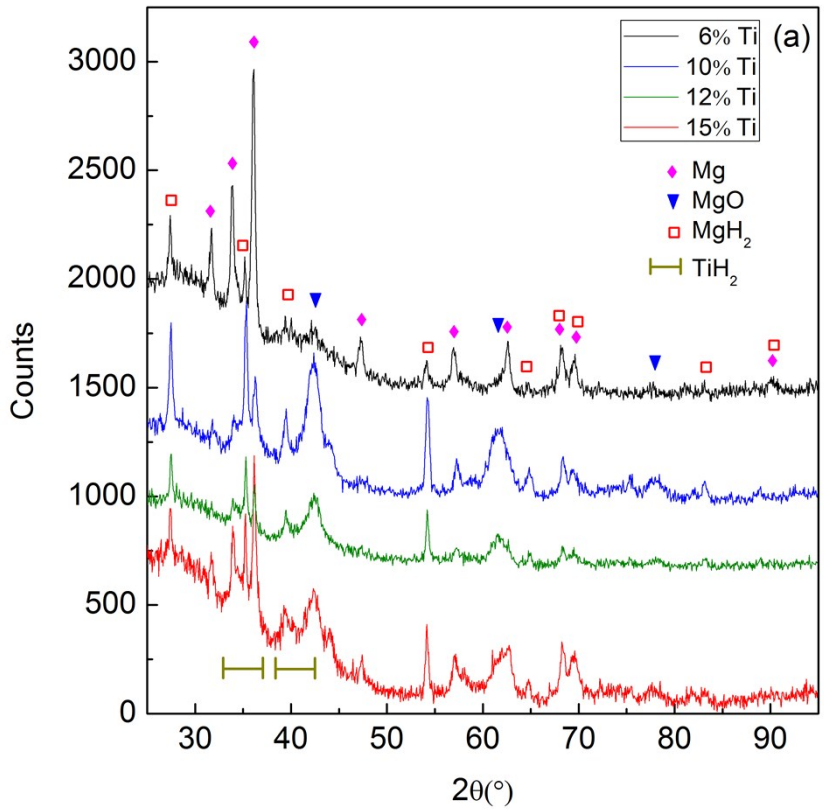
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Gas-phase synthesis of Mg-Ti nanoparticles for solid-state hydrogen storage

Supplementary informations

Table S1: Results of Rietveld analysis of the samples after cycling between 15 and 31 times in the HPDSC: phase abundance, crystallite sizes and lattice parameters of Mg and β-MgH_2.

Sample	Phase abundance (wt.%)				Cryst. size (nm)			β-MgH_2 cell parameters		Mg cell parameters	
	β-MgH_2	Mg	TiH_2	MgO	β-MgH_2	Mg	TiH_2	*a* (Å)	*c* (Å)	*a* (Å)	*c* (Å)
MgTi6	10(2)	49(5)	16(3)	25(4)	61(3)	53(5)	7(1)	4.5169(16)	3.024(2)	3.2109(8)	5.2132(14)
MgTi10	20(3)	6(1)	19(2)	55(4)	38(2)	39(6)	1.6(2)	4.5202(9)	3.0226(8)	3.2019(16)	5.203(5)
MgTi12	20(2)	6(1)	15(2)	59(2)	50(1)	100(30)	8 (1)	4.5186(9)	3.0219(10)	3.2109(12)	5.218(4)
MgTi15	13.4(6)	18(1)	22(2)	47(2)	46(4)	110(30)	4.1(2)	4.5191(11)	3.0212(12)	3.2064(10)	5.203(2)
MgTi9H	10.6(7)	1.7(2)	5.3(4)	82(3)	91(5)	53(14)	4.4(4)	4.5183(4)	3.0225(5)	3.2125(17)	5.223(6)
MgTi12H	7.3(5)	0	8.7(5)	84(4)	38(1)	-	4.7(1)	4.5190(12)	3.0232(13)	-	-
MgTi22H	8.6(6)	0	17(1)	75(4)	42(4)	-	6.1(7)	4.523(2)	3.027(2)	-	-



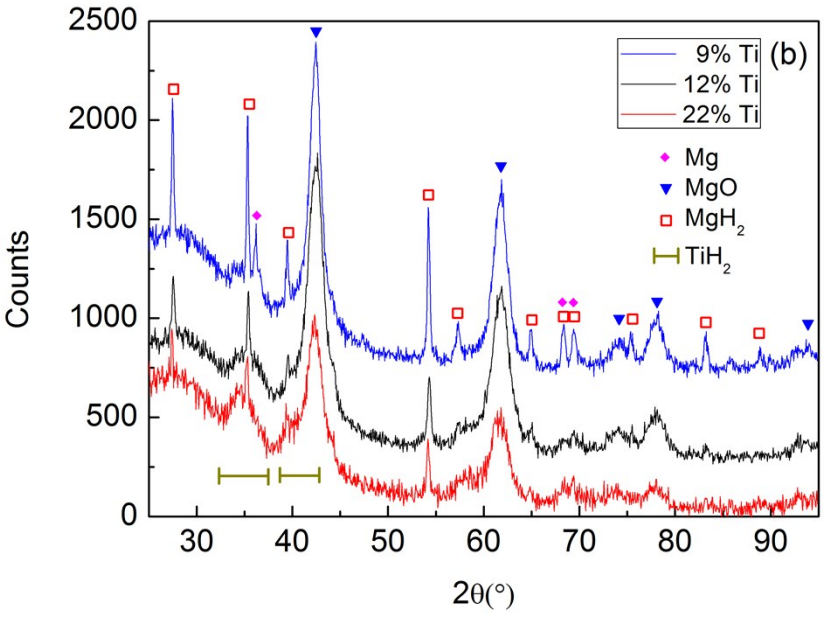


Figure S1: XRD profiles of MgTi# (a) and MgTi#H (b) samples after HPDSC cycles, ended with an absorption.

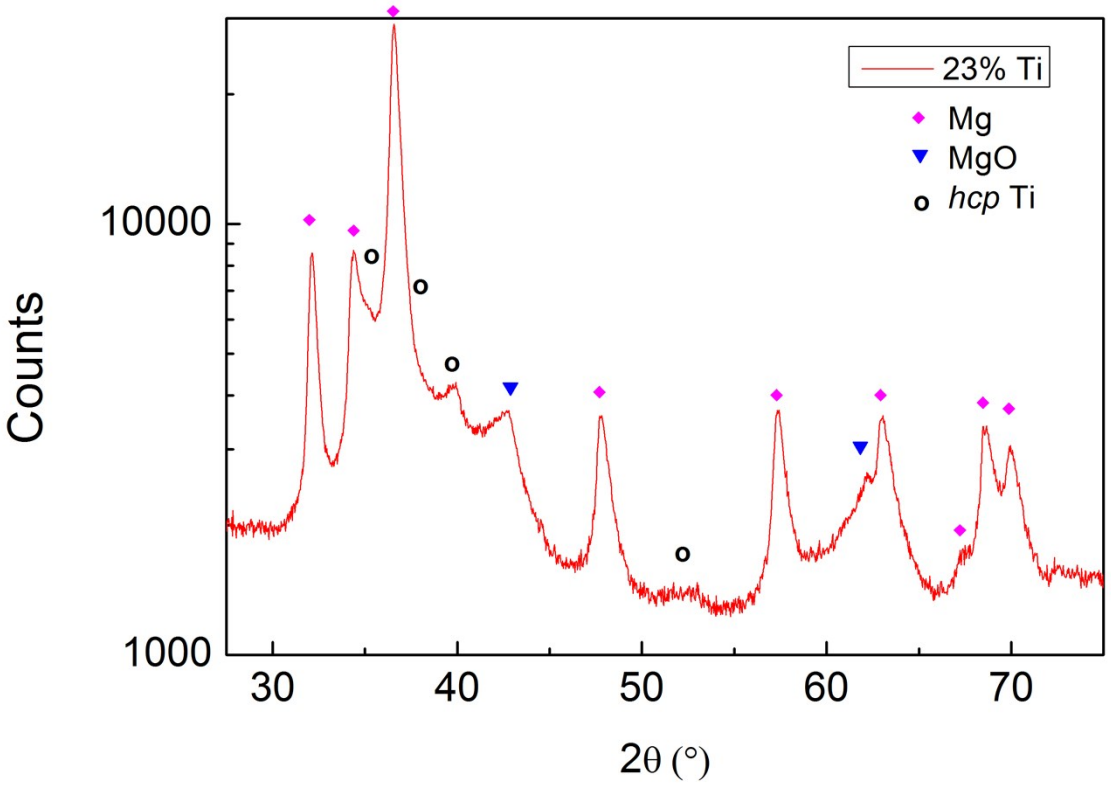


Figure S2: XRD profile of an as prepared sample without *in situ* hydrogenation with 23 at.% Ti.

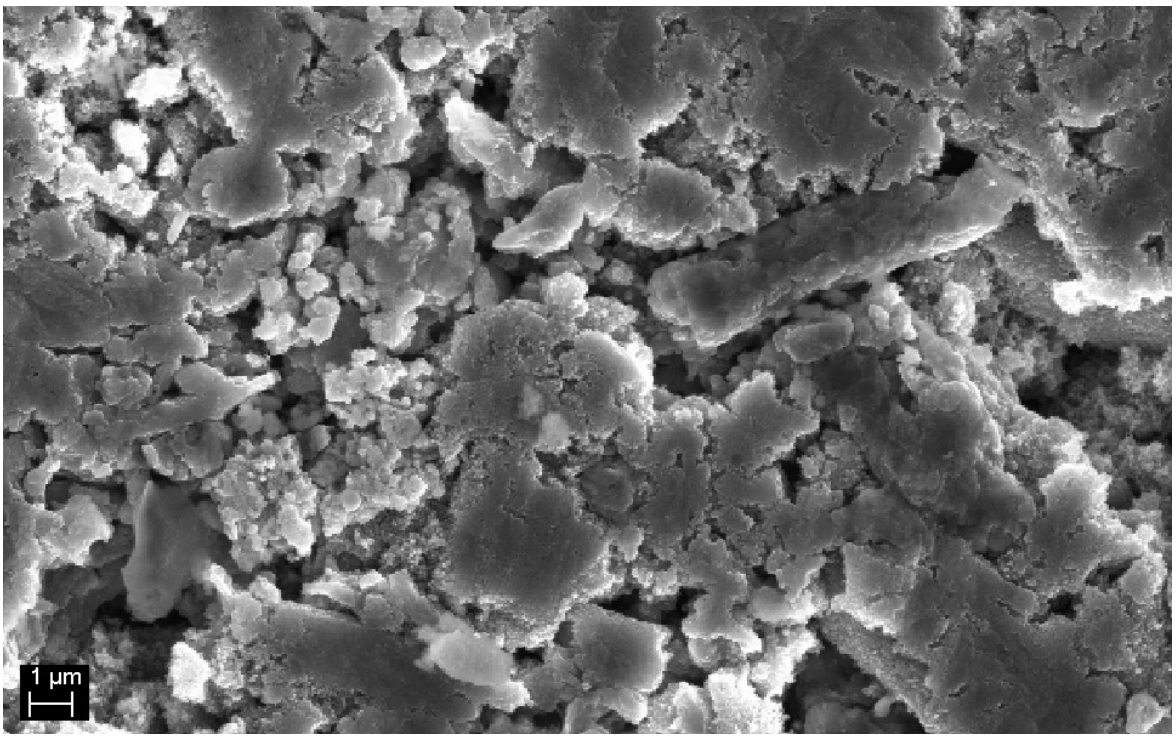


Figure S3: SEM image of sample MgTi15 after cycling in the HPDSC.