Supplementary Information

Remarkable hydrogen storage properties for nanocrystalline MgH₂

synthesised by the hydrogenolysis of Grignard reagents

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Figure S1. EDX analysis of H$_2$-DibutylMg (A) after hydrogenolysis - corresponding to Figure 5A and (B) after cycling - corresponding to Figure 8D.
Figure S2. TGA/DSC of H₂-DibutylMg after the first hydrogen cycle. Measurement done with a heating rate of 10 °C.min⁻¹ and under a 25 ml.min⁻¹ Ar flow.

H₂-DibutylMg released 7 mass % of hydrogen in agreement with the hydrogen storage capacity measured during cycling, i.e. 6.8 mass %.
Figure S3. XPS narrow-scan of C1s for H₂-DibutylMg (A) resulting from the hydrogenolysis of di-n-butylmagnesium and (B) after the first hydrogen absorption/desorption cycle.

The peak at 289.7 eV was assigned to CO₂ adsorption at the magnesium surface,¹ and the peak at 286.3 eV to C-O-C bond and thus hydrocarbon contamination²,³ (Such hydrocarbon contamination may come from THF vapor to be found in our glove box). The peak at 284.9 eV may correspond to C-C or C-H,²,³ and the peak at 289.7 eV was assigned to Mg-C bond.⁴
Figure S4. XPS wide-scan for H$_2$-DibutylMg (A) after hydrogenolysis and (B) after the first hydrogen absorption/desorption cycle.