Supplementary Information

Ultra-small MgH$_2$ nanoparticles embedded into an ordered microporous carbon

with rapid hydrogen sorption kinetics

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Content:

1) Pore size distribution of pristine carbon template CT

2) Hydrogenation of MgBu$_2$@CT followed by HP-DSC

3) N$_2$ sorption measurement at 77 K for all MgH$_2$@CT composites before and after HCl leaching

4) X-rays diffraction for pristine CT carbon and 50MgH$_2$@CT composite after leaching

5) Comparative study for determination of the activation energy of desorption of bulk MgH$_2$

6) $^3$H MAS NMR spectra from the CT and 15MgH$_2$@CT and related deconvolutions
1) Pore size distribution of pristine ordered microporous carbone CT

Figure SI-1. Pore size distribution of pristine carbon template CT from zeolite β.
2) Hydrogenation of MgBu$_2$@CT followed by HP-DSC

Figure SI-2. HP-DSC curve during hydrogenation reaction: Bu$_2$Mg@CT + H$_2$ → MgH$_2$@CT + 2C$_4$H$_{10}$↑ under 2.5 MPa H$_2$ with a constant heating rate of 5 K·min$^{-1}$. 
3) N\textsubscript{2} sorption measurement at 77 K for all MgH\textsubscript{2}@CT composites before (as-synthesized) and after HCl leaching

![Graph showing N\textsubscript{2} sorption isotherms at 77 K for MgH\textsubscript{2}@CT composites.](image)

Figure SI-3. N\textsubscript{2} sorption isotherms at 77 K for all MgH\textsubscript{2}@CT composites as synthesized (left) and after HCl leaching (right).
4) X-rays diffraction for the pristine CT carbon and the 50MgH$_2$@CT composite after leaching

![Graph showing X-rays diffraction](image)

Figure SI-4. X-rays diffraction of the pristine CT and the composite 50MgH$_2$@CT after leaching.

The X-rays diffractometer used is described in the experimental section. The diffraction peak at 7.5 ° strongly decreases after acid leaching of 50MgH$_2$@CT as compared to the pristine CT. This indicates a loss of structural ordering by insertion of MgH$_2$ nanoparticles, in agreement with previous results. [1]
5) Comparative study for the determination of activation energy of desorption of bulk MgH₂

Figure SI-5. Kissinger plot for bulk MgH₂ (left) and the comparison between the activation energies of desorption as calculated from Kissinger and Redhead methods (right).

The $E_{\text{des}}$ value calculated by Redhead method [2] for the slowest heating rate (1 K·min⁻¹) matches the one determined by Kissinger method suggesting that Redhead equation gives accurate results from our spectra recorded with low heating rates (1-2 K·min⁻¹).
6) $^1$H MAS NMR spectra from the CT, 15MgH$_2$@CT and 50MgH$_2$@CT and related deconvolution for 15MgH$_2$@CT

![1H MAS NMR](image)

Figure SI-6. $^1$H MAS NMR spectra from the CT, 15MgH$_2$@CT and 50MgH$_2$@CT (left) and related deconvolution for 15MgH$_2$@CT (right).

References: