Electronic Supplementary Information

A comprehensive study on Lithium-based reactive hydride composite (Li-RHC) as a reversible solid-state hydrogen storage system toward potential mobile applications

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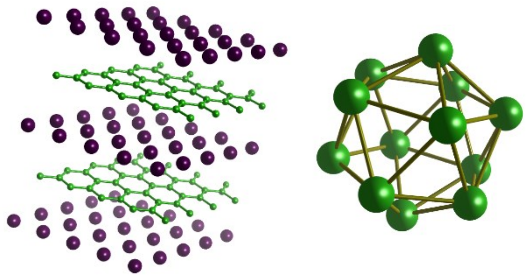

Figure S1. a) Layered structure of MgB_2 and b) Closo-structure of Boron Crystal structure.

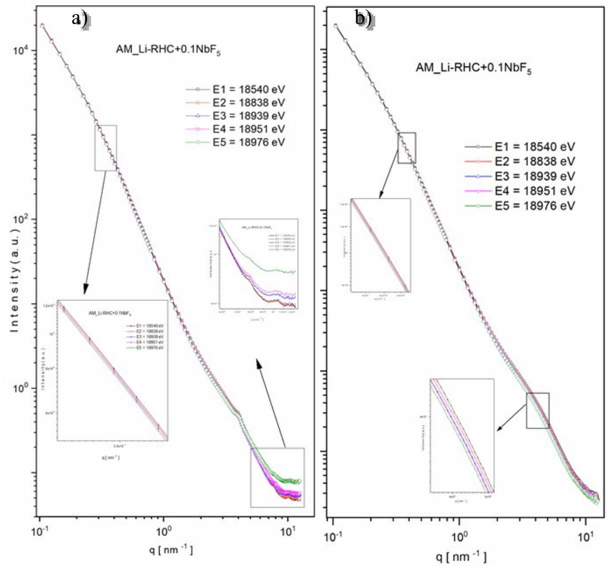

Figure S2. a) ASAXS curves collected at six energies close to the K-absorption edge of Nb (18.9 keV) b) ASAXS curves corrected for Kapton and incoherent scattering.

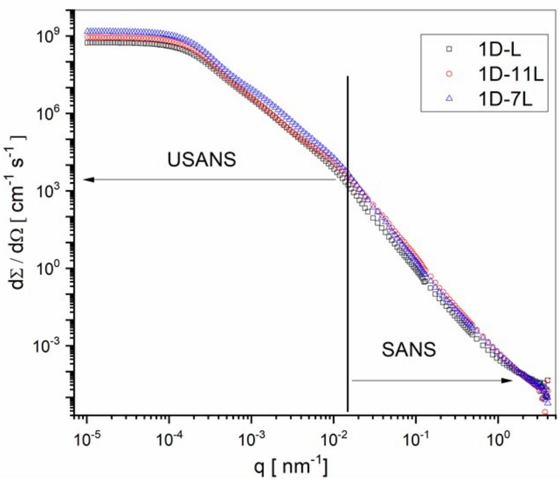

Figure S3. Merged SANS/USANS curves of pure $2LiBH_4+MgH_2$ with different isotopes after the first desorption.

Fitting model

For the SAXS/ASAXS and SANS/USANS scattering curves spherical particle distribution is assumed. The form factor of a sphere is given by:

$$F(q,r,\Delta\eta(E)) = 3\Delta\eta(E)\frac{\sin(qr) - qr\cos(qr)}{(qr)^3} \qquad (1)$$

and the size distribution of the spheres are assumed to be log-normal:

$$N(r) = \frac{1}{(2\pi)^2 r\sigma} exp\left(- \ln\left(\frac{r}{\mu}\right)^2 / 2\sigma^2\right) \qquad (2)$$

Table S1. Kinetic models for fitting the volumetric measurements of pure- and doped Li-RHC.[1-3]

Equation of the model	Model description
$\alpha(t) = kt$	Chemisorption/recombination on the particle surface is the rate-limiting step.
$[-ln(1-\alpha(t)]^{1/2} = kt$	2-dimensional growth of existing nuclei with constant interface velocity (2D-KJMA).
$[-ln(1-\alpha(t)]^{1/3}) = kt$	3-dimensional growth of existing nuclei with constant interface velocity (3D-KJMA).
$[-ln(1-\alpha(t)]^{2/3}) = kt$	Diffusion controlled 3-dimensional growth of existing nuclei with decreasing interface velocity (DC: 3D-KJMA).
$1-(1-\alpha(t))^{1/2}) = kt$	2-dimensional growth of contracting volume with constant interface velocity (2D-CV).
$1-(1-\alpha(t))^{(1/3)} = kt$	3-dimensional growth of contracting volume with constant interface velocity (3D-CV).
$1-(2\alpha(t)/3)-(1-\alpha(t))^{2/3}) = kt$	Diffusion controlled 3-dimensional growth of contracting volume with constant interface velocity (DC: 3D-CV).

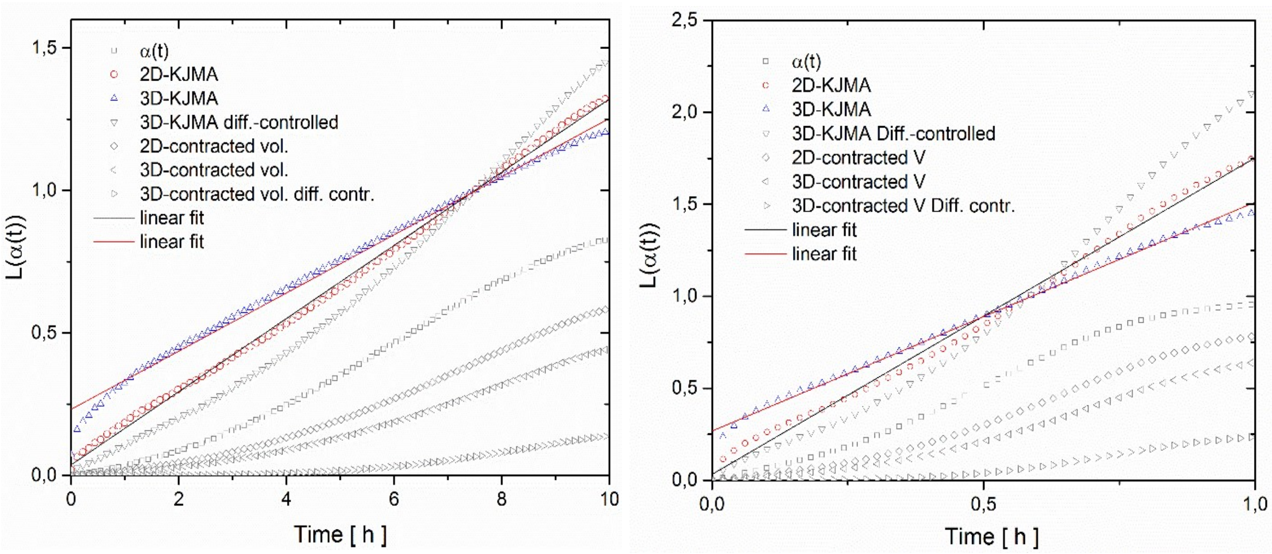

Figure S4. Kinetic models for the first desorption of a) pure Li-RHC and b) doped Li-RHC with the corresponding best fits.

References

1. M. Avrami, *The Journal of Chemical Physics*, 1939, **7**, 1103-1112.
2. M. Avrami, *The Journal of Chemical Physics*, 1940, **8**, 212-224.
3. M. Avrami, *The Journal of Chemical Physics*, 1941, **9**, 177-184.