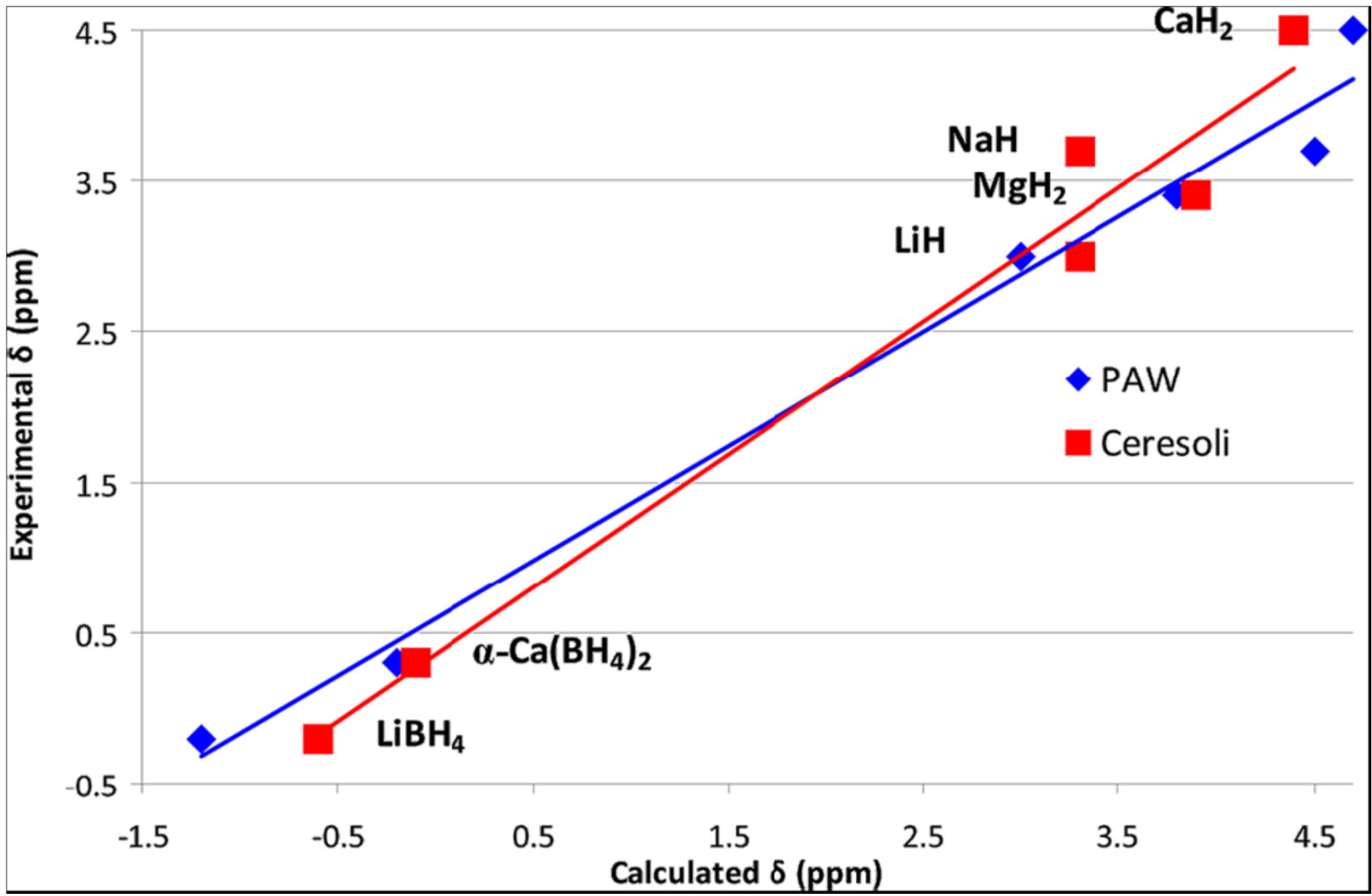
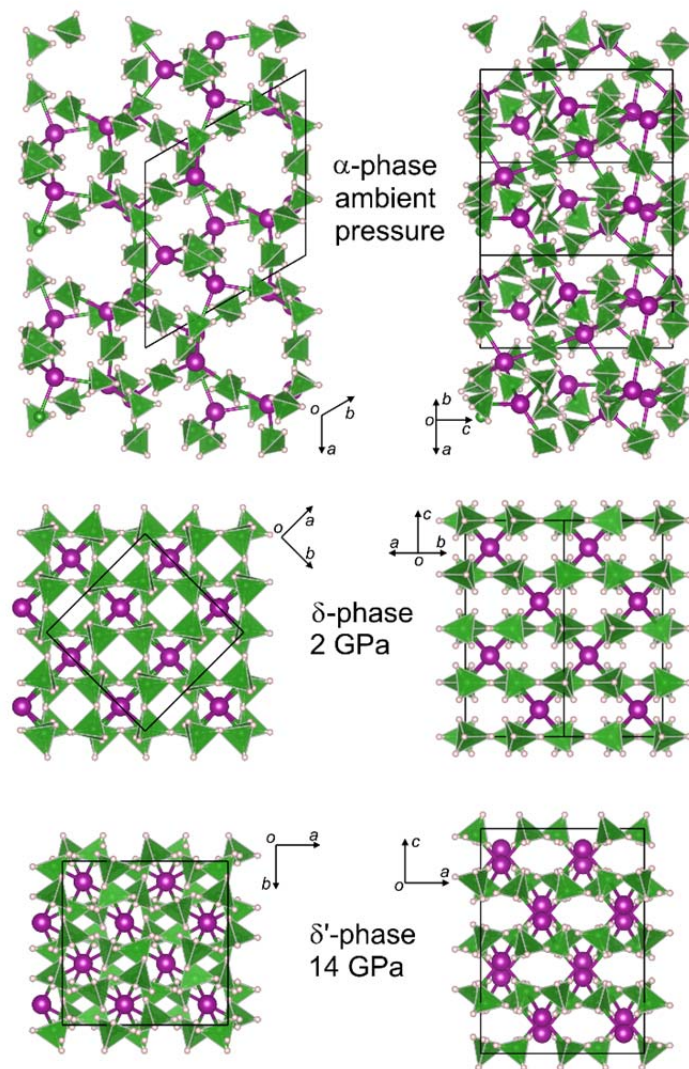


In line with this, diagrams or photographs illustrating and promoting the work of the project, as well as relevant contact details or list of partners can be provided without restriction.

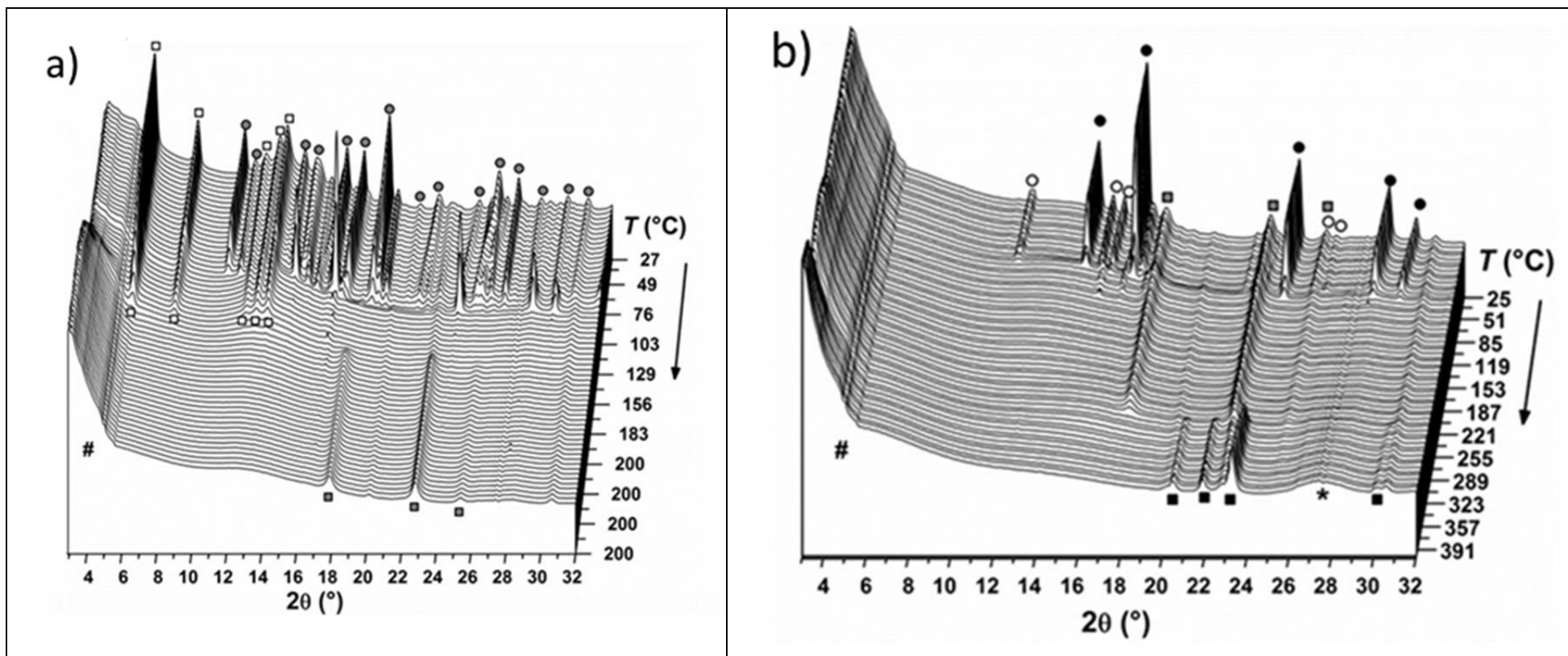




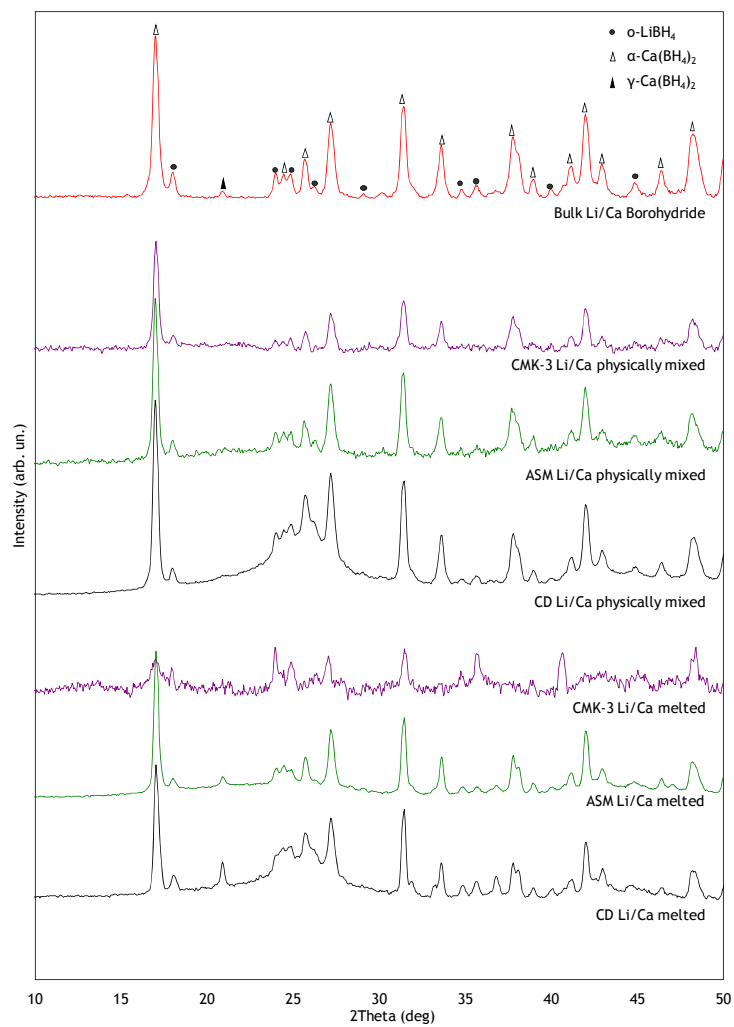
Modelling of boron hydride based hydrogen storage materials: experimental vs calculated ^1H chemical shifts in NMR spectroscopy (TMS as reference).



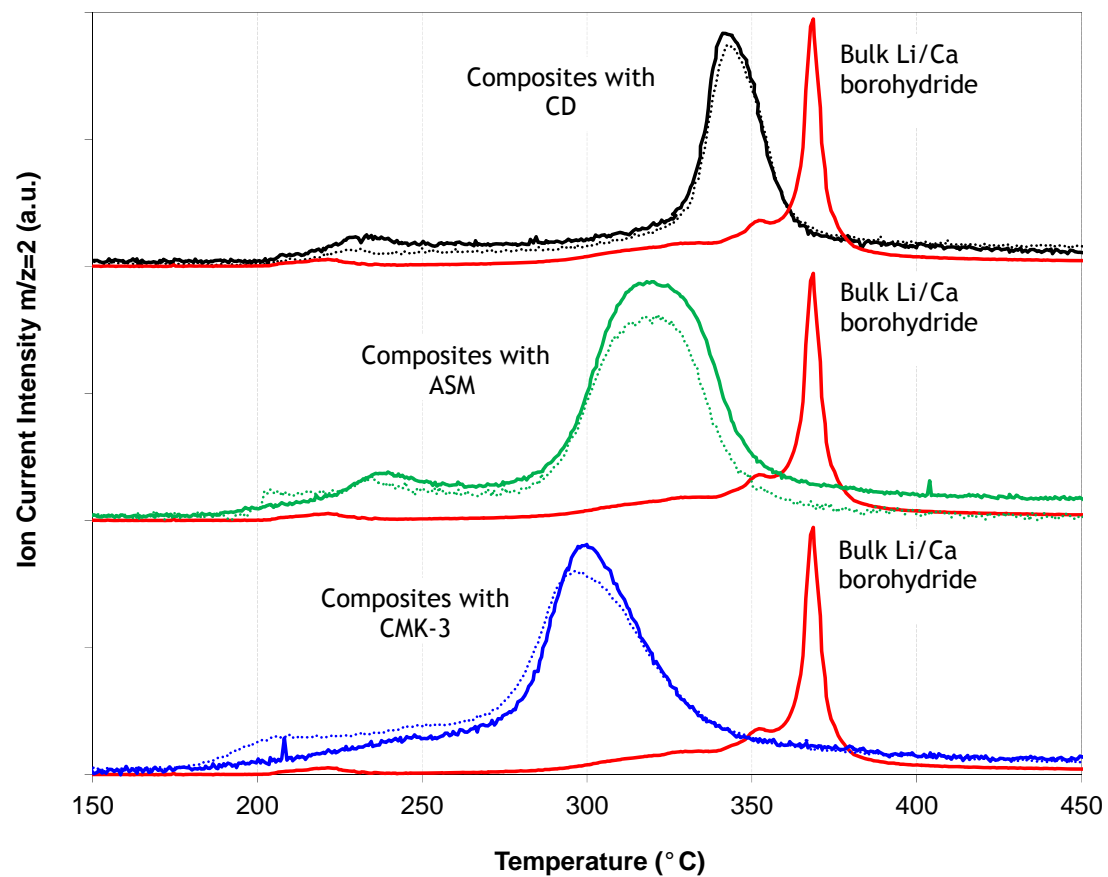
Crystal structures of α - $\text{Mn}(\text{BH}_4)_2$, high pressure δ - $\text{Mn}(\text{BH}_4)_2$ and higher pressure δ' - $\text{Mn}(\text{BH}_4)_2$, illustrating the increasing density of the material as function of pressure.



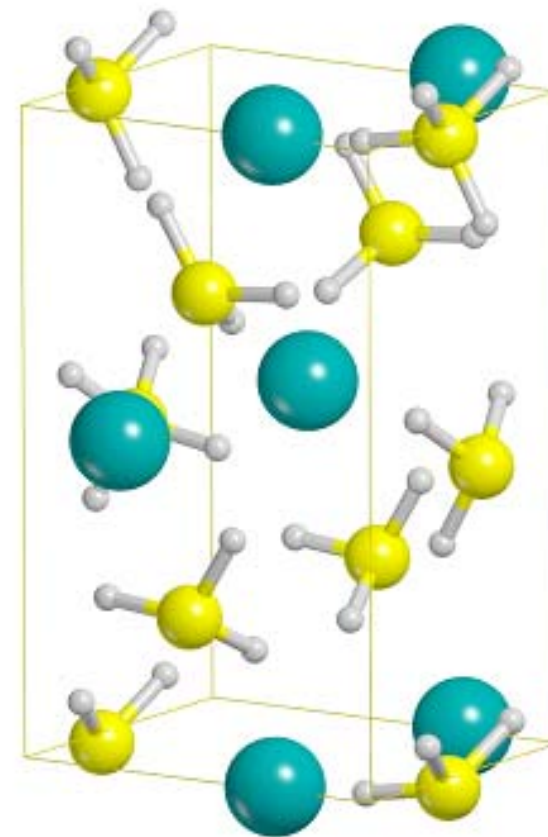
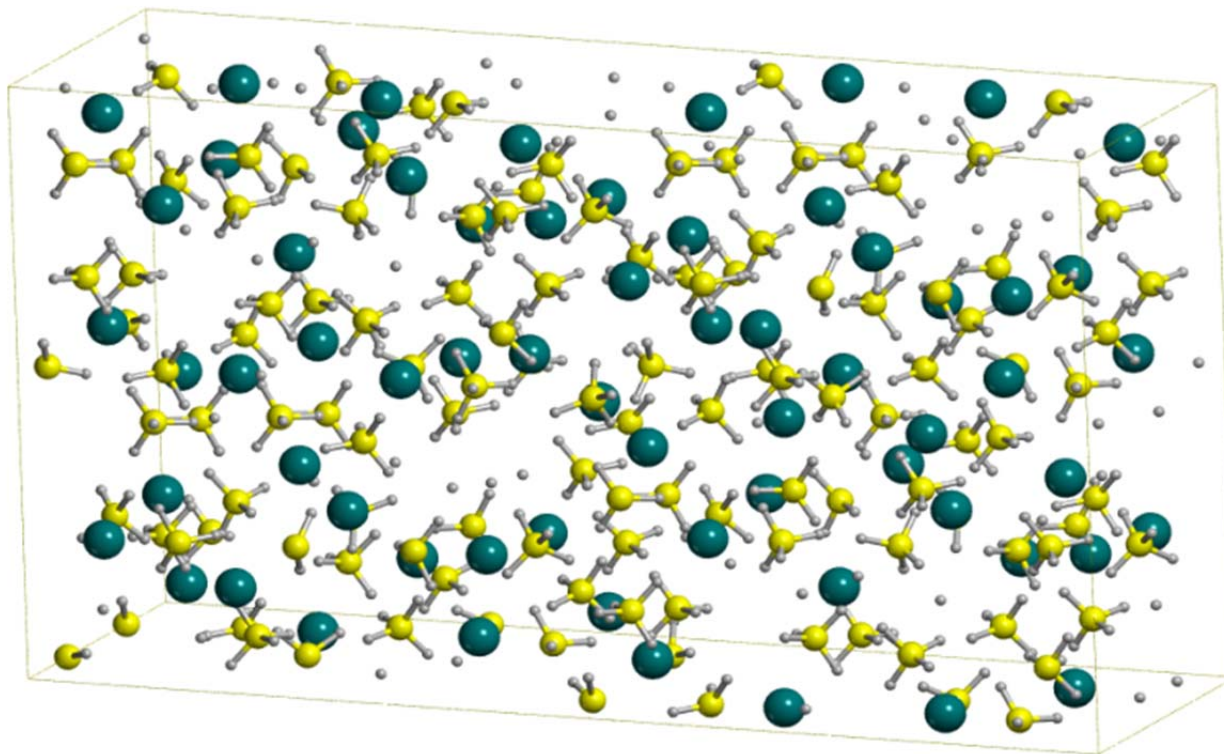
In situ SR-PXD measurements of $Mg(C_4H_9)_2$ infiltrated carbon aerogel scaffold X6 mixed with $0.725LiBH_4-0.275KBH_4$
(a) Melt infiltration, i.e. heating from RT to 200 °C ($\Delta T/\Delta t = 10$ °C/min) and kept isothermal at 200 °C for 15 min in $p(H_2) = 50$ bar.
(b) Hydrogen desorption, i.e. heating from RT to 400 °C ($\Delta T/\Delta t = 5$ °C/min), $p(H_2) = 10^{-2}$ mbar ($\lambda = 0.9919$ Å).
 Symbols: # Aerogel X6, □ $Mg(C_4H_9)_2$, ■ MgH_2 , ■ Mg, ● $LiK(BH_4)_2$, ○ $LiBH_4$, ● KBH_4 , * MgO.



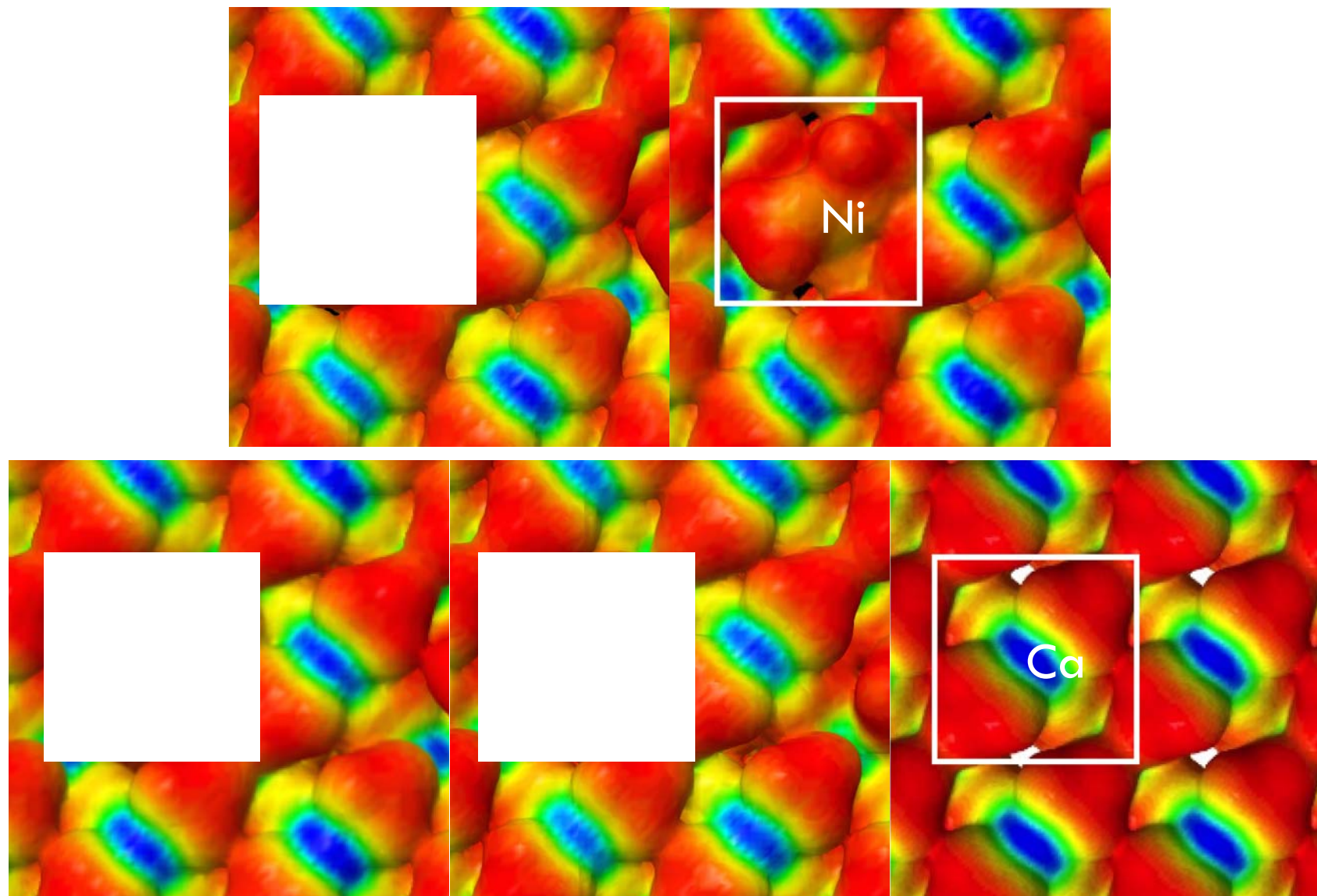
Powder X-ray diffraction patterns of bulk Li/Ca and Li/Ca carbon composites (60% Li/Ca mixture loading)



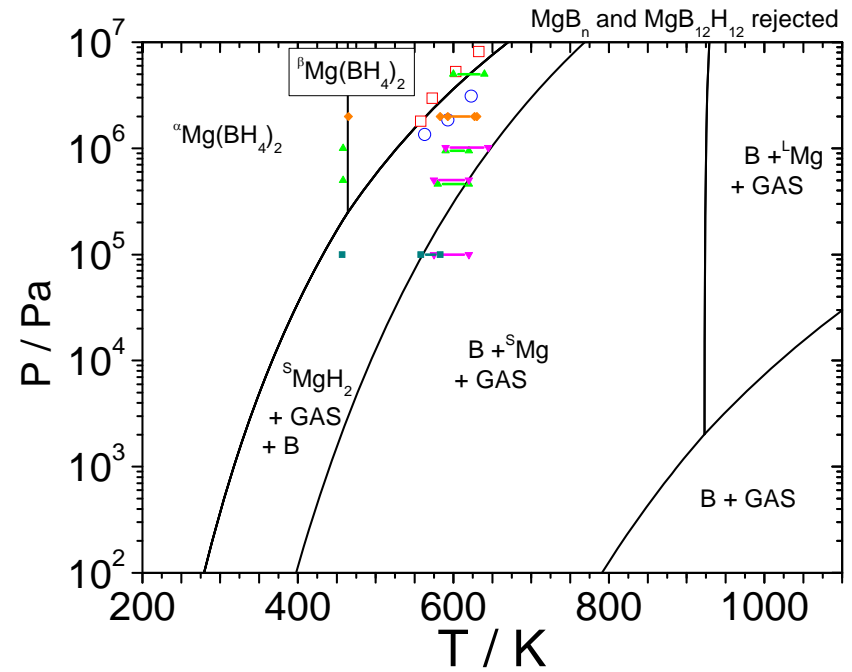
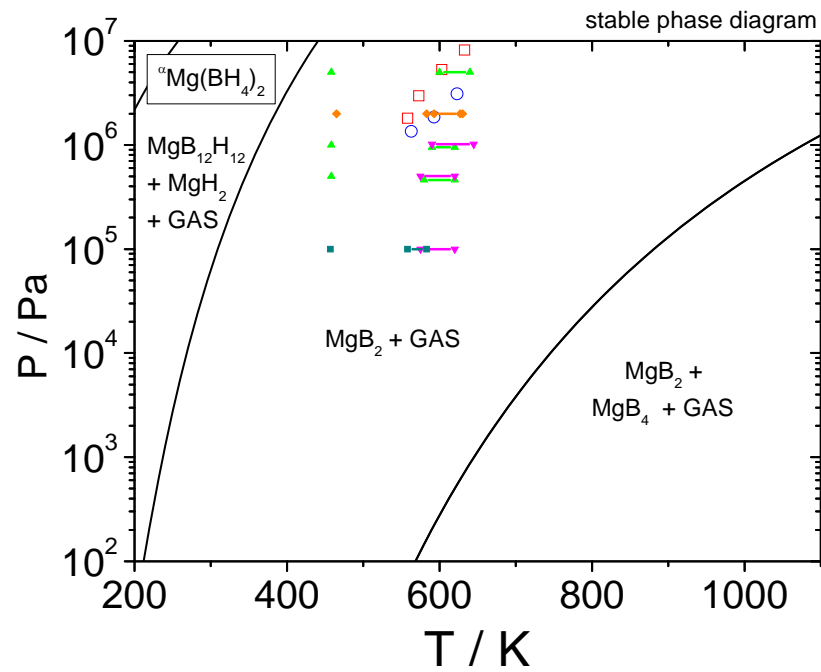
TPD-MS profiles. Dotted lines: physically mixed samples. Continuous lines: melted composites (60% Li/Ca mixture loading).



Unit cells of the high temperature $Fddd$ $Mg(BH_4)_2$ polymorph (left) and of the $Pmc2_1$ model system (right). Boron in yellow, calcium in green and hydrogen in white

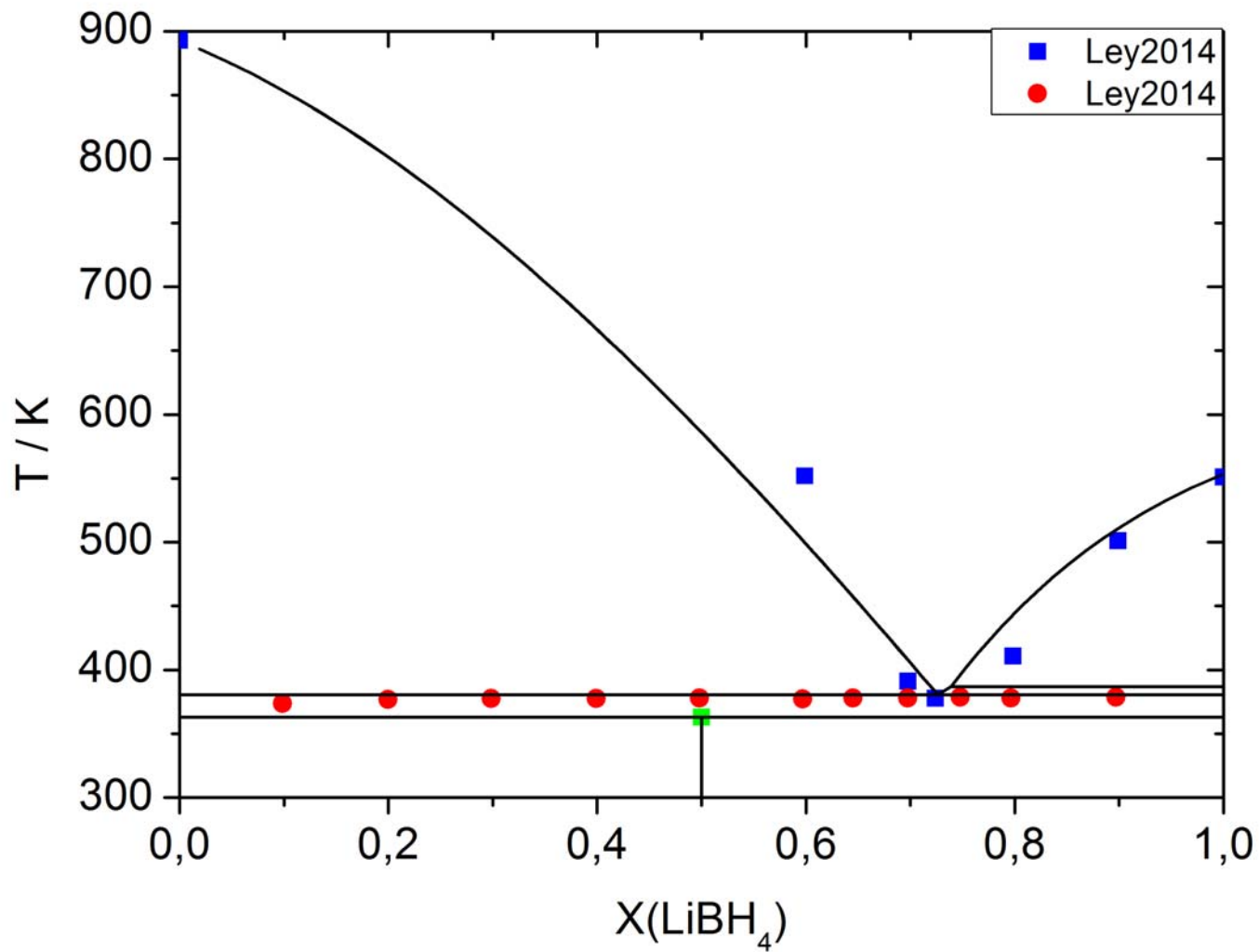


Top view of electrostatic potential (min: -0.029 a.u. (red); max: +0.246 a.u. (blue)) mapped on top of the charge density isosurface (i.e. 0.003 a.u.) for all the optimized structure. The region of interest is highlighted by the white box.



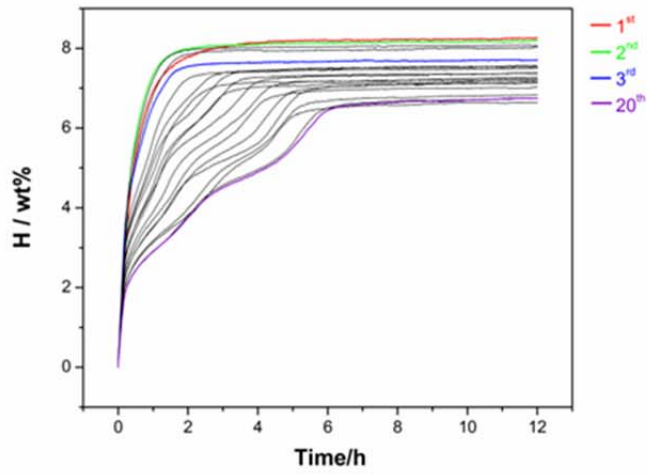
Calculated phase diagrams for $Mg(BH_4)_2$ composition. Stable phase diagram obtained considering all phases is shown on the left. Metastable phase diagram obtained rejecting $MgB_{12}H_{12}$ and magnesium borides is shown on the right. PCI and DSC data from literature are reported for comparison.

- Li, Acta Mater. 56(2008)1342
- Matsunaga, JALCOM 459(2008)583
- ▲ Hanada, J. Mater. Chem. 19(2008)2611
- ▼ Yan, Mat. Transactions 49(2008)2751
- ◆ Soloveichik, Int. J. Hydrogen Energy 34(2009)916
- Yang, Scripta Mater. 64(2011)225

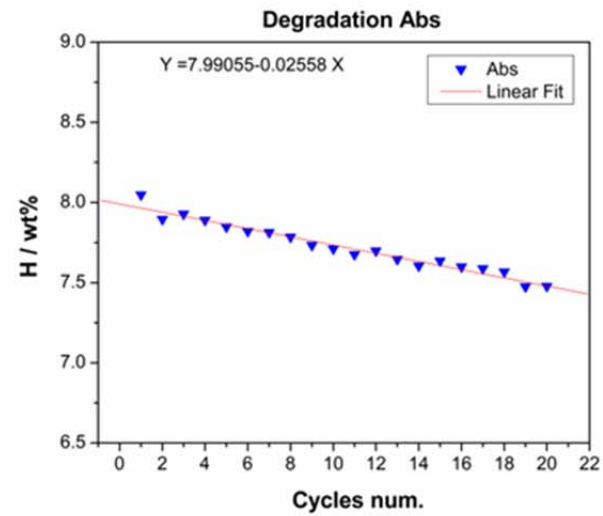
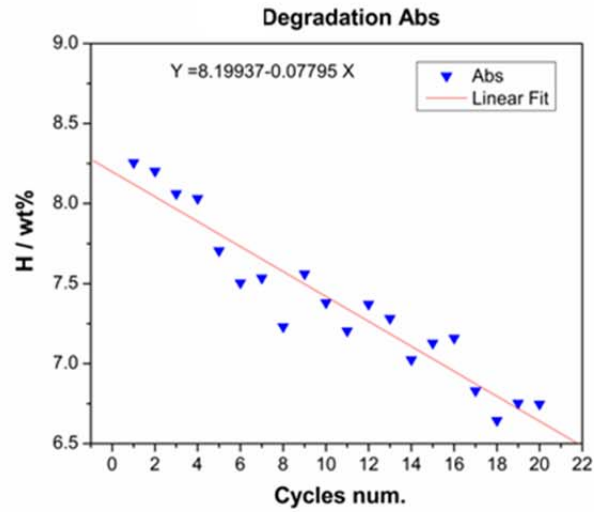
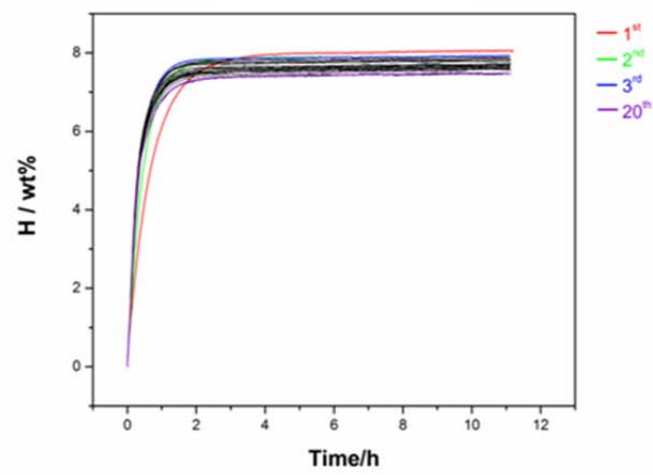


Calculated phase diagram for $\text{KBH}_4\text{-LiBH}_4$ system for $P_{\text{H}_2} = 1 \text{ bar}$ (lines). Experimental point obtained from the literature and from AU experiments (points).

2LiBH₄+1MgH₂+ 0.025 TiCl₃ (LiBH₄ 95 % purity)

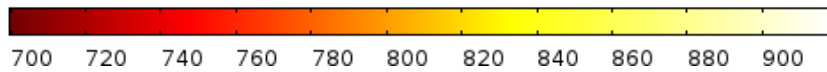
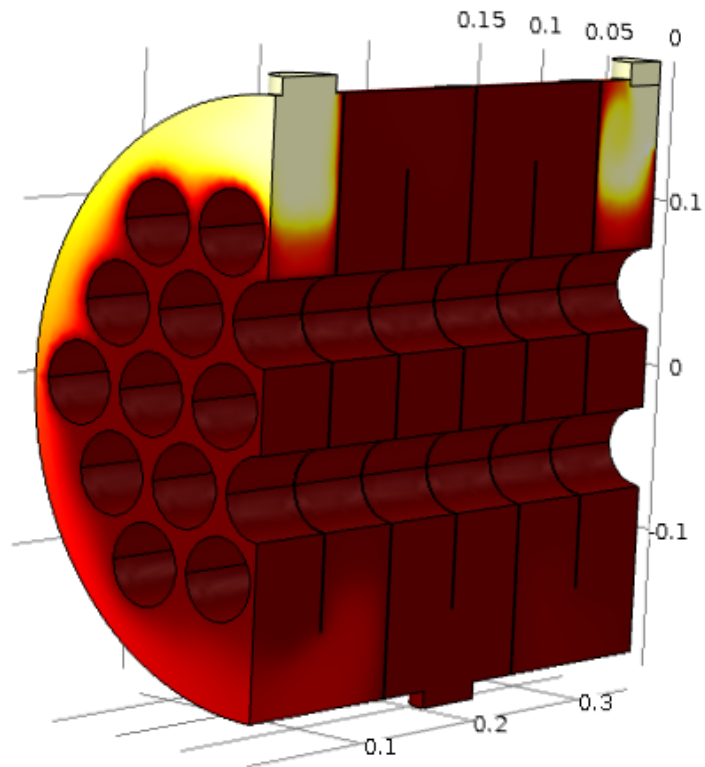


2LiBH₄+1MgH₂+ 0.025 TiCl₃ (LiBH₄ 85 % purity)

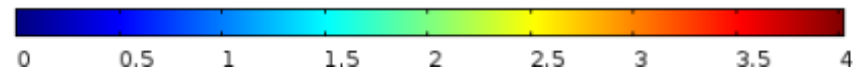
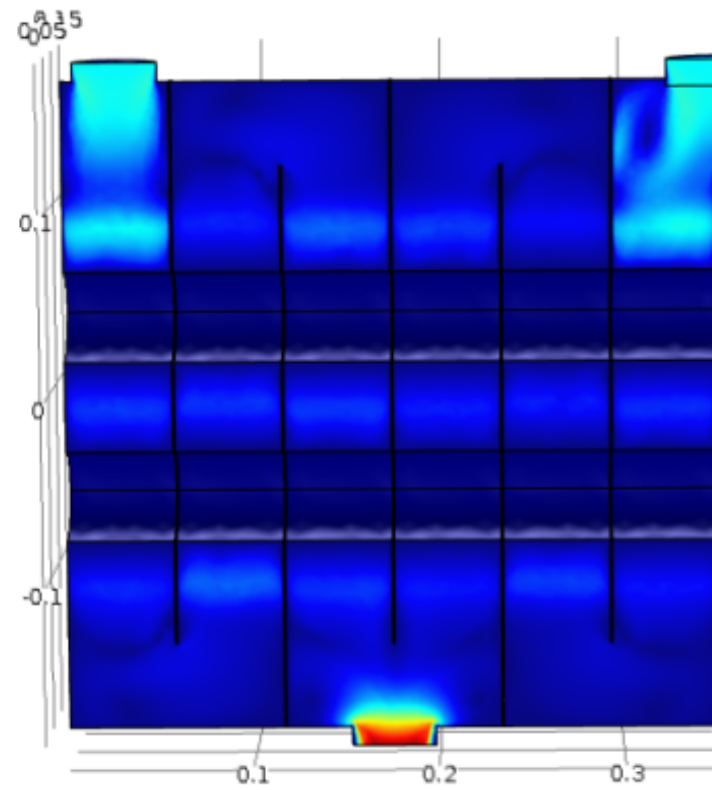


Absorption cycles 2LiBH₄+1MgH₂+ 0.025 TiCl₃ with LiBH₄ 85 % purity (right side) and with LiBH₄ 95 % purity (left side)

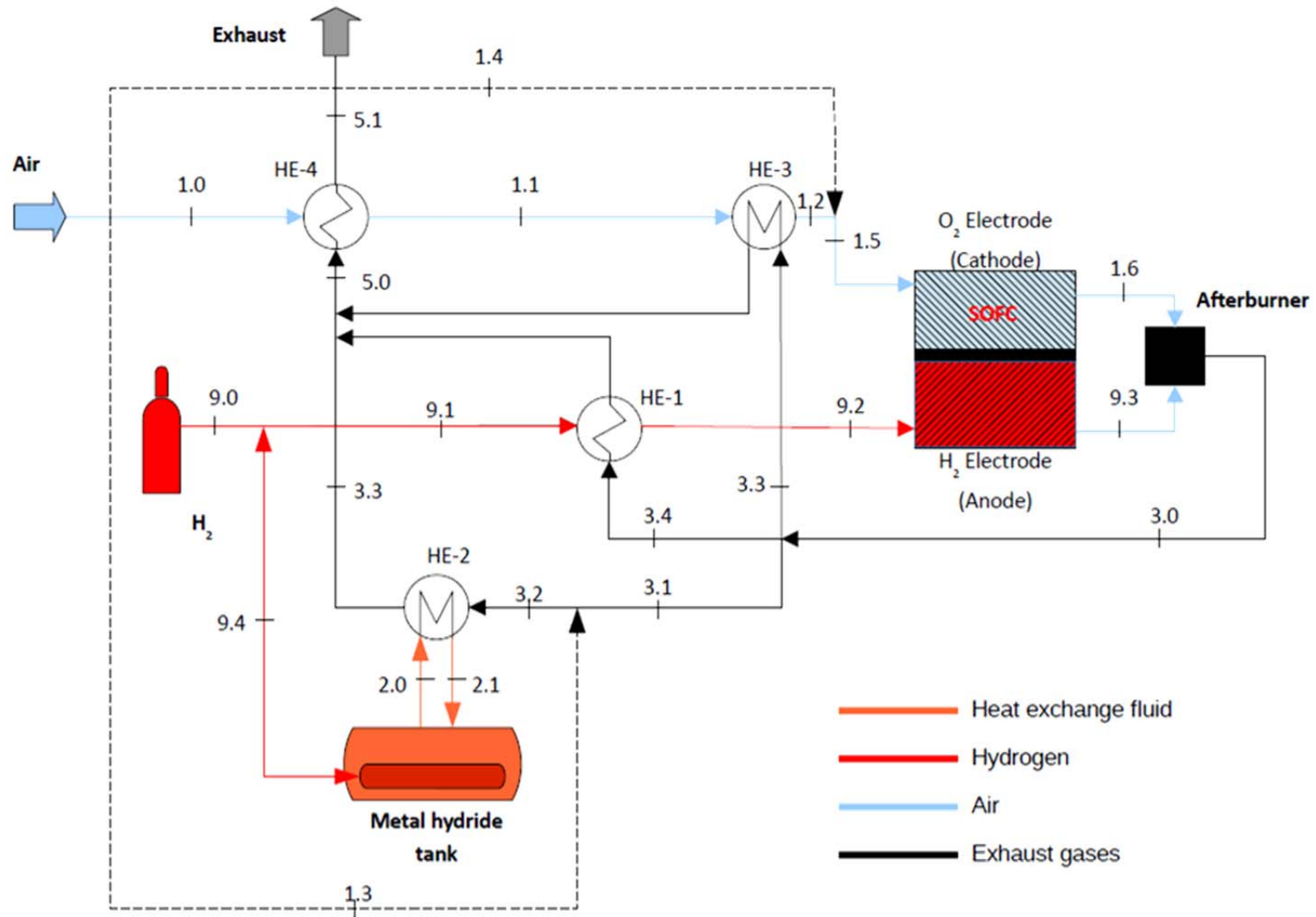
Time=20 s Surface: Temperature (K)



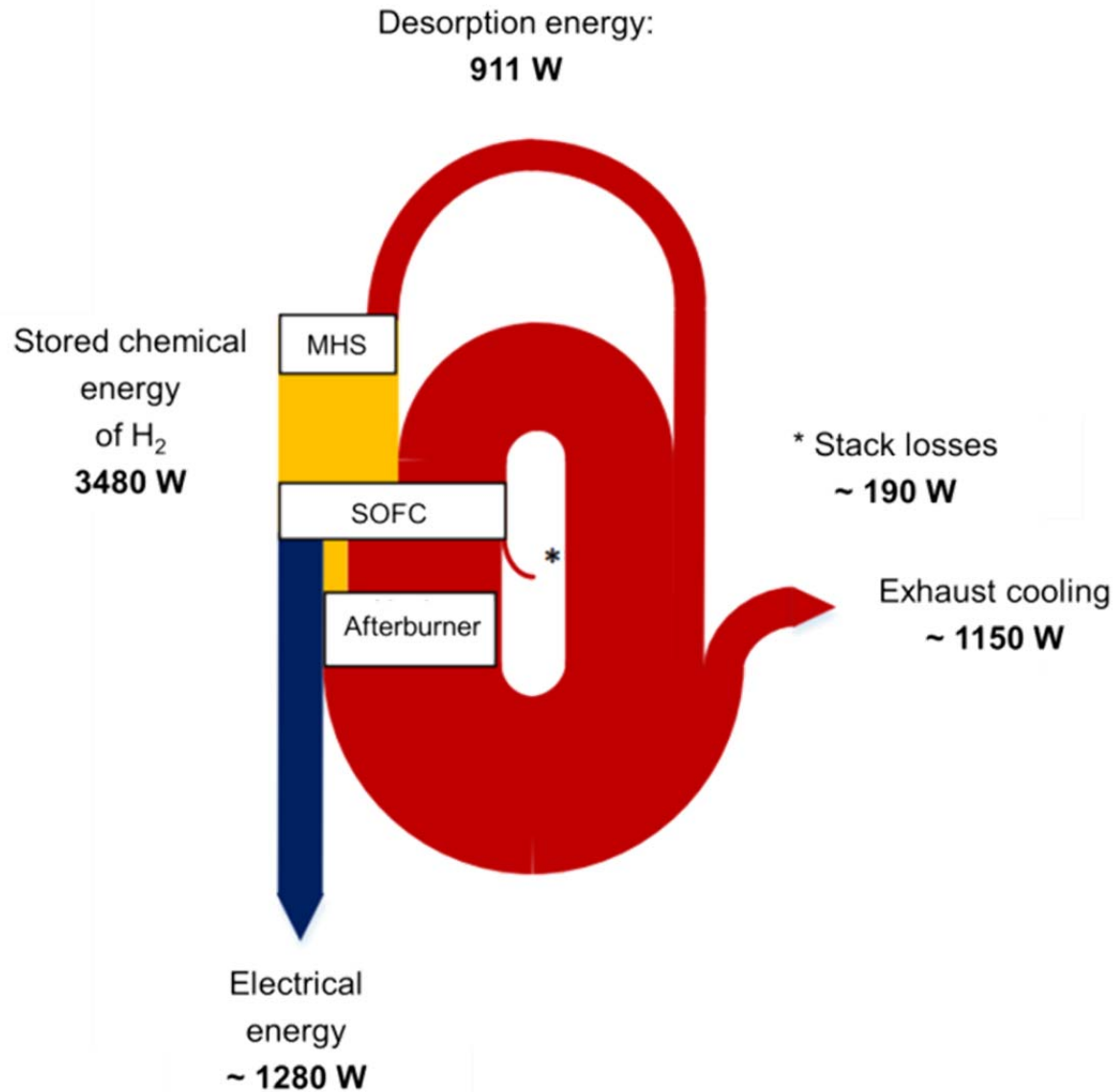
Surface: Velocity magnitude (m/s)



Temperature (left) and velocity magnitude (right) profiles within the helium heat exchanger designed by Helmholtz-Zentrum Geesthacht.



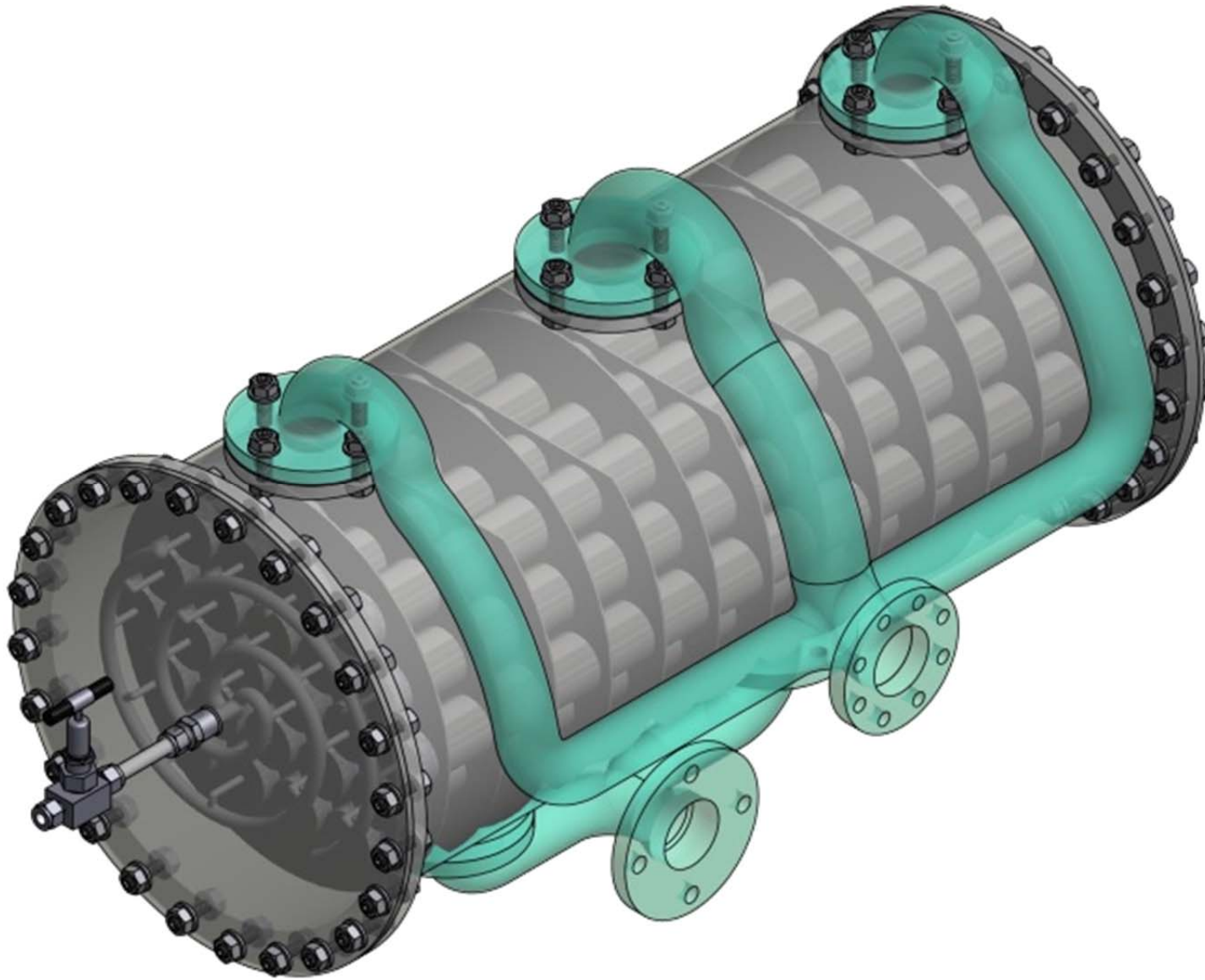
SOFC – MHT integration scheme (HE: heat exchanger)



Sankey diagram of the heat flows inside the integrated SOFC – metal hydride store (MHS) for the worst case scenario with MgH_2 ($\Delta H \sim 75 \text{ kJ}/(\text{mol } H_2)$), shown in Figure 43. The whole system can be operated without extra electrical heating of the MHS. For the Li-RHC ($\Delta H \sim 50 \text{ kJ}/(\text{mol } H_2)$) instead of MgH_2 , a smaller heat flow than 911 W, i.e. ca. 600 W, is required for hydrogen release. The simulation considered just the stationary case of continuous operation. Possible heat losses in the heat transfer system and of the MHS were neglected.



BOR4STORE single module tank (ZOZ name B4S-SM). Left and right heat shieldings for hydrogen supply and take-out line (left) as well as thermocouple lines (right). Image on heat shielding box shows cooling spiral in hydrogen line and flange of proper tank module



Multimodule tank design draft from HZG. Pressurised single tank modules (designed for 650°C and 100 bar) with welded ends. Outer hull contains heat transfer medium only and is designed for 650°C and 0.5 bar overpressure, closed by flanged ends for easy mounting of the single modules. Vertical plates guide the heat transfer medium around single tank modules.

