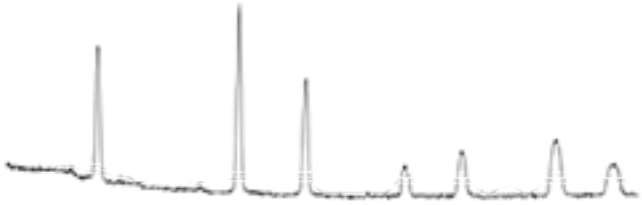

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Hydrogen motion in Li4(BH4)(NH2)3 investigated by Quasielastic Neutron Scattering (QENS)

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Fast and efficient hydrogen storage is one of the key components for the use of hydrogen in a sustainable energy economy. Reactive Hydride composites have been considered for some time as potential solid state storage systems, among others also the amide based mixture $Mg(NH_2)_2$ + 2 LiH. The kinetic performance of the hydrogen exchange reaction in this system is significantly enhanced by the addition of $LiBH_4$ [Gizer et al. Inter. J. Hydrogen Energy 44, 11920-11929 (2019)] and the subsequent formation of the amide-borohydride compound $Li_4(BH_4)(NH_2)_3$. Here, we present a study of the structure and of the anion motion of in $Li_4(BH_4)(NH_2)_3$ investigated with synchrotron radiation powder X-ray diffraction (SR-PXD) and quasielastic neutron scattering (QENS) at temperatures close to operating condition. SR-PXD confirms the recrystallization of $Li_4(BH_4)(NH_2)_3$ into the α-phase during cooling from the melt. The QENS measurements prove a long-range diffusive motion of hydrogen containing species at 514 K with the diffusion coefficient $D \sim 10^{-6}\,\frac{\mathrm{cm}^2}{\mathrm{s}}$. At temperatures below 514 K, localized rotational motions were observed which have been attributed to (BH_4^- tetrahedra units undergoing rotations mainly around C_3 axes. The activation energy for this thermally activated process is found to be $E_a = 15.5\pm0.9$ and $17.4\pm0.9\,\frac{\mathrm{kJ}}{\mathrm{mol}}$ for the two instrumental resolutions utilized in the QENS measurements, respectively, corresponding to observation times of 55 and 14 ps. The results will be discussed in the context of the improved hydrogen exchange reaction that is observed in $Mg(NH_2)_2$ + 2 LiH with $LiBH_4$ additions.

Authors: PISTIDDA, Claudia (Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon); GIZER, Gökan (Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon); ASLAN, Neslihan (GEMS at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); DORNHEIM, Martin (Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon); MÜLLER, Martin (Helmholtz-Zentrum Hereon); BUSCH, Sebastian (GEMS at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); Dr LOHSTROH, Wiebke (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München)

Presenter: Dr LOHSTROH, Wiebke (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München)

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