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QENS and in-situ SANS Investigations of Complex Hydrides

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With hydrogen as energy carrier, hydrides are in the focus of research for the application of energy storage and energy transportation. Within the complex hydrides, the metal hydride composite Mg(NH2)2 + LiH has recently gained in importance because of good properties for reversible hydrogen storage. Mg(NH2)2 + LiH has faster de- and rehydrogenation kintetics with the addition of LiBH4. So far Mg(NH2)2 + LiH + LiBH4 is a good candidate to be used for hydrogen storage with the high capacity (ca. 4 wt%) and good reversibility.
To understand the effect of the LiBH4 additive on the kinetics, neutron scattering experiments were applied at the Heinz Maier-Leibnitz Zentrum (MLZ). With this poster we present the investigated quasielastic neutron scattering (QENS) and in-situ small angle neutron scattering (SANS) measurements.
At the TOFTOF instrument the Time-of-Flight spectroscopy of Li4BH4(NH2)3 was investigated, which is an intermediate of the dehydrogenated Mg(NH2)2 + LiH + LiBH4-system. This product showed in the QENS measurement high degree of freedom for rotational and transversal motions. With the high mobility of the BH4-tetrahedron, the fast absorption/desorption kinetics of the complex hydrides are explained.
In-situ SANS of Mg(NH2)2 + LiH + LiBH4 at SANS-1 instrument was measured. The analyzed sizes of the nanoparticles are preserved after hydrogenation/dehydrogenation reactions. In addition, a model for these reactions are proposed based on the in-situ measurements.

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