

Hydrogen dynamics in β -Mg(BH₄)₂ in the picosecond timescale

Thursday, 18 June 2015 09:00 (20 minutes)

Among the complex hydrides, magnesium borohydride is attractive due to a quite good thermodynamic stability and high hydrogen storage capacity (14.9 H₂ wt %). Quasielastic neutron scattering (QENS) has been performed beta phase of Mg(11BH₄)₂ at the cold neutron time-of-flight spectrometer TOFTOF at FRM II, Munich. Spectra were reordered in the range of temperature from 11 to 500 K, in order to investigate the [BH₄] unit dynamics. At low temperature a strong inelastic contribution has been observed, whereas at higher temperatures the quasielastic contribution is predominating. A jump rotation dynamic has been identified, superimposed to a vibrational dynamic of the entire [BH₄] units. The quasielastic signal, as well as the vibrational signal, have been evaluated and used to determine the hydrogen motion in the scanned range of temperature and in the picoseconds time scale.

Primary author: SILVI, Luca

Presenter: SILVI, Luca

Session Classification: Material Science

Track Classification: Material Science