

Structure and dynamics of complex hydrides

Andreas Borgschulte

*Laboratory 138 Hydrogen & Energy, Empa - Materials Science & Technology
Überlandstrasse 129, CH-8600 Dübendorf, Switzerland*

The investigation of the structure and dynamic of solid helps in understanding the sought physical properties such as thermodynamic stability or ion conductivity. The pseudo-binary $\text{LiBH}_4\text{-LiI}$ system, which shows high Li-ion conductivity in the HT-phase of LiBH_4 , is studied by combined Raman and synchrotron X-ray diffraction, and nuclear magnetic resonance measurements. The vibrational properties measured as a function of composition and temperature corroborate the formation of a solid solution of the $\text{Li}(\text{BH}_4)_{(1-c)}\text{I}_c$ over the nearly entire phase diagram. The results shed light on anharmonic effects responsible for the structural phase transformation and its impact on the dynamic properties in this system. As a second example, I will discuss the vibrational properties of three allotropes of $\text{Ca}(\text{BH}_4)_2$ using density-functional theory calculations, infrared spectroscopy and inelastic neutron scattering. We show that the vibrational properties of $\text{Ca}(\text{BH}_4)_2$ depend on the specific phase and are hitherto the origin of their stability.