

ENERGYPOLIS SEMINAR

28. 11. 2016, 11:00 - 12:00, ENERGYPOLIS Sion, 4th floor, Seminar room

Structural studies of complex hydrides

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Detailed knowledge about the positions of the atoms is of major importance both for development of new compounds and for understanding of their properties. Neutron diffraction is a unique tool for studies of metal hydrides since it is the only method to determine the positions of the hydrogen/deuterium atoms in the crystal structures. The use of deuterium is crucial due to the challenge with incoherent scattering with normal hydrogen (protium). For studies of boron-based compounds, borohydrides, the ¹¹B isotope has to be used because of the strong absorption of neutrons in normal boron (mainly ¹⁰B). Most of our powder neutron diffraction (PND) experiments are performed with the high-resolution powder diffractometer PUS at the JEEP II reactor at IFE.

The combination of PND and X-ray diffraction is often important. In order to solve complicated structural features and to perform *in-situ* experiments, access to synchrotron radiation powder X-ray diffraction (SR-PXD) is crucial. SR-PXD is in particular important for detailed studies of crystalline phases during hydrogen absorption and desorption. Effects of additives are investigated by combined EXAFS/XANS and SR-PXD experiments. Our SR-PXD experiments are performed at the Swiss-Norwegian Beamlines (SNBL) at the ESRF, Grenoble, France.

Selected detailed structural studies and *in-situ* sorption diffraction experiments will be presented. The presentation will address recent studies of borohydrides and other complex hydrides. Selected examples of novel compounds, efforts to understand hydrogenation/dehydrogenation properties including effect of selected additives, will be described. The combination of neutron and synchrotron radiation X-ray scattering is in particular important and will be emphasized.

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CV: Prof. Bjørn C. Hauback

Hauback is Department Head and Chief Scientist of the Physics Department at IFE and adjunct professor of Physics at the University of Oslo in Norway. He has a PhD in physics at the Norwegian Institute of Technology from 1989. His main interests are structure-property relationships of hydrogen storage materials and neutron diffraction. At IFE Hauback is responsible for the neutron scattering activities in the research reactor JEEP II. He has contributed to 290 peer-reviewed articles and given 85 invited talks. Hauback led the Task 22 on hydrogen storage materials of the IEA HIA in 2006-12, and he was the co-chair of the Gordon Research Conference Hydrogen-Metal Systems in 2015.