École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis
Institute of Chemical Sciences and Engineering (ISIC)
Basic Science Faculty (SB)
Energypolis, Rue de l'Industrie 17, CH-1950 Sion, Switzerland

SEMINAR

Highlights in Energy Research

21. 9. 2017, 10:30 - 11:30, ENERGYPOLIS Sion, 4th floor, Seminar room

Electronic properties of Mg_2NiH_{4-x} across the metal-to-insulator transition for industrial hydrogen sensing

Dook van Mechelen

ABB Corporate Research, Segelhofstrasse 1K, 5405 Baden-Dättwil, Switzerland

Optical hydrogen sensors have a promising future in a society where hydrogen detection becomes increasingly essential. The traditional use of Pd as sensing material is disadvantaged by its small optical contrast and low sensitivity. A solution is found by complex metal hydrides that are structurally disordered and manifest a metal-to-insulator transition. The amorphous structure offers the sensor's reversibility and reproducibility. The metal-to-insulator transition translates through the electronic properties into an optical change that is uniquely linked to the hydrogen content, thereby avoiding cross sensitivity from the application environment.

In this talk I first present an optical and transport study on the metal-to-insulator transition in Mg-Ni-H. Experimentally, a significant electron renormalization is observed that increases towards the insulating phase. The lacking Drude weight is recovered in a series of mid-infrared bands. DFT calculations show that band flattening due to a decreasing hydrogen vacancy concentration cannot account for the observed mass. The calculations further suggest the presence of in-gap Ni 3d states that are hybridized with Mg and H. Transitions involving these states cause infrared spectral weight that qualitatively corresponds to the experiment. Subsequently, I discuss the materials science of making Mg-Ni-H amorphous by using the properties of Ni-Zr. The last part of the talk demonstrates the way from the basic electronic properties to a functional hydrogen sensor, where the hydrogen content is determined from the infrared behavior using fiber optic telecom technologies. Eventually I show the behavior of an amorphous complex metal-hydride in its industrial environment such an oil-filled power transformer.

CV: Dr. Dook van Mechelen
Born in 1980 in the Netherlands, Dook van Mechelen graduated with a MSc degree in Physics from the Vrije Universiteit Amsterdam in 2005. During his education, his research focused on the physics of complex metal hydrides. In 2010 he obtained a PhD degree in Physics from the University of Geneva. His thesis is in the field of quantum matter in perovskites probed with optical spectroscopy. From 2011, Dook has founded his THz spectroscopy lab at ABB Corporate Research where he aims at industrially and academically maturing THz technology to foster its societal implementation. In addition, he works on metal hydrides for the industrial application of an optical hydrogen sensor.