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NEUTRONS FOR SOCIETY

Hydrogen Dynamics in Elementary Reactions on Molybdenum Compounds

Hydrogen gas is an important energy carrier in connection with carbon-free energy production and as such part of a promising energy conversion storage concept: Alternately, hydrogen is produced from water when excess energy is available and reconverted when energy is in demand. Unfortunately, the water-splitting reaction in electrolysers requires the use of catalysts, which generally contain substantial amounts of expensive noble metals such as platinum. To reduce the need for platinum and to lower catalyst costs, several materials are being studied, among which we are concentrating on molybdenum disulphide MoS_2 and the molybdenum carbides MoC and Mo_2C. These catalyst materials are promising candidates for the cathode of polymer electrolyte membrane (PEM) electrolysers, but it is not clear how the hydrogen moves and how its transfer during the reaction takes place. Based on a multi-technique study of the dynamics on various length and time scales including experiments and computational modelling, we aim to find out how these catalysts can be optimised.

The main focus of this project is on neutron spectroscopy and diffraction, with which we will study hydrogen diffusion mechanisms, surface dynamics, and the structural evolution of catalyst particles. The data will be correlated with studies of electrochemical reactivity and macroscopic diffusion using hydrogen depth profiling as well as electrochemical impedance spectroscopy, cyclovoltammetry and X-ray diffraction. The experimental data will be compared to molecular dynamics and density functional theory simulations, which will be performed on the ILL computing cluster and with collaborating scientists. The research will be carried out at Institut Laue-Langevin and at Westfälische Hochschule. Several experiments at European neutron and synchrotron radiation sources are also foreseen.