



**Westfälische
Hochschule**

Gelsenkirchen Bocholt Recklinghausen
University of Applied Sciences



PhD Studentship

Westfälische Hochschule (Recklinghausen, Germany) and Institut Laue-Langevin (ILL, Grenoble, France) jointly invite applications for a three-year PhD programme focusing on

Motion of Hydrogen in Catalytically Activated MoS₂

This PhD project is part of a three-year collaboration between Westfälische Hochschule and the Institut Laue Langevin. The student will be based 1 year in Germany and 2 years in France. He or she will be attached to the Doctoral School of Physics of the University Grenoble Alpes.

Neutrons play a crucial role in the understanding of hydrogen sorption and dynamics in advanced catalyst materials. In this project we want to help understand how different activation strategies impact the chemical bonds and dynamics of hydrogen in MoS₂ catalyst powders, one of the most promising candidates for replacing Pt in the production of green hydrogen. In previous work we have made substantial progress in the identification of chemical processes and dynamics of hydrogen in MoS₂ single crystals, which will now allow us to classify motion observed on powders, where we expect to see much more complex dynamics. The PhD work will be centred on neutron research, but in view of the complexity of the chemistry involved, it will be essential that we combine the neutron scattering with several analysis techniques including electrochemical methods, X-ray scattering and photoelectron spectroscopy as well as ion beam techniques and electrochemical analysis.

In the first year commercial MoS₂ nano powders will be studied, for which the samples are readily available. As-received powders will be loaded by exposure to hydrogen gas in-situ as well as ex-situ, respectively. In a second approach, that is more relevant for technical applications, powders will be deposited onto porous electrodes and processed in electrolysis. Activation energies and mechanisms of hydrogen diffusion on the surface and inside the material will be studied using quasi-elastic neutron scattering. These results will be correlated to the surface chemistry as observed by the two complementary techniques photoelectron spectroscopy (XPS, NEXAFS) and inelastic neutron spectroscopy (INS). Chemically and electrochemically doped MoS₂ powders will be studied in the following step. For this, methods for chemical and electrochemical treatment will be optimized in the electrochemistry lab at WH. The new material will be characterized using all available supplementary methods. In the second and third year the student will proceed to the analysis of the mobility of hydrogen in modified and doped powders. Neutron spectroscopy will be performed to identify the effect of the treatment on the motion of hydrogen species and their availability for catalysis. For the third year it is planned to complete the experiments and complement the analysis using simulations conducted on the computing cluster of the scientific computing group of ILL and with our collaborators at Université d'Orléans. In particular, molecular dynamics and DFT simulations are planned that model the mobility of hydrogen in the substrates.

The PhD student will start the project (1 year) in Franziska Traeger's group (Westfälische Hochschule, Recklinghausen, Germany) including short external stays for specific training and experiments at large scale facilities. In addition, the candidate will attend online doctoral courses at the University Grenoble Alpes. During the last 2 years, the PhD student will be based at ILL, Grenoble, and will focus on neutron scattering experiments, data treatment and calculations.

We are looking for a highly motivated candidate with an MSc degree in physics, chemistry or materials science. The candidate must meet the requirements to be enrolled in the Doctoral School of Physics of the University Grenoble Alpes.

How to apply: please send an email to Franziska Traeger, Peter Fouquet, and Andrea Piovano (franziska.traeger@w-hs.de; fouquet@ill.fr; piovano@ill.fr) with the subject "Thesis-MAT-2023_32-your name". Attach a CV, a brief motivation letter and a contact person for a reference. For additional details about the specific conditions for the PhD and the application procedure, please consult the following link: <https://www.ill.eu/careers/all-our-vacancies/phd-recruitment/open-phd-position>