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QENS study of the diffusivity of hydrogen in MoS2

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With an increase in renewable energy production, the problem of energy storage becomes more and more significant. One of the most promising ideas is storage in form of hydrogen gas, which involves the production of hydrogen by electrolysis and later its reconversion into electricity in fuel cells. It is of great importance for these processes to be carried out most efficiently with the most readily accessible materials. Therefore, there have been intense studies in the search for catalyst materials for the hydrogen and oxygen evolution reactions.
Molybdenum disulphide, MoS_2, has shown promising behaviour as a catalyst in the hydrogen evolution reaction (HER), which is completely in line with its known activity for hydrogenation reactions. In this presentation we will show the results of our study of the diffusion of hydrogen adsorbed inside layered MoS_2 crystals, for which we used quasi-elastic neutron scattering, neutron spin-echo spectroscopy, nuclear reaction analysis, and X-ray photoelectron spectroscopy \[1\]. The neutron measurements demonstrate fast diffusion of hydrogen molecules parallel to the basal planes of MoS_2. A much slower hydrogen diffusion was observed perpendicular to the basal planes using nuclear reaction analysis.
1 V. Kuznetsov, W. Lohstroh, D. Rogalla, H-W. Becker, T. Strunskus, A. Nefedov, E. Kovacevic, F. Traeger and P. Fouquet, Physical Chemistry Chemical Physics 23 (2021) 7961 –7973.

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