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Hydrogen mobility and reactivity in MoS2 catalyst

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Catalyst materials are an essential component in hydrogen production and for the operation of fuel cells. Today, however, they are mostly based on platinum, which is expensive and rare. Molybdenum sulfide, MoS2, which is more abundant and significantly cheaper, has shown interesting catalytic activity and has been a focus point of research in recent years [2]. MoS2 is a van-der-Waals bonded 2d material that, theoretically, provides a high density of active sites, but little is known about the mobility and the reaction steps of hydrogen and water in MoS2.

In this presentation we will discuss our recent studies on hydrogen mobility and reactivity in MoS2 [1]. To shed light on the possible pathways for improving the performance of MoS2 and other layered catalyst materials, we have studied the diffusion of hydrogen and water by means of neutron scattering and X-ray photoelectron spectroscopy combined with nuclear reaction analysis and molecular dynamics simulations.

We observed a very fast hydrogen diffusion parallel to the basal planes and a very slow diffusion perpendicular to the MoS2 basal planes. Water, on the other hand, cannot penetrate the perfect crystal, but can intercalate within volume defects, where it can access edge sites of the material. MD simulations were essential for the identification of the contributions of the different hydrogen species (H(+), H2, H2O) to the chemistry in MoS2.

References

[1] D. Merki et al, Chemical Science 2, 1262, (2011), Y. Cao, ACS Nano 15, 11014, (2021), J. Aliaga et al., Molecules 24, 4631, (2019), J. Xu et al., Chemistry – A European Journal 27, 15992, (2021), Q. Yang, et al., J. Phys. Chem. C 123, 10917, (2019), G. Li, et al. ACS Nano 14, 1707–1714, (2020).

[2] V. Kuznetsov et al. PCCP 23, 7961-7973, (2021).

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