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Hydrogen mobility in layered materials: MoS_2 and Carbon

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The global climate challenges require a rapid suppression of fossil fuel use. Batteries are now widely used to replace petrol in cars, but they still have many disadvantages in terms of elevated price, long charging time, use of rare chemical elements and recycling. Therefore, hydrogen is still considered an important energy carrier for future mobile applications and much recent research efforts are invested in optimising hydrogen storage and catalysis.

Layered materials such as molybdenum sulfide (MoS2) are being studied intensively because they can serve as matrix for hydrogen storage and as catalyst or cat-alyst support in fuel cells thanks to their large surface area [1]. In addition, MoS2 is inexpensive and widely available, in contrast to platinum, which still is the standard catalyst material. MoS2 is a van-der-Waals bonded 2d material that 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 the progress that we achieved in identifying the translational and rotational diffusion in MoS2 [2]. To shed light on the possible pathways for improving the performance of MoS2 and other 2d catalyst materials, we have studied the diffusion of hydrogen and water by means of neutron scattering and XPS combined with nuclear reaction analysis and MD simulations.

References

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