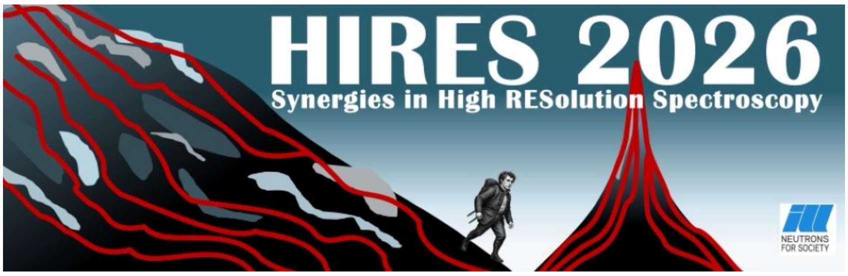

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From Atomic Motion to Catalytic Function: Unraveling Hydrogen Dynamics in MoS$_2$ through High Resolution Neutron Techniques

Hydrogen gas is a key energy carrier for a decarbonized energy system, especially when generated by water electrolysis. Molybdenum disulfide (MoS$_2$) offers a cost-effective alternative to platinum catalysts for the hydrogen evolution reaction (HER) [1], though its performance remains limited by slow hydrogen dynamics and incomplete understanding of adsorption and reactivity mechanisms. This study employs quasi-elastic (QENS), neutron spin-echo (NSE) and inelastic neutron scattering (INS) with XPS, XRD and EDX to elucidate how chemical doping and electrochemical activation control atomic-scale hydrogen motion in MoS$_2$ nanopowders and affect catalytic behavior [2,3]. Classical and ab initio molecular dynamics simulations support interpretation of these results [4].

For pristine MoS$_2$, QENS and NSE reveal distinct hydrogen and water mobilities operating on different time scales. INS identifies vibrational modes of water and S-H bonds, whose intensities rise after electrolysis, indicating enhanced surface hydrogenation and hydroxylation. Nitrogen doping greatly accelerates hydrogen diffusion, consistent with defect-induced, highly mobile adsorption environments. Complementary XPS, XRD and EDX confirm structural and electronic modifications underpinning the enhanced dynamics. Continuing work on Co-doped MoS$_2$ aims to further tune hydrogen transport pathways through compositional design.

[1] Cao et al., ACS Nano 15, 11014–11039 (2021)
[2] Yang et al., J. Phys. Chem. C 17, 10917–10925 (2019)
[3] Verma et al., Mater. Today: Proc. 102, 241–246 (2024)
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