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Advancing Spectroscopic Insights: Inelastic and Quasielastic Neutron Scattering for the Study of Hydrogen-Rich Materials

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Leveraging the unique interaction of neutrons with matter, neutron scattering techniques allow for the investigation of structural and dynamic properties that are often inaccessible by other means. Inelastic neutron scattering (INS) probes the vibrational modes of a system without the constraints of optical selection rules and is particularly effective in examining hydrogen-rich materials due to the large incoherent neutron scattering cross-section of hydrogen atoms. In the particularly small energy transfer regime, quasielastic neutron scattering (QENS) essentially studies the broadening of the elastic band given by the neutron scattering process [1]. This technique covers a sufficiently broad range in space and time to be able to study different dynamical processes, from fast vibrations and rotations to slow modes such as diffusion.

Here we present our recent study [2], in which we have used INS spectroscopy augmented by gas-phase and solid-state computational simulations to investigate the vibrational dynamics of methyl-β-D-ribofuranoside, a biologically significant carbohydrate with complex dynamic properties due to its five-membered furanose ring. Utilising the high-resolution capabilities of the TOSCA [3,4] spectrometer at the ISIS Pulsed Neutron and Muon Source, we obtained detailed INS spectra covering all vibrational modes up to approximately 500 meV with a good spectral resolution of 1.25% ΔE. Combining this with low temperature Raman and IR measurements, the dominating modes in condensed phase were characterised and spectroscopic evidence for a specific intermolecular H-bonding interaction in the unit cell was identified.

Taking advantage of the capabilities of QENS instruments to directly measure diffusive motions and dynamic processes of hydrogen-rich molecules over pico- to nanosecond timescales [5], we plan to combine the detailed vibrational information from INS with the dynamic data from QENS to study materials particularly relevant to catalysis research. Such studies will have broader implications in fields such as energy storage and sustainable chemical processes development.

References

[1] V. G. Sakai et al., *Current Opinion in Colloid & Interface Science*, 2009, **14**, 381. [2] M. Pascariu et al., *J. Phys. Chem. A*, 2024, **128**, 2111. [3] S. F. Parker et al., *J. Phys.: Conf. Ser.*, 2014, **554**, 012003. [4] R.S. Pinna et al., *Nuclear Instruments and Methods in Physics Research, A*, 2018, **896**, 68. [5] M. Kruteva, *Adsorption*, 2021, **27**, 875.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Condensed Matter