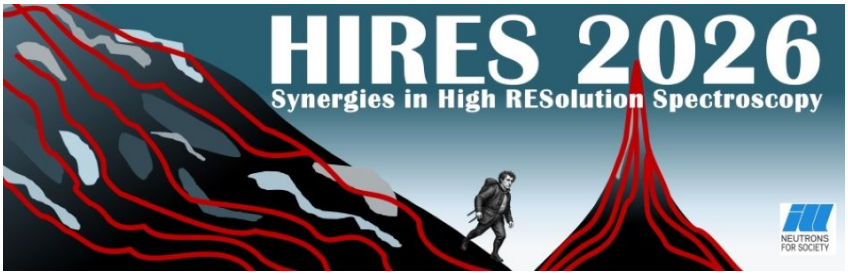

Contribution ID: **6** Type: **Oral**

Pressure dependent dynamical investigation of relaxations associated with hydrogen bonding in 1-propanol

Hydrogen bonds are ubiquitous in nature and play a central role in determining the microscopic dynamics of liquids. While water remains the most important hydrogen-bonded liquid, its peculiar behaviour and supercooling challenges motivate the study of simpler systems, such as mono-hydroxy alcohols,where hydrogen-bond dynamics are better separated from structural relaxation. Dielectric spectroscopy has shown that mono-hydroxy alcohols exhibit a dominant slow Debye relaxation, slower than the α-relaxation, and growing evidence suggests that poly-alcohols display a similar, though more merged, separation of processes. In this work, we investigate the relaxation dynamics of liquid 1-propanol and its 10% glycerol mixture above the glass transition using quasi-elastic neutron scattering (IN16B backscattering, wide-angle spin-echo, and IN5 time-of-flight) combined with dielectric spectroscopy. High-pressure measurements up to 6 kbar reveal that the slowest relaxation process shifts by orders of magnitude, whereas faster processes are largely unaffected, enabling their better separation. Selective deuteration demonstrates that this slow dynamic originates from intermolecular hydrogen bonds, while faster components are associated with methyl group motions and structural relaxation. Ongoing molecular dynamics simulations are used to calculate dynamic structure factors and support the interpretation of neutron and dielectric spectroscopy data, with the goal of disentangling the individual relaxation processes. Together, these experimental and computational efforts provide detailed insight into the pressure-,concentration-, and temperature-dependent hydrogen-bond dynamics of mono-hydroxy alcohols.

Session

Liquids

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