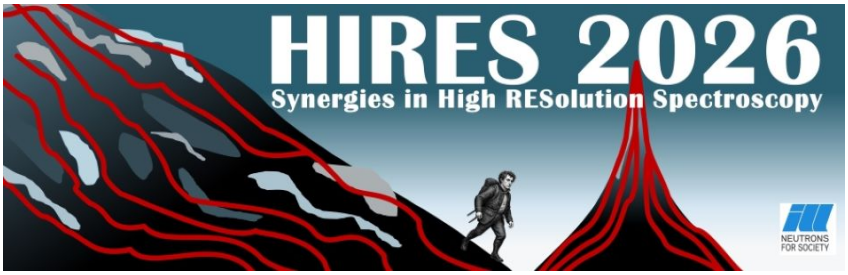

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Atomic dynamics studied with INS, QENS and large-scale atomistic simulations

Neutron scattering is an ideal probe of the atomic structure and dynamics in solids, from fast ionic diffusion in solid-state electrolytes to lattice dynamics and thermal transport in thermoelectrics, or structural distortions in metal-halide perovskites. Many of these phenomena bridge the time-scales probed by quasielastic and inelastic neutron scattering (QENS/INS). This presentation will illustrate the complementarity of QENS -both coherent and incoherent- and INS, as well as opportunities to leverage machine learning and large-scale atomistic simulations. Examples will focus on fast ion diffusion in superionic conductors [1-5] and dynamic structural fluctuations in metal-halide perovskites [6-8]. We investigated a series of halide and sulfide fast Na+/Li+ ion conductors, using a combination of coherent/incoherent QENS, INS, ab-initio molecular dynamics (AIMD), and machine-learning molecular dynamics (MLMD). In several instances, we find that soft anharmonic phonon modes play an important role in facilitating ionic hops, reflecting the softness in the potential energy surface. Further, the different coherent/incoherent components of QENS, supplemented with large-scale MLMD simulations, provide detailed insights into the diffusion process.

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Session

Hard Condensed Matter

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