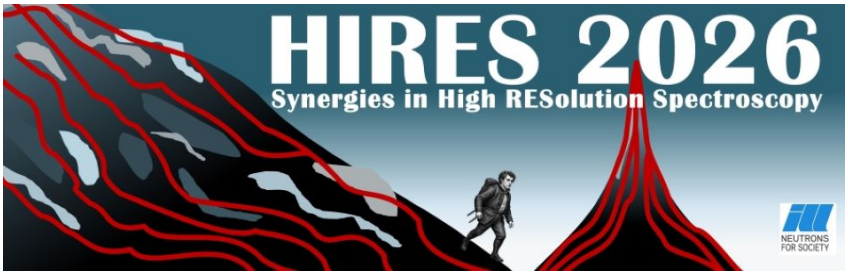

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A combined QENS and NMR study of the dynamics of the deep eutectic solvent ethaline

Over the past decade, Deep Eutectic Solvents (DESs) have garnered significant attention within the scientific community due to their remarkable functional properties. Yet their nanoscale organization remains challenging due to nanoscopic domains and dynamics heterogeneity.

We probed the molecular dynamics of the benchmark deep eutectic solvent ethaline, separating the motions of its two components choline chloride and ethylene glycol across a broad window of length and time scales (sub-nanometer to micrometers; picoseconds to milliseconds). Using pulsed-field-gradient NMR, time-of-flight QENS, and backscattering inelastic fixed-window scans (IFWS) on isotopically labeled samples, we obtained a species resolved view of the dynamics. At the micrometer scale, translational motion follows classical hydrodynamics: the two constituents exhibit distinct diffusion coefficients that reflect their different hydrodynamic sizes. This is no longer valid at the nanometer scale, where both components show similar short-range diffusivities, indicating strong supramolecular association. At sub-nanometer scales, we detect jump motions that precede Fickian diffusion and localized dynamics within transient molecular cages. The spatial amplitudes of these localized motions track each species molecular size and chemistry, while their correlation times differ from observations in other choline-based DESs (e.g., glyceline). Altogether, the results highlight how subtle differences in hydrogen-bonding propensity of the polyol donor control dynamics and why nanoscale behavior cannot be reliably inferred from macroscopic properties especially under varying environments such as confined media, interfaces, and porous catalysts.

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Session

Liquids

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