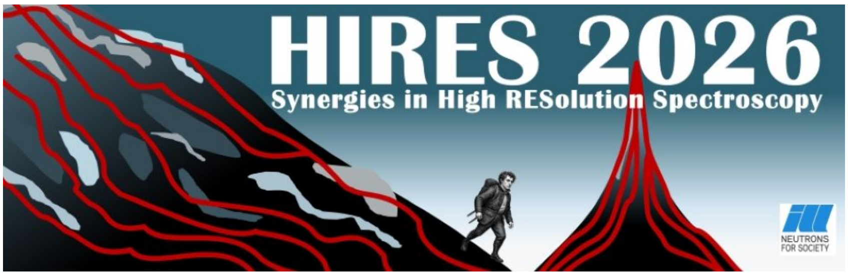

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Origin of Proton Conduction in Hydrated Sulfonated Porous Aromatic Framework: Insights from IN5B and IN16B QENS measurements

Understanding water diffusion in subnanometer pores is essential for designing next-generation proton-conducting materials. Sulfonated porous aromatic frameworks (SPAFs) offer a unique platform for this by combining rigid, permanently microporous carbon scaffolds with adjustable -SO3H densities. Their high proton conductivities, often comparable to fluorinated polymers, indicate that hydration and nanoscale dynamics differ markedly from bulk water, yet the microscopic basis remains unclear.
We address this question using complementary QENS measurements on IN16B (backscattering, λ = 6.2 Å, $\Delta E \approx$ 0.75 μeV) and IN5B (time-of-flight, λ = 4.9 Å, $\Delta E \approx$ 80 μeV) at ILL to resolve water dynamics in two fully hydrated SPAFs (93% RH) with nominal degree of sulfonation (DoS) 50% and 80%. Across all temperatures, the QENS data are consistently described by two separable motions: fast, local reorientation (resolved on IN5B) and a slower, translational jump-diffusion (resolved on IN16B). Because of the higher resolution, IN16B used for extracting the narrow translational linewidth Γ1(Q,T) via IFWS (3 and 6 μeV), which is then fixed in IN5B fits to isolate the broader rotational linewidth Γ2 and the EISF.
DoS_80% shows systematically slower translational diffusion and longer residence times than DoS_50%, indicating stronger water-acid interactions and reduced translational connectivity at higher acid density. Localized reorientations remain in the ps range, but vary in amplitude with DoS. Together, the combined TOF+BS dataset provides a continuous ≈10 ps - 1 ns dynamical window that links pore-scale dynamics to macroscopic, humidity-dependent proton transport and demonstrates the power of complementary neutron spectrometers for resolving ion conduction mechanisms in porous conductors.

Session

Soft Condensed Matter

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