22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

Hydrogen in Motion: From Confined Diffusion in MOFs to Collective Dynamics in Water

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Hydrogen is the lightest element and therefore exhibits pronounced quantum and collective effects that strongly influence transport phenomena in condensed matter. Understanding how hydrogen interacts with its local environment—through hydrogen bonding in liquids or confinement in nanoporous materials—is essential for revealing the microscopic mechanisms governing diffusion and relaxation processes. In this talk, neutron spectroscopy studies are presented that illustrate how hydrogen interactions control molecular transport.

Using neutron polarization analysis, we observe cooperative rearrangements of the hydrogen-bond network in bulk water beyond the independent-molecule picture. Enhanced correlations in the intermediate Q range (0.2–1 $Å^{-1}$) indicate picosecond reorientations involving several molecules, possibly associated with transient clusters and precursor processes for macroscopic transport such as viscosity and diffusion [1].

In nanoporous materials, quasi-elastic neutron scattering (QENS) reveals unusual hydrogen-isotope diffusion in flexible MOFs. Framework breathing and lattice-driven gating dynamically modify diffusion barriers, enabling kinetic quantum sieving and strong isotope-dependent mobility even at elevated temperatures [2,3]. Together, these studies show how hydrogen bonding and quantum confinement govern microscopic diffusion mechanisms.

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