Contribution ID: **20** Type: **Invited**

How the behavior of cations within interfacial layer can influence the water dynamics in confined media

Tuesday, 11 October 2022 10:30 (30 minutes)

The investigation of the processes taking place at the solid/aqueous solution interface in nanoconfinement media is an important key parameter to understand and predict the behavior of nanoporous materials. Indeed, understanding the water and ions behavior in such media can help to clarify the processes and chemical reactions occurring at this level of confinement. Recently, we highlighted how the dynamics and the structure of confined water in the presence of ions drive the alteration of mesoporous silica materials and glass [1−3]. This change of water properties is mainly due to the ions adsorption at the pore surface that structures water molecules [4−5].

In order to clarify this point, we investigated the impact of ions such as Li^+, Na^+ and Cs^+, on the structural and dynamical properties of water confined in silica materials (d_p=2.6 nm). To reach this goal, we studied the structural properties of the confined water using total X-ray scattering (ID15-A at ESRF) coupled with pair distribution function analysis. In addition, we performed empirical simulations to access the density profile in the pores [6]. Furthermore, we characterized the water dynamics at picosecond timescale using Quasi-Elastic Neutron Scattering (IN5 time-of-flight at ILL). The results clearly support the existence of ion-specific effects under confinement.

From such analysis, we will be able to propose an accurate structural description to understand the ions behavior and their impact on the structure and diffusion of water into silica confined space.

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Session Classification: Talks

Track Classification: Contributions