Contribution ID: **19** Type: **Poster**

Anisotropy of water dynamics confined in model silica material

Tuesday, 11 October 2022 18:40 (20 minutes)

The study of aqueous solution transport in nanoporous media such as clays, mineral and biomineral phases, cement, glass alteration layer ..., is of interest in the fields of construction, environment, geochemistry, effluent treatment, catalysis, energy storage, and nuclear wastes. Indeed, the strong interactions between water molecules and pore surfaces in these restricted nanomedia, modify the water structure and slow down its dynamics from nanoscale to macro-scale. Today, tortuosity, large pore size distribution and pore orientation make it difficult to link between these various scales. To reach this goal, highly oriented nanopores have to be used.

In this study, for the first time, we have used silica model systems made of highly oriented mesopores (4.8 nm) having a micrometric length [1] in order to characterize the water dynamics anisotropy at a picosecond timescale using Quasi-Elastic Neutron Scattering (IN5 time-of-flight spectrometer at ILL). The scattering intensity was collected in 2 orientations to obtain the mean dynamics of water molecules in both, parallel and perpendicular orientations. The sum over Q spectra show a slight broadening when rotating the sample from 45 to 135°. The data were fitted using a diffusive model with two translational diffusion coefficients, perpendicular and parallel, as fitting parameters [2]. The results show that the water molecules are slower in the axial pore direction than in the direction perpendicular to the surface (D =0.61$10^{-9}$ m^2/s *vs.* $D = 0.35 10^{-9}$ m^2/s). This finding shows that the confinement promotes the radial water dynamics, i.e. perpendicular, rather than the axial one.

These model systems open new perspectives to study the fluids dynamics at various timescales and to extend the solution transport in these model systems to the solution transport in nanoporous materials.

[1] G. Kickelbick, *Small* **1**, 168-170 (2005)

[2] N. Malikova et al., *Phys. Rev. Lett.* **101**, 265901 (2008)

Primary authors: KHODER, Hassan (CEA, ICSM - UMR 5257 CEA-CNRS-UM-ENSCM, 30207 Bagnols--sur-Cèze Cedex, France); ZANOTTI, Jean-Marc (Laboratoire Léon Brillouin (CEA-CNRS) / CRG SHARP); OLLIVIER, Jacques; LE GOFF, Xavier (CEA, ICSM - UMR 5257 CEA-CNRS-UM-ENSCM, 30207 Bagnols-sur-Cèze Cedex, France); PODOR, Renaud (CEA, ICSM - UMR 5257 CEA-CNRS-UM-ENSCM, 30207 Bagnols-sur-Cèze Cedex, France); REBISCOUL, Diane (CEA, ICSM - UMR 5257 CEA-CNRS-UM-ENSCM, 30207 Bagnols-sur-Cèze Cedex, France)

Presenter: KHODER, Hassan (CEA, ICSM - UMR 5257 CEA-CNRS-UM-ENSCM, 30207 Bagnols-sur-Cèze Cedex, France)

Session Classification: Poster session

Track Classification: Contributions