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Structuration, dynamics and diffusion of water in hydrophilic nanotubes

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An emblematic case of nanofluidics is the ultra-low friction of water in hydrophobic carbon nanotubes. But original behaviours of water molecules are also observed in hydrophilic nanotubes, such as imogolite nanotubes (INT), with nominal composition $GeAl_2O_7H_4$ and $SiAl_2O_7H_4$, noted Ge-INT and Si-INT. Inner diameter is 2.9nm for Ge-INT and 1.5nm for Si-INT. Investigations are based on both experimental and numerical approaches, namely X-ray scattering, quasi-elastic neutron scattering (QENS), inelastic neutron scattering (INS) and classical or ab-initio molecular dynamics simulations.

A unique structure of the water layer adsorbed inside Ge-INT is revealed [1]. Water molecules form an ordered triangular lattice on the inner surface of the nanotube. To the best of our knowledge, this structure differs from that of any kind of two-dimensional water. Analysis of the vibrational density of state measured by INS shows that the dynamics of INT and water are strongly interrelated, a fully original result with respect to the available experimental literature. Water dynamics remains harmonic from 10K to 300K, with no phase transition towards a liquid state up to room temperature.

In Si-INT, the adsorbed water layer is no more solid-like but it is structured periodically along the tube axis z. The influence of this structuration on water diffusion properties will be shown based on QENS experiments. Water close to the nanotube wall diffuses along a ring in the (x,y) plane, while water in the central section of the pore diffuses rapidly along the z axis.

The complementarities between the experimental and computational approaches will be underlined. Different behaviours of water in hydrophilic Si-INT and Ge-INT will be discussed.

[1] G. Monet et al., Nanoscale Adv. **2**, 1869 (2020)

[2] A. D'Angelo et al., article in preparation, as part of her PhD thesis under the supervision of S. Rols at ILL, E. Paineau and P. Launois at Laboratoire de Physique des Solides, Orsay.

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