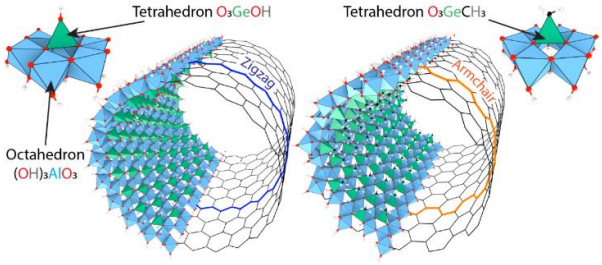
Multi-scale dynamics of water in geo-inspired nanochannels with variable hydrophilicity

PhD @ Institut Laue-Langevin (ILL, Grenoble) and Laboratoire de Physique des Solides (LPS, Orsay)
2019-2022

Project:



Imogolite nanotubes (INT) are natural clay nanotubes $SiAl_2O_7H_4$, capable of absorbing a large quantity of water, which could impact soil stability. In recent years, synthetic geo-inspired INTs $GeAl_2O_{7-x}C_xH_{4+2x}$, where the hydrophilicity of the inner wall is controlled by substituting internal hydroxyl groups by methyl ones, have been produced.

These geo-inspired nanotubes are ***model systems for studying new phenomena associated with water dynamics in nanoconfinement***. The objective of the thesis is to understand the role of geometric confinement and surface chemistry on the adsorption and diffusion properties of water molecules. Water filling will be studied thanks to ***in-situ X-ray scattering experiments*** in a dedicated humidity chamber at LPS, while ***quasi-elastic neutron scattering and neutron spin echo experiments*** will provide access to diffusion within time scales from picoseconds to hundred of nanoseconds. In addition to the experiments, the PhD student will carry out ***molecular dynamics simulations***, made possible by the determination of the structure of INTs in 2018 (figure above), in order to analyze the processes of water adsorption and diffusion at different time scales. External collaborations will allow him/her to put the results in perspective with thermodynamics insights from adsorption isotherms and with complementary diffusion experiments (NMR dispersion experiments performed at laboratoire PHENIX in Paris). The ambitious objective of the thesis is to obtain a consistent set of experimental and simulation data about the multiscale dynamics of water confined in model hydrophilic or hydrophobic nanoporous media and to present a global picture of the associated phenomena.

Candidate and supervision – The ILL in Grenoble and the LPS in Orsay jointly advertise a 3-year PhD position in France, of which ***about the first 12 months will be spent in Orsay and the subsequent 24 months in Grenoble, both with regular visits to the complementary place***. The thesis will be defended at Paris-Saclay University. The PhD project builds on a well-established collaboration between the supervisors who have co-supervised PhD students with publications in high rank journals. Two of them have been awarded by the Société Française de Neutronique in 2013 and by the Association Française de Cristallographie in Physics, in 2014. The candidate must have a ***broad knowledge of physics*** and he/she should be ***highly motivated by both experimentation and numerical simulations***. He/she should possess organizational skills as well as the ability to work both independently and as part of a team.

Some related publications of the supervisors – **Nature Comm.** 9, 2033 (2018) : *the structure of INT*; **JACS** 138, 10437 (2016): *water dynamics and H bond network in carbon nanotubes*; **Chem. Mater.** 27, 1488 (2015): *custom-made hydrophilic/hydrophobic nanotubes*; **Phys. Rev. Lett.** 101, 065507 (2008): *new dynamics of fullerenes confined in carbon nanotubes*. One can also find here an illustrative movie about the dynamics of a hydrated INT.

Supervisors and contact info – Dr/HdR Pascale LAUNOIS, Dr Erwan PAINEAU and Dr Stéphane ROLS
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How to apply – Please send a cover letter, a detailed CV including academic records, and the names and contacts of two referees to the supervisors.