Deuterated clathrate hydrates as novel moderator material for a source of very cold neutrons

(PhD studentship at Institut Laue-Langevin, enrolled at Université Grenoble Alpes)

This PhD studentship is located within ILL’s group for Nuclear and Particle Physics and funded by the European project HighNESS, whose main mission is "Development of High Intensity Neutron Sources at the ESS". The goal of this thesis is to investigate promising moderator materials for a development of a source of very-cold neutrons (VCN), with energies well below the intensity maximum of well-established cold-neutron moderators. Ultimately, this will enhance the capabilities of various neutron scattering techniques and the scientific reach of particle-physics experiments employing beams of slow neutrons.

Clathrate hydrates are inclusion compounds consisting of a network of water molecules, which form cages of different sizes that are able to host small guest molecules. Fully deuterated, they seem particularly well suited as a moderation medium, as they possess low-energy modes with sufficiently large inelastic neutron scattering cross sections. Earlier works have already measured spectra of low-energy incoherent excitations of methane and tetrahydrofuran (THF) clathrates [1]. While THF occupies only large cages in the clathrate structure II, the twice more abundant smaller cages can still be filled with smaller molecules, providing a binary clathrate [2]. Particularly interesting is oxygen, which offers an additional path for neutron slowdown via a cooling cascade mechanism exploiting the zero-field splitting of the magnetic triplet ground state of molecular oxygen [3].

The works planned within this PhD thesis include measurements of the neutron scattering function $S(q,\omega)$ for fully deuterated clathrates in absolute units, using ILL’s neutron diffraction and time-of-flight instruments. In the beginning, allocated beam times on the TDF:D2O clathrate are foreseen to be executed in the first half of 2021, followed by data analysis. Results will serve as a benchmark for molecular dynamics (MD) simulations of clathrate hydrates by collaborators of the HighNESS consortium and enable model calculations of yields in realistic moderator/reflector geometries. In parallel, new instrumentation will be developed to prepare samples of binary TDF:O2:D2O clathrates to be investigated with neutron scattering techniques during the second half of the PhD thesis.

For more information, please contact Prof. Dr. Oliver Zimmer (zimmer@ill.fr). Applications including a letter of motivation should be sent to the two contacts given with the reference “PhD project SPEC-2-2020” in the subject line.