ESRF	**Experiment title:** Structure of nanoconfined supercooled water	**Experiment number**: SC-4452
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Names and affiliations of applicants (* indicates experimentalists):

Felix Lehmkühler*,[1], Jakob Benedikt Mietner*,[2], Avni Jain*,[1], Florian Otte*,[3], Christian Sternemann[3], Michael Fröba[2]

1 Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
2 Institut für Anorganische und Angewandte Chemie, Universität Hamburg, Hamburg, Germany
3 Fakultät Physik/DELTA, TU Dortmund, Dortmund, Germany

Report:

Compared to bulk water, nano-confined water is known to show different equilibrium and dynamical properties. In particular, it has significant lower melting point depending on pore size and material. Despite its manifold occurrence in nature and a rising number of nano-cage materials for application in industry and research, little is known on the water hydrogen bond structure in confinement and the origins for the differences to bulk water. In this experiment, we studied water confinement in a new class of nanopores (periodic mesoporous organosilicas, PMO) allowing for modifications of the water-pore material interaction and thus supercooling below 200 K [1]. We performed a temperature-dependent Compton scattering experiment in order to study changes in the hydrogen bond network of confined water upon cooling.

The experiment was performed at beamline ID31. We used the standard Compton scattering set-up with the 13-element Ge solid state detector. The samples were filled to a glass capillary (sample thickness around 2 mm), sealed afterward, and placed onto the sample stage. Temperature was controlled using a cryo jet. We took spectra from water filled in silica MCM-41 as well as different differently functionalized pores. Each sample was measured at at least five different temperatures between 295 K and 160 K. The 13-element Ge solid state detector was mounted at a scattering angle of about 160°. To keep a constant flux, we used a wedge shaped absorber in front of the sample. The samples were controlled by x-ray diffraction patterns measured at least every 60 min during a Compton measurement

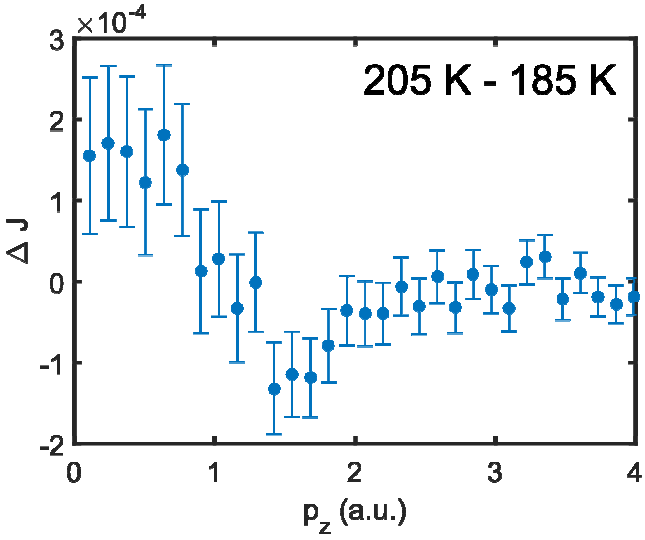

Figure 1: Compton profile difference of water confined in funcionalized PMO between 205 K and 185 K.

run. The Compton scattering data was stored every 10 minutes and checked afterwards for consistency. During the analysis, the spectra were corrected for background scattering, relativistic cross section and absorption, before summing up.

A first result is shown in Figure 1. Here, a Compton profile difference between 205 K and 185 K is shown for water in a funcionalized pore. The difference shows a rather broad feature, suggesting intramolecular changes of the water structure [2]. Further data analysis anf modelling is currently ongoing.

[1] J.B. Mietner et al. Angew. Chem. Int. Ed. 56, 12348 (2017).
[2] F. Lehmkühler et al. Phys. Chem. Chem. Phys. 18, 6925 (2016).