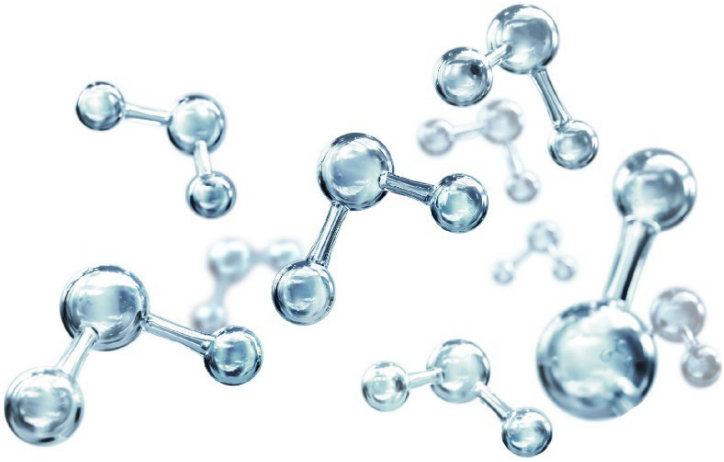
Seminar

CMWS Centre for Molecular Water Science

18th of April 2024
12:00 h (CEST)

Zoom Virtual Meeting:
https://tuhh.zoom.us/j/82631283465
Meeting-ID: 826 3128 3465
Password: 978444

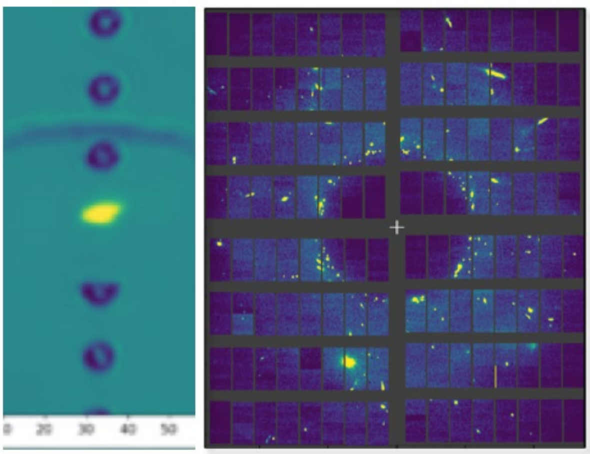


Jonas Sellberg
KTH Royal Institute of Technology

Probing structural motifs in water that control crystallization using x-ray scattering

The structure of metastable water and its ability to nucleate into ice are relevant for many research fields, such as cryobiology, astronomy and atmospheric science. We have over the past decade used x-ray scattering at x-ray free-electron lasers to study the structure of water upon deep supercooling and the structure of ice during subsequent crystallization. This is achieved by evaporative cooling of micron-sized water droplets in vacuo down to ~230 K and intersecting the droplets with the ultrabright, coherent x-ray beam. The initial experiments [1] revealed a continuous increase in tetrahedral coordination among the structural motifs in the liquid upon deep supercooling. Simultaneously, crystallization increases rapidly, suggesting that the barrier to form an ice nucleus of critical size is quickly reduced at these temperatures.

In this talk, I will present recent work on the structure factor of water upon deep supercooling [2] as well as homogeneous ice nucleation rates, which can be used to extract the interfacial energy between water and ice. We have also analyzed individual Bragg peaks upon coherent illumination [3], showing that ice grows heterogeneously throughout the droplet. Finally, I present a proof-of-concept experiment [4] to use fluctuation x-ray scattering in order to obtain 3D structural information about the precursor liquid and thus reveal structural motifs that aid or frustrate spontaneous nucleation and subsequent crystal growth.



[1] J. Sellberg *et al. Nature* **510**, 381 (2014).
[2] N. Esmaeildoost *et al. J. Chemical Physics* **155**, 214501 (2021).
[3] N. Esmaeildoost *et al. Crystals* **12**, 65 (2022).
[4] Microscope image (left) of the ultrafast x-ray pulse hitting a micron-sized water droplet and the virtual powder diffraction pattern (right) that occur from ice inside 3 µm water droplets at 30 mm from the nozzle. Results taken from proposal 3378 performed at SPB/SFX, EuXFEL in April, 2023.