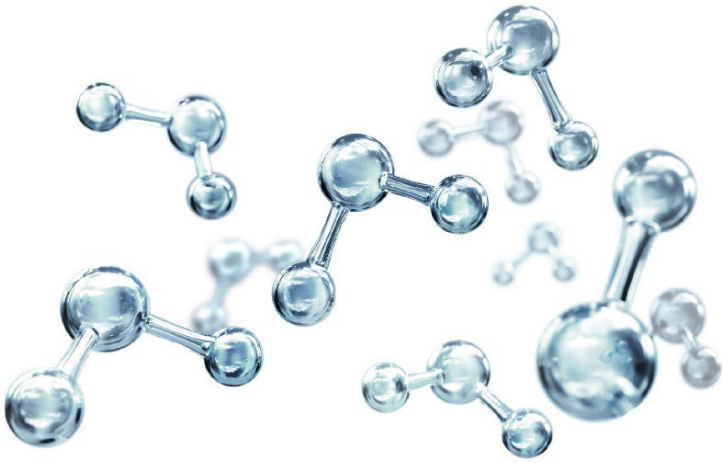
Seminar

CMWS Centre for Molecular Water Science

27th of April 2023
12:00 h (CEST)

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



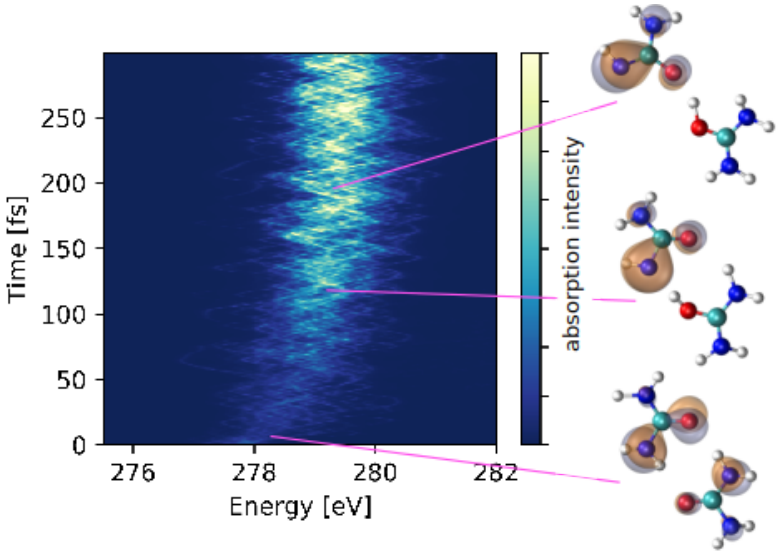
Ludger Inhester

Center for Free-Electron Laser Science CFEL
Deutsches Elektronen-Synchrotron DESY

Tracing Radiation Damage in Water and Aqueous Solutions via X-ray Absorption Spectroscopy and Simulations

The immediate response of matter to ionizing radiation is of crucial impact to many areas. Using ultrafast x-ray spectroscopy, we are able to gain new insight into the first steps of these radiation damage processes. When ionization occurs in a solution, radicals are produced in an extremely short timescale that set the stage for a chain of further reactions. In our earlier work [1], we have demonstrated how the creation of OH radicals can be traced via x-ray absorption spectroscopy.

In this talk, I will present recent extension of our theoretical modeling, disentangling the x-ray absorption signal of other ions and radicals in liquid water. I will also present our recent work [2,3] addressing the ionization response in an aqueous, highly concentrated urea solution. Via time-resolved x-ray absorption spectroscopy, we are able to follow the immediate ionization-triggered dynamics of molecules in the solution. It turns out that the direct response to ionization is a proton transfer reaction, in which the ionized urea molecule gives away a proton to a neighboring urea molecule. This reaction leaves a trace in the x-ray absorption transition from a core level to the unoccupied valence hole.



[1] Loh, Z.-H., Duomy, G., *et al. Science* **367**, 179–182 (2020).
[2] Shakya, Y., Inhester, L. *et al. Struct. Dyn.* **8**, 034102 (2021).
[3] Yin, Z., Chang, Y.-P., *et al.* In Review