## Seminar

COMPS Centre for Molecular Water Science

12th of December 2024 12:00 h

Zoom Virtual Meeting:

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



## Giulia Giubertoni

University of Amsterdam

## D<sub>2</sub>O: problem or opportunity for research on protein assembly? The strange case of collagen and other proteins

The building blocks of functional biomaterials, such as human tissues, are often fibrillar proteins that self-assemble into hierarchical structures. These structures serve as a scaffold and underpin the mechanical properties of the biomaterials. Infrared spectroscopy is one of the most commonly employed experimental methods to investigate the structure and formation of these protein assemblies. The molecular vibrations of amide groups act as informative markers, enabling researchers to monitor conformational changes during the assembly process.

Just like NMR measurements, infrared measurements are usually performed on proteins dissolved in heavy water (D<sub>2</sub>O) instead of water, and this isotope replacement is generally assumed to have no significant impact on biomolecular structure. In this talk, I will present experimental evidence that replacing H<sub>2</sub>O by D<sub>2</sub>O can in fact have profound impact on the assembly of fibrillar proteins, in particular of collagen- the main building block of the human body [1]. We will see that such isotope effects are not isolated incidents: there are many studies showing a substantial impact of D<sub>2</sub>O on the structure and dynamics of proteins and protein assemblies[2]. Finally, we will explore the potential causes of the H<sub>2</sub>O/D<sub>2</sub>O isotope effect on biomolecular structure, and whether this "elephant in the room" might be transformed into an opportunity to investigate protein self assembly.

To you, then, the final verdict: D<sub>2</sub>O, problem or opportunity for research on protein assembly?

[1] Giubertoni et al., PNAS, 2024, https://doi.org/10.1073/pnas.2313162121
[2] Giubertoni et al., JPCB, 2023, https://doi.org/10.1021/acs.jpcb.3c04385