Contribution ID: **28** Type: **Oral Presentation**

Structural biology using neutrons: introduction and how to get started

Wednesday, 24 March 2021 15:00 (40 minutes)

The method of choice for obtaining detailed, high resolution structural information macromolecules is X-ray crystallography. The magnitude of X-ray scattering from the electron cloud around an atomic nucleus is related to the Z number of that element, i.e., the more electrons an atom has, the better it will scatter X-rays. Due to this it is very challenging in theory and practice to determine the position of H atoms in crystal structures. Neutron diffraction offers a highly complementary approach in that the neutrons are scattered from atomic nuclei of all elements to a similar extent. This means that in practice the nuclear density maps for C, N, H (and its isotope Deuterium, or D), and O atoms all appear to a similar extent, even at medium (˜2 Å) resolution. H atoms are very important in biology as they are involved with everything – including hydrogen bonds, protein folding, solvation, electrostatics, amino acid side chain charge state, ligand binding, and enzyme catalytic mechanisms. To profit from neutron scattering properties and to be able to "see" these H atoms, it is crucial to deuterate (i.e. replace all H with isotope D) the materials to be studied. Multiple approaches to biological deuteration will be explained as well as the growth of large protein crystals for neutron diffraction. Finally, some practical aspects of what beamlines are available, and how to get access to neutron scattering facilities will be covered.

Primary author: FISHER, Zoe (European spallation source ERIC)

Presenter: FISHER, Zoe (European spallation source ERIC)

Session Classification: Structural biology II

Track Classification: Structural biology II