

Invited Lecture

Neutron Diffraction and Quantum Crystallography: tool or opportunity?**Silvia C Capelli***UKRI-STFC ISIS Neutron and Muon Source**silvia.capelli@stfc.ac.uk*

The effect of isotope substitution on the properties of materials is quite difficult to study with x-ray diffraction, especially when it involves H/D substitution and the property to investigate is related to the hydrogen bonding in the solid state. Neutron diffraction, is in fact a much better probe to locate the position of light atoms even in the presence of heavy ones. Furthermore, the fact that the neutron scattering length depends only on the interaction of the neutron with the nucleus and is completely independent of the atomic number, means that every single isotope in the periodic table has its own specific scattering length. In the case of hydrogen and deuterium the contrast is huge: b is -3.74 barns for H and 6.67 barns.

Most of the time, in Quantum Crystallography, neutron diffraction data are used only as a reference to check whether new calculation methods can reproduce the Anisotropic Displacement Parameters (ADPs) obtained in the experiment. In this talk I would like to show how neutron data could be used in combination with Quantum Crystallography to gain better insights of molecular systems. For example in computing the topological properties of the same material with different isotopic substitutions or to determine the energy range in which specific transformations occur.