Dr hab Matthew Krzystyniak

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Dr Krzystyniak completed his PhD in medical physics at the Faculty of Physics of the Jagellonian University in Cracow, Poland. He continued his research career as a postdoctoral research associate at Free University of Berlin and Technical University Berlin, followed by a fellowship of the German Research Foundation at the Rutherford Appleton Laboratory and postdoctoral positions in Durham and Oxford Universities. In 2011 he was appointed Senior Lecturer in Physical Chemistry at the School of Science and Technology, Nottingham Trent University. Since 2012 Dr Krzystyniak has been a visiting fellow at the same faculty and a visiting fellow the Rutherford Appleton Laboratory. In 2015 he obtained a position of an instrument scientist in electron volt neutron spectroscopy at the Rutherford Appleton Laboratory. His area of expertise includes NMR and EPR spectroscopy and relaxation theory as well as neutron spectroscopy, including Compton scattering in condensed matter systems and molecules.

Abstract

Mass-resolved neutron spectroscopy

Neutron Compton scattering (NCS) is a unique experimental technique made possible by the development of epithermal neutron sources, such as the ISIS source of the Rutherford Appleton Laboratory in the UK [1, 2]. The measurement of nuclear momenta by high-energy neutron Compton scattering relies on the fact that the energy and momentum transferred in the scattering process are sufficiently large, such that the so-called impulse approximation (IA) is an accurate starting point. In the IA limit, the dynamic structure factor measured in NCS for a given nucleus is determined by the nuclear momentum distribution (NMD). In the picture of purely classical nuclei, the NMD shape is determined by whole energy spectrum of the motional modes, including translational and rotational modes, followed by lattice and internal molecular vibrations. However, more and more experimental evidence has been accumulated over the years that nuclear quantum effects, with nuclear zero point motion being the most prominent, also contribute to the NMDs. Since its birth, the NCS technique has been employed to study proton momentum distributions in quantum fluids and solids, metal hydrides and gas and charge-storage media, etc. Beyond the proton, recent instrument developments towards MANSE (Mass-resolved Neutron Spectroscopy) offer the prospects of access to the NMDs of heavier nuclides including deuterium, helium, lithium, carbon, oxygen, and fluorine. I will present some examples of recent MANSE work advocating the use of a combination of ab initio tools and neutron scattering techniques for the characterisation of nuclear chemical dynamics in the solid state with the special emphasis on hydrogen bonded molecular crystals (see [3] and Fig 1).

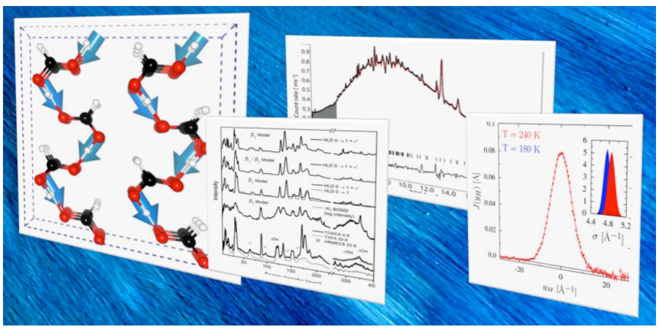

Fig. 1. Neutron Compton Scattering applied concurrently with inelastic neutron scattering and neutron diffraction and augmented with DFT calculations (adopted from [3]).

[1] Electron-volt neutron spectroscopy: beyond fundamental systems, Adv Phys (2017): 1-73. doi:10.1080/00018732.2017.1317963 [2] "Atomic Quantum Dynamics in Materials Research ", Felix Fernandez-Alonso and David L. Price Eds., Academic Press, 2017 (in press). [3] Nuclear dynamics and phase polymorphism in solid formic acid, Physical Chemistry Chemical Physics, 2017, 19, 9064 - 9074.