

Keynote Lecture

KN05

Synchrotron radiation macromolecular crystallography: our science and spin offs

J. Helliwell¹

¹*School of Chemistry, University of Manchester, Brunswick Street, Manchester, UK*

I will give an overview of synchrotron radiation (SR) in macromolecular crystallography (MX) instrumentation, methods and applications from the early days to the present, including the evolution of SR sources and on to the 'ultimate storage ring'. The build of dedicated beamlines for resonant anomalous scattering, large unit cells, ever smaller crystals and studies up to ultra-high resolution are core benefits. Results include a high output of PDB depositions, the successful use of microcrystals, pushing the frontiers of using high and low photon energies and time-resolved structural studies at even sub-nanosecond resolutions. These intensively physics based developments will be complemented by biological and chemical crystallography research results, encompassing catalysis and marine coloration, as well as the public understanding of our science and its impacts. Spin off benefits include services to the pharmaceutical industry and helping develop chemical crystallography uses of SR. The development of the Laue method with SR has led to pioneering spin off developments in neutron MX, including transfer of the well validated Daresbury Laue software to various neutron facilities worldwide. Neutron MX is gathering pace as new instrumentation and dedicated sample preparation facilities are in place at reactor and spallation neutron sources; smaller samples and much larger molecular weight protein complexes are now feasible for investigation so as to establish their protonation states and bound water structure. With the X-ray lasers, closely linked to the SR developments, we anticipate the use of ever smaller samples such as nanocrystals, nanoclusters and single molecules, as well as opening up femtosecond time-resolved diffraction structural studies. At the SR sources, a very high throughput assessment for the best crystal samples and tackling sub-micron crystals will become widespread.

Keywords: Synchrotron radiation, Neutrons, Macromolecular crystallography