

1st National Congress of the Mexican Society of Synchrotron Light & 1st International Congress of Synchrotron Light Techniques



Contribution ID : 24

Type : **Presentation**

THE FUTURE OF SYNCHROTRON DATA COLLECTION

Saturday, 26 June 2021 12:30 (1:00)

Abstract

This talk will attempt to see into the future of synchrotron data collection with a focus on macromolecular crystallography (MX) but not forgetting other fields of research which are enabled by synchrotron radiation. MX is a field with a nearly 90 year history of which the last 50 years have included work at synchrotron X-ray sources. To enlighten my futuristic crystal ball, I will take a brief retrospective look at MX developments that have advanced the field and shaped current trends and practice. Recent breakthroughs such as those in protein structure prediction using AlphaFold2 [1] and the resolution revolution in cryo-electron microscopy [2] must be embraced when considering the future science best addressed by synchrotron radiation.

About

Elspeth graduated with a D.Phil (Ph.D.) in nuclear physics from Oxford University in 1980 and switched to Biochemistry only later in her career, in 1987, when she joined the research staff at the Laboratory of Molecular Biophysics in Oxford. Since 1999 she has been faculty at the Biochemistry Department at Oxford University, where she holds a position as Professor of Molecular Biophysics and has also served as Director of the Systems Biology Programme at the Doctoral Training Centre. At Brasenose College she is a Nicholas Kurti Senior Research Fellow in Macromolecular Crystallography and until recently was Tutor for Graduates there. Elspeth's research on cryo-cooling and radiation damage has had a profound impact on crystallography. Armed with a rigorous approach inherited from her physics background and her natural inventiveness, she optimized cryogenic tools and cooling parameters, introducing a methodical approach to cryo-cooling that greatly improved diffraction data. Since radiation damage emerged as a serious problem in crystallographic structure calculation in 2000, she has spearheaded the studies dedicated to the issue, introducing mitigating measures such as the use of small molecules as radical scavengers. She experimentally determined the maximum x-ray dose that can be delivered to a macromolecule before compromising its structure -a parameter that is now called "the Garman" limit- and presented a method to predict the lifetime of proteins exposed to certain radiation doses. She also pioneered the use of an online UV-visible spectrometer to detect the early signs of radiation damage. Besides these studies, she developed the proton induced X-ray emission (PIXE) technique, which allows precise identification of trace metal elements within a protein structure, and she determined the structure of many proteins involved in infectious diseases.

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Session Classification : Plenary Lecture