Poster Presentation

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Chemical Crystallography at the Australian Synchrotron MX Beamlines

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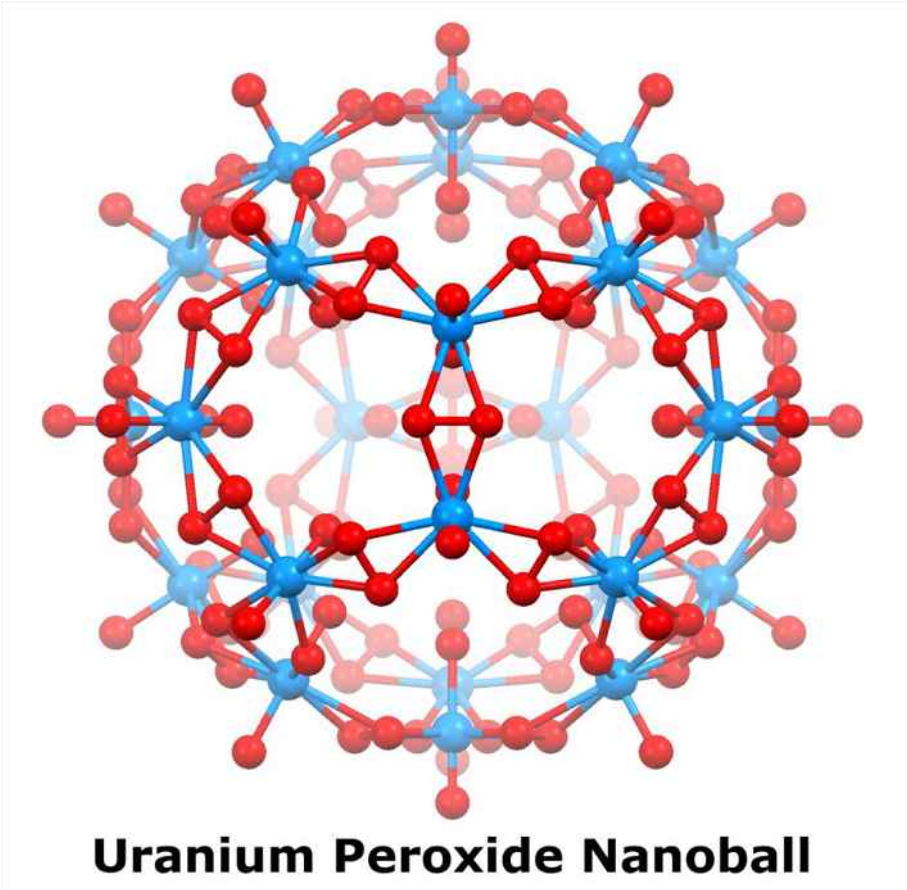
The Macromolecular Crystallography (MX) Beamlines at the Australian Synchrotron collect data on protein samples (PX) and chemical samples (CX). This broad range of sample types requires us to consider a number of experimental and data processing considerations. Protein samples have very large unit cells but diffract weakly, the chemical samples on the other hand have very small unit cell and diffract comparatively strongly. From an experimental point of view, this requires substantially different geometrical considerations which can be handled by changing the energy of the monochromated X-rays and detector distance. Another consideration is detector type, the detectors at the MX beamlines are from the Area Detector Systems Corporation (ADSC) and they have generally been used for PX data collections. This has lead to investigation regarding high incidence angle phosphor thickness corrections. As the detectors have mainly been used for PX work, the software for sample handling has also been developed with PX considerations rather than CX. For example, the software for space group determinations is set my default to assumes that your space group is only ever one of the 65 space groups that don't contain mirror, inversion or glide operations. Another area of interest is the way data scaling is handled. The data is often scaled with PX data for a number of reasons, with the most common scaling of data is due t the prevalence of radiation damage to the samples. By contrast the most common form of scaling for CX data is for sample anisotropy in strong absorbers. A discussion of the challenges faced for the chemical crystallography experiments at the Australian Synchrotron will be presented.



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