MS051.O06

XAFS, Fluorescence, XANES, RIXS, XERT data formats and coding

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In the XAS field, database formats and coding are much less well-defined and in general in much less consistent unity in format or structure, leading to challenges regarding analysis, reanalysis, validification, and robust programming.

Regarding the high-accuracy X-ray Extended Range Technique XERT for XAS, and in general, the format varies between beamlines and depending upon policy from e.g. USA, Japan, Europe and other areas. Standard software can be in Spec, EPICS, IDL, Python, Fortran, C++, Microsoft basic, and other heterogeneous formats.

The XAS and XAFS for challenging structural problems. This has led to the proposal, now coming to fruition, for a new Volume of the International Tables for Crystallography, Volume I on X-ray Absorption Spectroscopy and X-ray Absorption Fine Structure. Recently, this has led to the Q2XAFS Satellite and separate workshop series, which most recently is a Satellite of this Congress and was held in Diamond, UK. I will report a few of the successful outcomes of that series and a way forward to assist the world-wide community in producing stronger data, information content, validification and deposition with publication.

Keywords: XAFS, fluorescence detection, data collection and processing