Novel advanced methods in XAS – XERT and Hybrid Techniques

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Developments over the last two decades have achieved accuracies in attenuation coefficient and X-ray absorption fine structure of below 0.2%. This generally requires careful sample characterisation, monochromator and detector characterisation and additional experimental components to measure and correct for a range of systematics. More recently similar levels of accuracy have been obtained in fluorescence measurement. These techniques, XERT developed by Chantler, Barnea, Tran and group; and Hybrid, developed by Chantler, Tran, Best et al. offer accuracies and insight for disordered systems up to 100x more than previous work. To bring them to standard routine implementations for all users would strengthen hypothesis discrimination and testing for molecular and disordered structure and dynamics including for ideal crystals. In this they are complementary to XRD and ND investigations.

Over the past two years parts of this system have been implemented at the Australian Synchrotron with excellent precision and control of a range of systematics using XERT and Hybrid techniques in both transmission and fluorescence geometries.

Insight includes high accuracy of derived dynamical bond length, thermal parameters, consistency and inconsistency of energy offsets revealed from the data, and structural determination of nearby shells approaching an ab initio manner with XAS. It has allowed exploration of atomic form factors [1], XAFS dynamical bonding [2], electron inelastic mean free paths [3] and nanoroughness [4] appropriate for circuit quality control for microcomputers, with technological offshoots into detector and synchrotron diagnostics. As a consequence, the accurate characterization of fluorescence spectroscopy is developing [5], together with the accurate investigation of organometallic complexes. Further it has allowed investigation of several types of dynamic behaviour including the investigation of the reaction coordinate [6], thermal isotropy, and potentially Debye behaviour. The reaction coordinate investigations permit study of catalytic paths in Amyloid beta, and other electrochemical studies of ifficult or fragile organometallic systems in solid or solution form, at room temperature or in a cryostat.

Perhaps intriguingly, it has permitted the first X-ray measurements of electron inelastic mean free path [7]. This paper will explore the requirements for and applicability of higher accuracy in XAFS, the advantage of theory simultaneously fitting XANES and XAFS [8], and the opportunities for advanced dynamics and Debye studies, in addition to the potential for resolving challenges in catalytic and active centres.

The quality of XAFS data and the intrinsic information content can be outstanding, and its ability to determine bonding and dynamical modes can be unsurpassed. The talk will also look towards future opportunities not yet realised in advanced analysis and disorder measurement.

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Keywords: XAFS, XERT, high accuracy, organometallics, disorder