Putting it all Together: How Modelling Multiple Experiments can enhance our Structural Understanding of Liquids and Disordered Materials

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Recent advances in the modelling of diffraction and spectroscopy data now provide the structural scientist with a powerful tool to maximise the benefit of experimental data. By developing a single three dimensional model that simultaneously accounts for the differing sensitivities of a range of experimental probes, it becomes possible to circumvent many of the difficulties that can limit individual measurements. For highly disordered systems such as liquids and glasses, critical challenges that must be accounted for in any comprehensive model include the chemically specific understanding of the atomic and molecular interactions, and an appropriate account of the continuous nature of the structural distribution functions. In this presentation I will illustrate with a range of examples, how the approach of Empirical Potential Structure Refinement can now add considerable value to the analysis of neutron and X-ray scattering, and EXAFS spectroscopy data obtained from disordered systems.