[MS27-P08] Total Scattering Measurements of 'Complex' Systems: Disorder and Reduced Dimensionality.

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In order to understand fully the behaviour of functional materials or pharmaceutically-active substances, structure determination is essential. Traditionally, this has been the domain of single-crystal and powder crystallography. However, there are materials where the functionality arises from short-range correlations that are undetectable by conventional crystallographic methods, and there are others that do not exist in a crystalline form at all [1].

Total scattering is capable of measuring both long-range correlations (the average crystal structure) and local structural fluctuations that reflect instantaneous deviations from the average structure. A crystalline sample is not necessary. Furthermore, these data can be modelled using a reverse Monte Carlo (RMC) approach resulting in atomistic configurations that are consistent with long-and short-range structural data [2,3].
Reverse Monte Carlo models, derived from neutron and X-ray total scattering data, will be discussed for two different systems: cyclohexane [4] and a layered double hydroxide. Both these systems are united by the fact that they can be considered 'complex' in terms of the structural challenges they pose for RMC modelling -namely extreme rotational disorder and reduced dimensionality. The differences between the local and average structures in both these materials will be discussed as well as the more subtle, yet important, features that are revealed by examining local structure.

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