Understanding Order and Correlation in Liquid Crystals by Fluctuation Scattering

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Characterising the supramolecular organisation of macromolecules in the presence of varying degrees of disorder remains one of the challenges of structural research. Discotic liquid crystals (DLCs) are an ideal model system for understanding the role of disorder on multiple length scales. Consisting of rigid aromatic cores with flexible alkyl fringes, they can be considered as one-dimensional fluids along the stacking direction and they have attracted attention as molecular wires in organic electronic components and photovoltaic devices [1].

With its roots in single-particle imaging, fluctuation x-ray scattering (FXS) [2] is a method that breaks free of the requirement for periodic order. However, the interpretation of FXS data has been limited by difficulties in analysing intensity correlations in reciprocal space [3]. Recent work has shown that these correlations can be translated into a three-and four-body distribution in real space called the pair-angle distribution function (PADF) – an extension of the familiar pair distribution function into a three-dimensional volume [4]. The analytical power of this technique has already been demonstrated in studies of disordered porous carbons and self-assembled lipid phases [5,6].

Here we report on the investigation of order-disorder transitions in liquid crystal materials utilising the PADF technique and the development of facilities for FXS measurements at the Australian Synchrotron.



Figure 1. Three-dimensional intensity correlations between detector pixels are determined in reciprocal space. Intensity correlations are converted into the real-space PADF function which encodes three-and four-body correlations with distances r, r' and internal angle θ . Discotic molecules can be approximated as rigid aromatic discs surrounded by flexible alkyl chains; a common transition observed in DLCs is between ordered and disordered columnar structures (adapted from [1,5]).

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