

Micelles & Monolayers: Exploring use of models to understand scattering data

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With the continuing improvements to small angle scattering instruments it is now possible to routinely collect data out to 1 \AA^{-1} or even higher in many SAS experiments. In addition, instruments such as NIMROD at ISIS are extending their low angle range into the small angle range. This extended range of data brings new opportunities for data analysis, which can potentially cover structures from molecular level, or at least coarse-grained levels through to colloidal particles. The major question is how to efficiently fit experimental data with atomistic models on feasible timescales. I will present some of our work on analysing micelle structure using Empirical Potential Structure Refinement (EPSR) and on looking at appropriate levels of coarse graining and potentials for generating models of lipid monolayers at the air-water interface.