Computational Reverse Engineering Analysis of Scattering Experiments (CREASE) for Soft Materials

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Computational Reverse Engineering of Scattering Experiments (CREASE)' is a computational method that we have developed for analysis of small angle scattering profiles and interpretation of the structure in soft materials. In this talk I will share examples of how we have applied CREASE to experimental small angle X-ray and neutron scattering profiles obtained from different soft materials [e.g., methylcellulose fibrillar structures (Macromolecules 2022, 55, 24, 11076–11091), micelles in amphiphilic polymer solutions (ACS Polymers Au (2021) 1, 3, 153–164), segregation in binary nanoparticle mixtures (JACS Au 2023, 3, 3, 889–904 and ACS Central Science 2022, 8, 7, 996–1007)] to test various hypotheses regarding the domain shapes and sizes within the structure and identify the relevant structural dimensions. CREASE is useful to interpret structural detail at a range of length scales for soft materials without relying on fitting with off-the-shelf analytical models that may be too approximate for novel polymers and/or unconventional assembled structures. I will also show how one can take CREASE's structural interpretation as an input for other computational methods that predict macroscopic properties (e.g., color, reflectance profiles) thus serving as a valuable tool for predicting structure-property relationships.