Utilizing coarse-grained modelling and Monte Carlo simulations to understand and predict SAXS-data for intrinsically disordered proteins

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Computer simulations and modelling in combination with small angle X-ray scattering (SAXS) is a fruitful approach to achieve a molecular understanding of the underlying physics of a system. In this talk I will present how coarse-grained modelling in combination with Monte Carlo simulations can be used to understand and predict solution behavior of intrinsically disordered proteins (IDPs). The model used is based on the primitive model,[1] which is sometimes also referred to as the bead-necklace model. In this model each monomer corresponds to a bead with a given radius. In addition, each individual bead can be appointed a charge. The water is always treated as a dielectric continuum.

First an introduction to coarse-grained modelling will be given with emphasis on pros and cons utilizing this approach. Thereafter I will show examples of how it can be applied to study dilute as well as concentrated IDP solutions, where the effect of electrostatic interactions and oligomerization will be highlighted.[2-4] Throughout the talk, comparisons will be made with SAXS-experiments, and when applicable, also atomistic molecular dynamics simulations and polymer theory.[5-7]

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