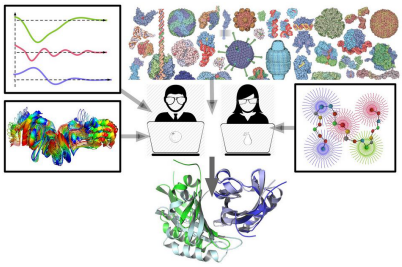

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Computer simulations of intrinsically disordered proteins - What are we missing?

Intrinsically disordered proteins (IDPs) lack well-defined three-dimensional structure in solution under physiological conditions. Despite this they are functional and participate in the regulation of many biological processes, in which disorder can enable interactions of high specificity coupled with low affinity. Phosphorylation is one of the most abundant types of post-translational modifications of IDPs. The addition of a phosphoryl group can act as a regulatory mechanism, for example by inducing changes in secondary structure or the association state. Computer simulations and modelling in combination with small angle X-ray scattering (SAXS) is fruitful approach to achieve a molecular understanding of the underlying physics of a system. In this talk I will present how atomistic and coarse-grained modelling in combination with Monte Carlo and molecular dynamics simulations can be used to understand and predict the structure and solution behavior of IDPs, but more importantly, focus will be on "what are we missing". After setting the stage and introducing the models used for the monomeric IDPs under dilute conditions, four different cases will be discussed:

1. Temperature effects
2. Phosphorylations
3. Self-association
4. Crowding

Throughout the talk, comparisons will be made between models with different degrees of details, and SAXS-experiments. The talk is based on the experience from research performed in Skepö research group during the last ten years.

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