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«Protein complexation driven by electrostatic interactions»

Protein complexation is a topic of interest in several fields including material sciences, food technology, pharmaceutical formulations, medical and bioprocess technology. The often observed strong dependency of such complexes formation on salt and pH indicates that electrostatic interactions are their main driving forces. It is clear that the interplay between the (bio)colloidal characteristics (especially size and charge), pH, salt concentration and the thermal energy results in a unique collection of “mesoscopic” forces of importance to the molecular organization and function in biological systems. On biological machineries there are systems that show attraction in the weak-coupling regime where the expected behavior is repulsion (as predicted by the classical DVLO theory). The theoretical background for the physical interpretation of such systems goes back to Kirkwood’s structure sensitive electrostatic forces, where attractive forces between biomolecules arise from fluctuations in proton charge due to the acid–base equilibrium.

Quantitative insights into the physical basis of these molecular mechanisms can be provided by computer experiments. Coarse-grained models were specifically derived to capture the main particular features of such phenomenon. These models are intermediate in details, describing only the most relevant features of the chemical heterogeneity of the proteins. This includes, for example, a description of protein shape at the residue level, but also a description of the location of the charges at the level of individual chemical groups. Conversely, these models also include details of the OH and H⁺ association and dissociation equilibria that are crucial for the complexation. This is often ignored, even in simulations with atomic details and explicit solvent.

By means of Monte Carlo and classical molecular dynamics simulations, this talk will outline the main physics behind such systems. Protein-protein, protein-polyelectrolyte, protein-nanoparticles and protein-RNA will be used as examples. A particular focus will be on milk proteins and the N-terminal domain of the Major Ampullate Spidroin

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SALLE DE CONFÉRENCES