

Modeling protein adsorption on soft interfaces

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Understanding and quantifying the physical mechanisms behind protein adsorption on soft interfaces, such as polyelectrolyte (PE) brushes or gels, pose a major challenge to experiments and theory. While it is clear that Coulombic and hydrophobic interactions are two of the major driving forces of adsorption, it is typically difficult to separately quantify those in experiments, where only average, macroscopic observables can be measured. In this talk I firstly discuss current work on the interpretation of isothermal titration calorimetry (ITC) data of protein adsorption on charged hydrogels and show how electrostatic leading order contributions can be quantified by an extended Langmuir model. Secondly, I present preliminary results from Brownian dynamics computer simulations of protein adsorption on PE brushes from which a more microscopic insight into the electrostatic mechanisms of protein adsorption is possible.