JOHANNES KEPLER
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über

Simulations of reaction equilibria in macromolecular systems

Abstract:

Molecular simulations have become an indispensable tool in chemical research and materials science. However, most molecular simulations are performed assuming a fixed chemical composition. They focus on structural and conformational changes and intermolecular interactions, while neglecting the possible chemical changes which may occur simultaneously. In this lecture, we present an overview of our modeling work, addressing how reversible chemical reactions affect the properties of macromolecular solutions. In particular, we discuss the effect of acid-base equilibria on the net charge of peptides, synthetic polyelectrolytes, polyelectrolyte hydrogels, and proteins. By comparing with experiments, we show that our models can quantitatively predict how this net charge depends on pH of the solution. Next, we show that a change in the pH can trigger attraction between macromolecules, resulting in the formation of condensates, precipitation or gelation. Finally, we show how changes in the pH control the uptake of charged proteins into coacervates, or how the pH affects the properties of protein solutions during purification processes used by the pharmaceutical industry: dialysis and ultra- or dia-filtration.

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