Abstract:

Polypeptides are an essential part of biological systems. If they contain amino acids with acidic or basic side chains, they can carry a charge due to dissociation reactions depending on the pH. Polypeptides can thus be considered weak polyelectrolytes, and their pH-responsive behavior, which is important in terms of describing their biological functioning as well as potential applications, can be studied in this context. Molecular simulations in particular have a long history in this regard. In this work, a coarse-grained computer model of the polypeptide is created and it is investigated how parameters of the model such as the level of detail in it or system parameters such as chain length and salt concentration affect the behavior of the polypeptide. The goal is to get results from simulations that could later be compared with experimental results in order to determine whether the created model is suitable for the study of these systems in the future.