PHYSIOCHEMICAL BEHAVIOR AND NETWORK MORPHOLOGY OF CHITOSAN: A MARTINI3 COARSE-GRAINED MOLECULAR DYNAMICS STUDY

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Chitosan-based hydrogels have emerged as advanced materials for wastewater remediation applications due to their high absorption capacity, biodegradability, and structural flexibility [1]. The presence of amine and hydroxyl groups in chitosan, as well as their distribution along the polymer chain, plays a crucial role in determining ¢its solution behavior. Additionally, the network morphology and physicochemical properties of chitosan are influenced by factors such as the degree of acetylation, water/chitosan ratio, degree of polymerization, and pH [2]. Therefore, understanding and predicting the effects of these design parameters on morphology and physicochemical behavior in solution is key to developing tailored hydrogels for wastewater remediation.

In recent years, all-atom molecular dynamics studies have emerged as effective and accurate tools for studying such phenomena and their underlying molecular mechanisms. However, due to computational limitations, coarse-grained approaches, particularly those based on Martini 3 polysaccharide and carbohydrate force fields [3] have shown strong agreement with both experimental results and all-atom simulations, enabling the study of higher degree polymerization chains over longer timescales.

In this work, Martini coarse-grained molecular dynamics simulations were employed to investigate the physicochemical behavior of chitosan in solution. This study analyzes the radius of gyration and persistence length of chitosan as functions of degree of polymerization, degree of acetylation, and amino group distribution. The results demonstrate a scaling behavior of the radius of gyration and persistent length with respect to degree of polymerization and acetylation, consistent with experimental findings. Furthermore, the study reveals a transition from rod-like chitosan oligomers to more flexible chain conformations in solution. Moreover, the network morphology was systematically examined for varying degrees of acetylation alongside the effect of pH on structural organization. The acetylation influence on the chain interactions, aggregation and swelling behavior and overall network architecture are studied for varying pH.

Keywords:
Chitosan, Deacetylation, Network morphology, Coarse Grain molecular dynamics

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