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**A Coarse-Grained Model for Simulating Chitosan Hydrogels**

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University of Maryland, College Park — Hydrogels are biologically-derived materials composed of water-filled cross-linking polymer chains. It has widely been used as biodegradable material and has many applications in medical devices. The chitosan hydrogel is stimuli-responsive for undergoing pH-sensitive self-assembly process, allowing programmable tuning of the chitosan deposition through electric pulse. To explore the self-assembly mechanism of chitosan hydrogel, we have developed an explicit-solvent coarse-grained chitosan model that has roots in the MARTINI force field, and the pH change is modeled by protonating chitosan chains using the Henderson-Hasselbalch equation. The mechanism of hydrogel network formation will be presented. The self-assembled polymer network qualitatively reproduce many experimental observables such as the pH-dependent strain-stress curve, bulk moduli, and structure factor. Our model is also capable of simulating other similar polyelectrolyte polymer systems.

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