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Multiscale modeling of salt-responsive polyelectrolyte morphologies[1]

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Responsive materials, which react to changes in the surrounding environment through specific property adjustments, will play an increasingly important part in a diverse range of applications. However, the mechanisms of responsiveness is difficult to characterize due to its inherent complexity and multiscale nature: stimuli triggers atomistic-level molecular changes that cause macroscopic response in physical and chemical properties of material. Modeling a responsive material presents a challenge with a large number of unknown variable parameters, such as chemical reactions kinetic or conformational changes as a function of environment, that is hard to measure directly. We have recently developed a method which is parameterized based on a single set of parameters, which allows for large-scale simulations of self-assembling polyelectrolytes materials and their morphological response to the changes in salt concentration. Polyelectrolyte block copolymers, which combine structural features of polyelectrolyte, block copolymers and surfactants, can self-assemble in a variety of nanoaggregates in aqueous environment, such as micelles, vesicles, lamellar mesophases or micellar aggregates. The morphology and size of formed aggregates are determined by the characteristically complex equilibrium of noncovalent forces and depends on variations in ionic strength or/and pH in the aqueous solution. In this talk, I will illustrate our recent progress in prediction of responsive morphologies of polyelectrolytes on the example of the DNA-based materials. Our methodology permit us to construct a morphological diagram of polyelectrolyte block copolymers and evaluate the size of aggregates obtained along with their responsive morphological transitions and scaling relation.

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