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Stimuli-responsive biopolymeric morphologies: effect of salt and temperature

Abstract: 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, such as drug delivery, tissue engineering, artificial organs, coatings, separation techniques, and soft actuators. Most of the biological materials are innately responsive. For example, in plant Venus fly trap it is believed that mechanical stimuli of plant follicles transfer into electrical signal that causes the leaf to close. 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. However, when we applied a similar approach for modeling temperature-responsive elastin-like polypeptides (ELP) materials, the success was much limited due to more complex parameter space. In this talk, I will discuss progress in modeling of DNA-based salt-responsive materials and temperature-responsiveness of ELP-based materials.

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Yaroslava G. Yingling is Professor of Materials Science and Engineering at North Carolina State University. She received her University Diploma in Computer Science and Engineering from St. Petersburg State Technical University of Russia in 1996 and her PhD in Materials Engineering and High Performance Computing from the Pennsylvania State University in 2002. She carried out postdoctoral research at Penn State University Chemistry Department and at the National Institutes of Health National Cancer Institute prior to joining North Carolina State University in 2007. She received the National Science Foundation CAREER award (2012), American Chemical Society Open Eye Young Investigator Award (2012) and was named a NCSU University Faculty Scholar in 2014. Research interests in Prof. Yingling's group are focused on the development of soft materials informatics, advanced computational models and novel algorithms for multiscale molecular modeling of soft and biological materials and aim to provide a fundamental understanding of the structure-property relations of a variety of soft materials systems that are formed through the process of self-assembly.