Stony Brook University

Department of Materials Science and Chemical Engineering

In-Person Departmental Colloquium

Wednesday
October 12, 2022
1:00 – 2:00 p.m.
Old Engineering Room 301

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Distinguished Professor

Materials Science and Engineering
North Carolina State University
Raleigh, NC

Understanding and predicting stimuli-responsive biopolymeric morphologies

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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.

Biosketch

Prof. Yingling is a Kobe Steel Distinguished Professor of Materials Science and Engineering at North Carolina State University. She also serves as an Associate Department Head, Director of Undergraduate Program and Director of Graduate Certificate in Materials Informatics. 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. Prof. Yingling leads an active interdisciplinary research program that focuses on the development of materials informatics approaches, advanced computational models and novel multiscale molecular modeling methods for investigations of properties and processes in composite, soft and biological materials. Prof. Yingling and her students have engaged actively in a variety of projects exploring assembly of biomolecules on surfaces and interfaces, ab-initio design of nanomaterials for industrial and pharmaceutical applications, de novo biomolecular structure prediction, and development of advanced multiscale methods for the prediction of properties and responsive behavior of functional complex materials and application of data-science techniques to heterogeneous data. In data science, her research aims to solve critical bottlenecks in materials informatics, which include connecting heterogeneous data, such as data from various computational and experimental techniques, and organization of databases and formulation of appropriate descriptors. She has published more than 100 papers, gave more than 100 invited talks and seminars, organized more than 10 professional symposia and workshops and is serving as an Editor for Journal of Materials Science and as an Editorial Board Member of ACS Biomaterials Science and Engineering and ACS Applied Materials and Interfaces. She received the National Science Foundation CAREER award, American Chemical Society Open Eye Young Investigator Award, named a NCSU University Faculty Scholar, received the 2021 NC State Alumni Association Outstanding Research Award and was inducted into the NC State Research Leadership Academy.