"Predicting Structure and Thermodynamics in Macromolecular Materials with Specific and Directional Intermolecular Interactions"

Wednesday
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3:00 p.m.
Wu and Chen Auditorium
Levine Hall

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Abstract

In this talk, I will present my group's recent work aimed at developing predictive coarse-grained (CG) models for investigating structure and dynamics in soft materials with chemistries that have specific and directional molecular interactions. Although computational studies have been tremendously useful in understanding molecular phenomena and guiding synthesis of new macromolecular soft materials for a wide variety of applications, the inability to capture small scale specific and directional interactions (e.g., hydrogen bonds) alongside *macromolecular* length and time scales represents a key limitation of most studies to date. We address this limitation by developing coarse-grained models that capture the anisotropic, directional and specific interactions (e.g., hydrogen bonding interaction) governing the structure and thermodynamics in many polymer systems of interest. In this talk, I will also present our recent work using a combination of atomistic molecular dynamics simulations, PRISM theory and molecular simulations with these new coarse-grained models for two specific systems: 1) thermo-responsive biopolymers, specifically, elastin-like peptides and collagen-like peptides, and 2) polymer nanocomposites composed of polymer grafted nanoparticles in a polymer matrix, with hydrogen bonding donors and acceptors in the graft and matrix polymers. The successful development of qualitatively, and, *in some cases*, quantitatively accurate CG models is enabled by synergistic feedback from experiments conducted in the labs of our collaborators, specifically Prof. Kristi Kiick (University of Delaware), Prof. April Kloxin (University of Delaware) and Prof. Ryan Hayward (University of Massachusetts). I will present some of these key experimental results alongside the computational results from my group.

Bio

Arthi Jayaraman received her B.E. (Honors) degree in Chemical Engineering from the Birla Institute of Technology and Science, Pilani, India in 2000. She received her Ph.D. in Chemical and Biomolecular Engineering from North Carolina State University in 2006, and from 2006-2008 conducted her postdoctoral research in the Department of Materials Science and Engineering at University of Illinois-Urbana Champaign. In August 2008, she joined the faculty of the Department of Chemical and Biological Engineering at the University of Colorado at Boulder, and held the position of Patten Assistant Professor. In August 2014, she joined the faculty at the University of Delaware as an Associate professor of Chemical and Biomolecular Engineering and Materials Science and Engineering. She has been awarded the Saville Lectureship at Princeton University (2016), the AIChE COMSEF division Young Investigator Award (2013), the ACS PMSE division Young Investigator Recognition (2014), the University of Colorado Provost Faculty Achievement Award (2013), the Department of Energy (DOE) Early Career Research Award (2010), the University of Colorado outstanding undergraduate teaching award (2011) and the Graduate Teaching Award (2014) in Chemical and Biological Engineering. Her research expertise lies in development of theory and simulation techniques and application of these techniques to study polymer functionalized nanoparticles and polymer nanocomposites, and to design macromolecular materials for biomedical applications.

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