Amgen Seminar Series in Chemical Engineering

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Theory and Simulations of Macromolecular Soft Materials: Linking Molecular Design to Macroscale Morphology and Function

By

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We use theory and simulation techniques to connect molecular features of macromolecular materials, specifically polymers, to their morphology and macroscopic properties, thereby guiding synthesis of materials for various applications in the energy and biomedical fields.

In the first part of my talk I will present our recent theory and simulation studies of polymer functionalized nanoparticles in polymer nanocomposites. The goal of this work is to control spatial arrangement of nanoparticles in a polymer nanocomposite so as to engineer materials with target mechanical or optical properties. One can tailor the inter-particle interactions and precisely control the assembly of the particles in the polymer matrix by functionalizing nanoparticle surfaces with polymers, and systematically tuning the composition, chemistry, molecular weight and grafting density of these grafted polymers. We have developed an integrated self-consistent approach involving Polymer Reference Interaction Site Model (PRISM) theory and molecular simulations to study polymer grafted nanoparticles in polymer matrix, and understand the effect of heterogeneity, such as monomer chemistry, monomer sequence, and polydispersity, in the polymer functionalization on the effective interactions, and dispersion/assembly of functionalized nanoparticles in a polymer matrix.

In the second part of my talk I will present our molecular simulation studies aimed at designing polycations for DNA delivery. DNA delivery involves successful transfection of therapeutic DNA by a vector into target cells and expression of that genetic material. Viral vectors, while effective, can elicit harmful immunogenic responses, thus motivating ongoing research on non-viral transfection agents. Cationic polymers or polycations are a promising class of non-viral vectors due to their low immugenic responses and low toxicity, and their ability to bind to the polyanionic DNA backbone to form a polycation-DNA complex (polyplex) that is then internalized in the target cell. Combinatorial approaches have generated many polycations with differing DNA transfection efficacies, but there is a need for general design guidelines that can relate the molecular features of the polycation to its DNA transfection efficiency. Using atomistic and coarse-grained molecular dynamics simulations of DNA and polycations composed of polypeptides, we connect the thermodynamics of polycation-DNA binding and structure of the polycation-DNA complexes, both of which impact transfection efficiency, to polycation chemistry and architecture.

Biography: *Arthi Jayaraman received her B.E (Honors) degree in Chemical Engineering from 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 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 Associate professor of Chemical and Biomolecular Engineering and Materials Science and Engineering. She has received the AIChE COMSEF division young investigator award (2013), ACS PMSE division young investigator recognition (2014), University of Colorado Provost Faculty Achievement Award (2013), Department of Energy Early Career Research Award (2010), ACS Women Chemists Committee Lectureship Award, the University of Colorado outstanding undergraduate teaching award (2011) and 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 engineer polymer functionalized nanoparticles and polymer nanocomposites for optics and organic photovoltaic applications, and to design polymers for gene delivery and biomedical applications.*

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