PURDUE UNIVERSITY

PURDUE MATERIALS ENGINEERING

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Winchell Seminar Series

Frontiers in Polymer Science and Functional Materials

Friday, February 21
3:30 Coffee
3:45 Seminar
ARMS 1010

Theory and simulation studies of structure and thermodynamics in macromolecular materials

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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 target applications. 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 ligands such as polymers, and systematically tuning the composition, chemistry, molecular weight and grafting density of the ligands. We have developed an integrated self-consistent approach involving Polymer Reference Interaction Site Model (PRISM) theory and Monte Carlo 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 potential of mean force between functionalized nanoparticles, and the dispersion/assembly of functionalized nanoparticles.

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. 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.

Arthi Jayaraman received her B.E (Honors) degree in Chemical Engineering from Birla Institute of Technology and Science and Ph.D. in Chemical and Biomolecular Engineering from North Carolina State University working with Dr. Carol Hall and Dr. Jan Genzer. She conducted her postdoctoral research with Dr. Kenneth S. Schweizer in the department of Materials Science and Engineering at University of Illinois-Urbana Champaign. She has received the AIChE COMSEF division young investigator award (2013), ACS PMSE division young investigator recognition (2014), Department of Energy Early Career Research Award (2010), ACS Women Chemists Committee Lectureship Award and the University of Colorado outstanding undergraduate teaching award in Chemical and Biological Engineering (2011). 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.