My research group uses 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 first 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 recent simulation work linking molecular features of conjugated polymers to morphology, and in turn efficiency of organic solar cells. Organic solar cells consist of an active layer made of an electron donating species (e.g. conjugated polymer) and an electron accepting species (e.g. fullerene derivative). The efficiency of a solar cell is dependent on the morphology of the donor and acceptor materials. For high efficiency the morphology must have a) large interfacial area to facilitate charge separation, while being small enough so charge carriers can diffuse to the donor-acceptor interface before their energy is dissipated and b) continuous pathways for charge carriers to reach their respective electrodes. Donor-acceptor morphology is dependent on the chemistry and architecture of the conjugated polymer and its interactions with the acceptor material (fullerene derivatives). We use molecular simulations to understand the effects of varying conjugated polymer architecture, polymer chemistry, fullerene derivative chemistry, and processing conditions on order -disorder transition and morphology within blends of conjugated polymer and fullerene derivatives used in bulk heterojunction solar cells.

Biography: Arthi Jayaraman received her B.E (Honors) degree in Chemical Engineering from Birla Institute of Technology and Science, Pilani, India in 2000. In 2006 she received her Ph.D in Chemical and Biomolecular Engineering from North Carolina State University working with Dr. Carol Hall and Dr. Jan Genzer, and was awarded the Edward M. Schoenborn award for outstanding doctoral research. She conducted her postdoctoral research with Dr. Kenneth S. Schweizer in the department of Materials Science and Engineering at University of Illinois-Urbana Champaign from 2006 to 2008. In August 2008 she joined the faculty of the Department of Chemical and Biological Engineering at University of Colorado at Boulder, where she currently holds the Patten Assistant Professor position. 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 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 metamaterials and organic photovoltaic applications, and to design polymers for gene delivery and biomedical applications.