

## DEPARTMENT OF MATHEMATICS AND SIMCENTER present

### “UNDERSTANDING ELECTROSTATIC CORRELATIONS IN POLYMERS”

given by **Dr. Rajeev Kumar**

Research Scientist, Oak Ridge National Laboratory  
November 6<sup>th</sup>, 3:30 p.m., UTC SimCenter Auditorium\*

*Public Invited*



Fundamental and applied research on neutral non-polar homopolymers as well as block copolymers over the last four decades have played major roles in advancing various areas such as organic electronics, photonics, cosmetics and chemical separation/filtration. Nonetheless, increasing energy demands and novel technologies require significantly improved materials for modern applications such as in the area of energy storage, polymer batteries and water purification membranes, to name a few. Ionic and zwitterionic polymers synthesized by introducing charges on the monomers have been shown to be promising materials with desirable responses to various stimuli in applications such as actuators, capacitors, membranes and polymer batteries. However, the simple introduction of charges leads to dramatic changes in structure and dynamics of the polymers. These changes get reflected in the responses of the polymers to temperature, applied electric fields and solvents used in the processing. Presence of a large parameter space and lack of our understanding about the fundamental electrostatic correlations greatly hinder any hope for systematic designs of the ionic and zwitterionic polymers for various energy applications. In this talk, I will present our recent theory and simulation work in developing fundamental understanding of electrostatic correlations in ionic and zwitterionic polymers. In particular, importance of often-neglected gradients/non-local effects of electric polarization in affecting electrostatic correlations in polar polymers will be discussed. Furthermore, effects of electrostatic correlations and their close connections to polarization will be discussed in light of experimental results obtained using scattering and reflectivity measurements, broadband dielectric spectroscopy, and atomic force microscopy-based measurements.

Rajeev Kumar is a Research Scientist at the Oak Ridge National Laboratory (ORNL), Oak Ridge, TN. He received his B. Tech. in Textile Technology from Indian Institute of Technology, Delhi, India in 2002 and Ph.D. in Polymer Science and Engineering from the University of Massachusetts, Amherst, MA in 2008. After his Ph.D., he worked at the Materials Research Lab, University of California, Santa Barbara as a post-doctoral fellow. He joined ORNL in 2010 as an American Recovery and Reinvestment Act (ARRA) Fellow at the National Center for Computational Sciences. His current research interests include dynamics of polar polymers, self-assembly of charged and neutral polymers, and scattering from polymers.