

RESEARCH SUMMARY

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My research interests center on soft condensed matter and statistical physics. Soft condensed matter physics deals with soft materials like colloids, complex fluids, liquid crystals, and polymers that are "soft" to touch and for which thermal fluctuations dominate over quantum fluctuations. It is a discipline with a wide range of phenomena and materials that are both intellectually challenging and of importance in fields ranging from oil recovery to biology and medicine. Soft materials provide an ideal testing ground for many fundamental ideas of physics such as the relation between elasticity, low-frequency dynamics, topological defects and broken symmetry, critical phase behaviours, and self-assembly of complex materials. Statistical physics provides us with a language and tools to describe everything from fluctuations in ferromagnets to charge distribution and size variations in polyelectrolytes, and it is critically important for the study of soft materials.

My postdoctoral research (Adviser: Prof. Murugappan Muthukumar) concentrates on the physics of polymers in various physical environments. Polymeric materials are unique in nature as they can assume structures and conformations of astonishing variety, both in biological and synthetic systems. Due to their connectedness and flexibility, polymers possess very rich statistical behaviour and are treated as candidate structures to apply the very basic concepts of statistical and soft matter physics. A tremendous thrust from the experimental community in recent years has explored a multitude of new equilibrium and dynamic properties of both neutral and charged polymers, and that has led to the discovery and synthesis of novel materials such as nano-composites and bio-templates. These polymeric materials have notable impact on modern technology and medicine, especially in the fields of bio-technology (such as gene therapy or drug delivery), and material science (such as electrical circuit industry) - to name a few. A synergistic integration of the observations from these experiments with theoretical and computational approaches can provide much insight into these complex processes, and the gleaned physical insight can facilitate further applied research. To that end, I have used the techniques of statistical mechanics to theoretic-

cally study the physics of polyelectrolytes, the polymers with charged groups having Coulomb interactions between them. These long-range electrostatic interactions lead to significant conformational modification of the polymer chains to the uncharged systems. I study both the equilibrium and dynamics of these systems, ranging from a single molecule to gels in solutions, both in the presence and absence of small electrolytes (salts). The salts can have counterions to the polyelectrolyte of equal or different valency to that of the charged monomer, and depending on the physical parameters (temperature, the heterogeneity of the dielectric constant of the surrounding solvent in the vicinity of the polymers and proteins, the amount of salt etc.), there can be substantial variation in the ion distribution around the polymer as well as within the solution. Depending on the prevailing Coulomb strength, which in turn is regulated by the relative importance of the electrostatic interactions to the thermal fluctuations, a sizable number of counterions might adsorb on to (also known as counterion condensation) the charged groups of the monomer. This charge complexation modifies the effective charge of the polymer and consequently affects its size and density in the solution. Very recently, I have demonstrated the presence of the phenomenon of charge reversal (in which the original polymer charge is reversed) resulting from this adsorption process and also a first-order chain collapse due to electrostatic bridging mediated by divalent counterions between non-bonded monomers for a single flexible polyelectrolyte. I plan to further apply the theory to analyze the volume collapse transition in synthetic or bio-polymer gels, polyelectrolyte brushes, semi-flexible polymers (DNA compaction), and to phenomena involving complexation of charged objects.

The kinetics in polymeric systems in the presence of charge can be fascinating. I study the kinetics of swelling and solvent diffusion in polyelectrolyte gels, and focus on especially two important physical possibilities - one in that physical stress relaxation is the dominant mechanism (e.g., in polar solvents), in which the distribution of inhomogeneous stress determines the time-scale for the conformational changes of the polymers, and the other in that chemical interaction (e. g., for new-generation photo-resists in aqueous-base developers) is the key process that controls the rate of polymer swelling and dissolution. Polyelectrolyte gels are observed to undergo sudden volume changes of immense order when the solvent quality is changed either chemically or thermally. I have been studying the role of the counterions in

modifying the solvent quality and the effective osmotic pressure, and that has been a very challenging theoretical problem of late in the polymer community. The theoretical study of the volume change and the related kinetics of gels and other polyelectrolyte systems has immediate application to the fields of drug delivery, photo-lithography and various others.

In the early phase of my postdoctoral research, I studied the role of the conformational entropy of chains in polymer crystallization. I developed a continuum theory applicable to polyethylene type systems starting from the basic premises of the theory of small molecular crystallization. I proposed a kinetic model involving entropic barriers that recovers both the limits of nucleation and diffusion control for polymer crystal growth in both melts and solutions. We numerically calculated the growth details of a single crystal in dilute solutions, and recovered conventional experimental traits of concentration and molecular weight dependencies. The concept of an entropic barrier will have critical relevance to biological phenomena such as protein crystallization. For the kinetic problems - both the crystallization in uncharged systems and the swelling of polyelectrolyte systems - I used numerical techniques to solve diffusion equations in the presence of moving boundaries. In addition, using a very similar methodology, I have developed numerical programs involving moving boundary conditions in non-trivial, multi-dimensional geometries to calculate the temperature diffusion and related volume changes in polymeric materials.

The primary focus of my doctoral and predoctoral studies were on equilibrium and non-equilibrium physics of soft condensed matter systems. In my doctoral thesis (Adviser: Prof. Tom Lubensky), I calculated using a generalized Abrikosov vortex lattice theory the detailed nature of smectic and director ordering in twist-grain-boundary-C (TGB_C) phases in liquid crystals, and the nature of transitions to them from the cholesteric phase. In my master's thesis (Adviser: Prof. Chandan Dasgupta), I studied using computer simulations the presence of extended self-similarity (ESS) and multi-exponent scaling ("multi-scaling") in the height fluctuations in atomistic surface growth models.