NORTHWESTERN INSTITUTE ON COMPLEX SYSTEMS PRESENTS

Wednesdays @NICO

Domain Formation and Morphologies in Polymers with Self-Regulating Charge

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Wednesday, February 11th, 2009
12:00 – 1:00 PM
Chambers Hall, 600 Foster Street, Lower Level Classroom

In this presentation we will discuss the properties of polylelctrolytes end-grafted to solid surfaces. This original motivation of this study was to understand the properties and interactions of aggrecans, which are one of the main components of cartilage. Aggrecans are supramolecular aggregates composed by polysaccharides, a biological natural type of polyelectrolyte. Polyelectrolytes are molecules composed by many repeat units (monomers) that each could be charged. The properties of these molecules are determined by the interplay between electrostatic interactions, the conformational entropy of the polymers (i.e. its flexibility) and the interactions with the environments. Furthermore, we will concentrate the discussion on weak polylelectrolytes, namely where the charges in the polymer segments are determined by a chemical equilibrium between charged and uncharged species. The polymer backbone does not like to be dissolved in water, while the charges tend to solubilize the molecules. This competition leads to a range of temperatures and surface coverages where the homogeneous grafted polyelectrolyte layer becomes unstable and domain formation is the favorable state of the system. We will show how different morphologies evolve depending upon the thermodynamic state of the solution in contact with the surface. The study of the thermodynamic and structural properties of the grafted weak polyeletrolytes layers are carried out using a molecular theoretical approach that explicit considers the conformational properties of the chain molecules, the chemical equilibrium between the charge and uncharged states of the polymer segments and the intra and inter molecular interactions. The theory is formulated in terms of the free energy of the system, which is written as a functional of the different density components and whose minimization provides with explicit expressions and equation that enable the determination of the different interaction fields. We will show how the variety of domains that are found from the theory are the result of the delicate balance between the different interactions in the systems. Furthermore, we will discuss in detail how the complexity of the system is due to the non-additivity of the different interactions. Namely, the optima structures and their distribution of charges is the result of the coupling that exists between the different interactions and the chemical equilibrium in the system. The relationship between these couplings to biological system will be discussed.

NICO Coffee Hour will follow for questions, networking, and collaboration.

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