pH Responsive Polymers at Curved Surfaces

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Natural and man-made pores and channels of nanoscale dimensions display unique ionic and protein transport behavior. Nanopores modified with supramolecular chemical species (such as polyelectrolyte brushes) have dimensions that are similar to the range of the electrostatic interactions, and also to the molecular size of the tethered macromolecules. Chemical equilibrium within these confined environments is very different from bulk solution and that strongly affects the molecular organization and transport behavior within the pores. In cells, Nuclear Pore Complexes (NPC) control the transport of species between the cytoplasm and the nucleus using disordered proteins as gate keepers. The competition between molecular and interaction length scales, as well as the geometry of the surfaces, creates interesting possibilities for stimuli responsive gates and ion channels and for the fundamental understanding of the interplay between molecular organization and charge transport in nanoconfined environments. In this talk we will discuss recent theoretical developments that enable us to study the structural properties of the modified pores and the coupling that exists between the chemical (protonation) state of the polyelectrolytes and ionic transport through them. The predictions from the theory are in excellent agreement with experimental observation and they provide a direct understanding of the important coupling that exists between protonation state, molecular organization and transport. We will demonstrate how the molecular organization within the pore is a strong function of the pore geometry and how these effects translate into the transport behavior. Finally, we will show predictions for the interactions between nanoparticles and NPC. The importance of considering explicit molecular details of the surface modifiers as well as the coupling between chemical equilibrium, physical interactions and molecular organization will be discussed in detail, in particular as it leads to highly non-additive behavior.