# Mesoscopic Simulations of Confined Polyelectrolyte Electrophoresis and Depletion Induced Chromosome Collapse

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In this talk, I shall present our mesoscopic models and results for two distinct biopolymer systems.

Depletion forces play a role in the compaction and de-compation of chromosomal material in simple cells but it remains debatable whether they are sufficient to account for chromosomal collapse. We present coarse-grained molecular dynamics simulations of a flexible chain of large structural monomers immersed in an explicit bath of smaller depletants. Our results verify that depletion induced attraction is sufficient to cause collapse. We quantitatively cast the action of depletants on bacterial chromosomes as an effective solvent quality. Both the theoretical framework and simulation results point to a continuous phase transition for flexible chromosomes.

The study of confined, electrophoresing polyelectrolytes in a buffer solution is crucial to the advancement of DNA separation techniques. The electrophoretic motion of deformed DNA molecules in narrow channels is of particular interest, since conflicting experimental results have reported both a decrease and increase of mobility with confinement. Our hybrid multi-particle collision dynamics and molecular dynamics simulations of polyelectrolytes with finite Debye layers electrophoresing in an axisymmetric, wall-less confining well show that electrophoretic mobility increases with confinement in a length dependent manner, though the chains remain "free-draining", as seen explicitly from the elctro-osmotic flow within the coil. I shall explain these results and propose an experimental setup to utilize these phenomena to separate DNA on a simple microfluidic chip.