Simulations of DNA condensation

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The effects of the presence of a mixture of counterions, with different valances, on DNA condensation are investigated with Monte Carlo simulations. It is well known that charged chains decrease in size forming condensed conformations when the strength of the electrostatic interactions is increased, e.g. by adding multivalent counterions.

For flexible charged polymers, this decrease in chain size is a smooth function of the amount of added salt. For DNA, a very stiff polyelectrolyte, the behaviour is qualitatively different. When a small amount of multivalent salt is added, stiff polyelectrolytes are only observed in elongated conformations, while for high amounts of salt only compact toroidal or rodlike structures are found. We have been able to show how, for intermediate amounts of multivalent salt, there is coexistence between the elongated and compact conformations. In this region a single chain is found in either of the two conformations, but does not show a gradual decrease in size as the flexible chain does. In terms of the free energy, the simulations show how a flexible chain always has one minima as a function of chain size, while the stiff chain has two for certain amounts of added multivalent salt.