Microscopic modelling of DNA: From Chromatin to Nanomachines

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Charged polymers such as DNA exhibit a number of different complexation modes when mixed with other charged objects such as spheres or cylinders. A simple model for the complexation of semiflexible polyelectrolytes with oppositely charged spheres is considered, which can exhibit tightly wrapped polymer structures. Using the appropriate parameters for DNA-histone complexes, we find complete wrapping for intermediate salt concentrations only, in agreement with experiments. The obtained structures resemble the experimentally observed chromatin morphologies. The forces needed to pull the DNA off from the histone show a plateau at 10-40 pN (depending on salt concentration).

From the characteristic force-extension profile at larger forces one can learn a lot about the elastic behavior of a stretched polymer that is bound between surface and AFM tip. The enthalpic stretching modulus of different synthetic and biopolymers is obtained from ab-initio quantum-chemical calculations and compares well with experimental data at high forces above 400 pico-Newton.[1] At smaller forces, entropic contributions are well described within the discrete-chain model, whereas the commonly used worm-like-chain model is shown to be inadequate for describing experimental stretching data on synthetic chains.

We also consider stiff polymers in various non-equilibrium situations. Polymers that are anchored to surfaces, so-called brushes, are subject to shear flow and as a result deform and screen the hydrodynamic flow to various degrees, as relevant for glycocalix layers at endothelial cells in the blood stream. Conversely, stiff polymers at surfaces that are beating back and forth can be used to pump liquids over surfaces, which is a concept realized by ciliae but also attractive for synthetic designs. Elasticity is important here because for rigid rods the pumping efficiency is zero.

[1] *Highly Stretched Single Polymers: Atomic-Force-Microscope Experiments Versus Ab-Initio Theory,* T. Hugel, M. Rief, M. Seitz, H. Gaub, R.R. Netz, , Phys. Rev. Lett., **94**, 048301 (2005)