Example Systems

Here we give examples of other systems of interest which also highlight methods and capability. The four examples are

•Self-assembled monolayers (SAMs)

•Rhodopsin

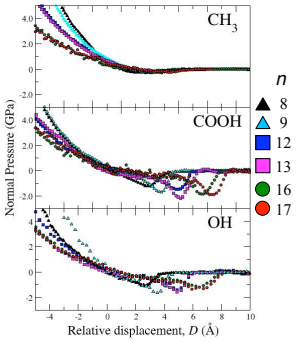
•microtubules

•DNA condensation

All of this work involves molecular dynamics (MD) simulations typically using our massively parallel code LAMMPS. The simulations of SAMs and rhodopsin are atomistic simulations. The microtubule and DNA simulations use coarse-grained models.

Self-Assembled Monolayers

We have treated alkanethiol and alkylsiloxane SAMs focusing on the adhesion and friction properties. MD simulations are performed to calculate the interaction between two SAM coated surfaces. Recently, we have studied SAMs with different endgroups. Below we show some results for the dependence of the adhesion curves on the chain length and endgroup. The bottom images of OH terminated alkanethiols show the structure of the SAMs at different separations. *D* is the separation between the two SAMs. The offset for *D* is chosen such that *D* = 10 Å when the terminal C atoms have separation of 10Å. The images show that the chain tilt less due to hydrogen bonding at *D* = 3Å and tilt more at high compression.



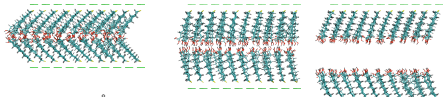
•Little *n* dependence for CH_3

•Small attractive minima for CH_3

•Large attractive minima for OH and COOH

•Significant *n* dependence for OH and COOH

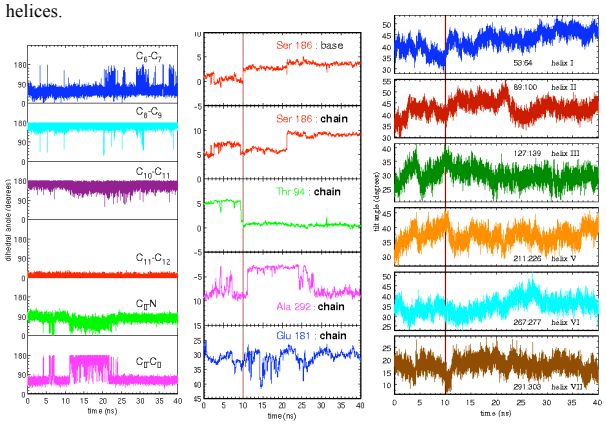
•minimum position increases with *n*



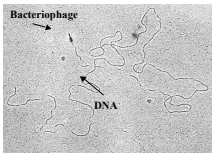
D = -4Å *D* = 3Å *D* = 10Å

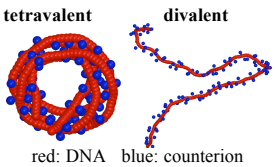
Rhodopsin

Rhodopsin is a membrane protein that is part of the visual system consisting of 7 transmembrane alpha helices. A retinal molecule is bound within rhodopsin and undergoes a light activated cis-trans isomerization. The transition for dark to light adapted rhodopsin involves structural changes which affect the G-protein associated with rhodopsin and results in a signaling cascade. We performed 40 ns MD simulations of the dark-adapted structure of rhodopsin within a DOPC bilayer. While the retinal molecule does not undergo a transition as expected, we find many dihedral transition in the retinal molecule and neighboring amino acid side chains. These are related to changes in hydrogen bonds. Ultimately, this local dynamics results in larger scale motion of the transmembrane helices.



Packaging DNA





red: DNA blue: counterion

DNA is *huge* compared to its host. DNA is one of the most highly charged polymers known with each base containing a negatively charged phosphate group. These charges repel each other resulting in an extended structure. Collapsing DNA into a volume that fits inside a bacteriophage capsid would involve enormous pressures.

How is DNA packed into a small volume overcoming the enormous Coulomb repulsion?

Experimentally, we knew the answer is multivalent counterions, but we did not know why.

Simulations of a simple, bead-spring model of DNA reproduce the spontaneous formation of toroids in the presence of tetravalent counterions (e.g. spermine), but divalent ions (e.g. Mg^{2+}) do not collapse the DNA.

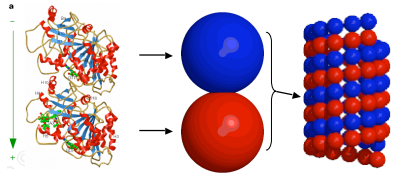
The mechanism for 'DNA packaging' involves only electrostatic interactions, i.e. independent of base pair sequence.

For the higher valence counterion, the electrostatic interactions dominate all other and prefer to charge order the system so that the ions alternate +–+–+–. This yields the toroids.

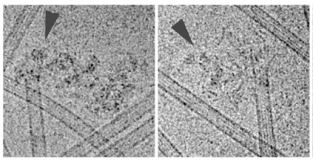
Microtubule Modeling

Microtubules are long polymers that form 'train tracks' for motor proteins within cells. They are thus a fundamental element of a transport system. In addition, self-assemble and disassemble depending on the environment (active assembly). We are presently developing coarse-grained models that we expect will yield active assembly of microtubules. Microtubles are polymers of tubulin protein dimers. We model each tubulin protein as a single bead.

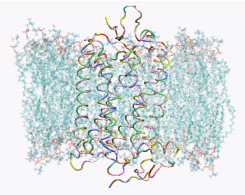
tubulin dimer (known structure) monomers as single particles microtubule



What is the minimal set of interactions that will yield the correct microtubule structure?



microtubule formation Kinoshita *et al.*, Science 2001



rhodopsin