unfolds in at least two major steps. Whether the kinetics of the transitions are influenced by the presence of capsid proteins is a subject of further detailed investigations.

863-Pos Board B632
Hydrogen Bond Strength Modulates the Mechanical Strength of Ferric-Thiolate Bonds in Rubredoxin
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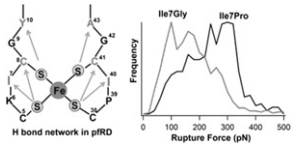
It has long been recognized that hydrogen bonds formed by protein backbone amides with cysteinyl Sulfur atoms play important roles in modulating the functional and structural properties of the iron-sulfur centers in proteins. Here we use single molecule atomic force microscopy, cyclic voltammetry and protein engineering techniques to investigate directly how the strength of N···H-Sγ hydrogen bonds in the secondary coordination sphere affects the mechanical stability of Fe(III)-thiolate bonds of rubredoxin. Our results show that the mechanical stability of Fe(III)-thiolate bonds in rubredoxin correlates with the strength of N···H-S hydrogen bonds as reflected by the midpoint reduction potential, providing direct evidence that N···H-S hydrogen bonds play important roles in modulating the mechanical and kinetic properties of the Fe(III)-thiolate bonds of iron-sulfur proteins and corroborating the important roles of the protein environment in tuning the properties of metal-thiolate bonds.



864-Pos Board B633
Synthesis of Functionalized Microspheres with High Magnetic Concentration for Microscale Force Application
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Magnetic microspheres are commercially available in a wide range of diameters and with a variety of chemical functionalities for applications such as cell sorting, protein isolation, or microscale force spectroscopy. The most commonly-used products are magnetic spheres one micron in diameter or larger. These spheres generally consist of a polymer core which is swollen in a solvent and saturated with a solution of iron oxide nanoparticles. This top-down process tends to result in incomplete saturation of the polymer spheres and therefore a diminishing magnetic concentration as spheres grow larger since the magnetic content does not scale with volume.
We present here a bottom-up approach to microsphere fabrication which begins with a high-permeability magnetic fluid consisting of magnetite nanoparticles complexed with poly(dimethyl siloxane-co-aminopropylmethyl siloxane). The magnetic content of the fluid may be adjusted smoothly from 0 - 50% wt. without any nanoparticle aggregation, resulting in a highly-magnetic silicone fluid which is homogenous at scales well below 100 nm. Using this material, we demonstrate the production of solid, spherical microbeads in diameters ranging from 2 - 30 microns. Since magnetic nanoparticles are distributed uniformly throughout the material, magnetic content scales directly with volume, resulting in a significant advantage over competitors in terms of magnetic force application at larger sizes. Controlling for diameter, the high magnetic content of these spheres results in nearly four times the force-generating capabilities of the leading 2.8-micron competitor, with advantages increasing in larger spheres. In addition, we use a cell-targeting assay to demonstrate our ability to functionalize the microsphere surface with a variety of ligands.

Molecular Dynamics I

865-Pos Board B634
Covering All the Bases: A Martini Coarse-Grained Force Field for DNA
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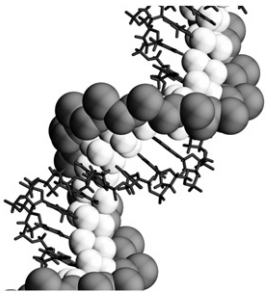
University of Groningen, Groningen, Netherlands.
Deoxyribonucleic acid or DNA is not only important as the keeper of our genes but due to its self-recognition properties and programmability it has found use in technical applications like nanostructures, crosslinkers and tethers. One of the tools used to study the conformational dynamics and interactions of DNA are molecular dynamics simulations. DNA is most often simulated using all-atom force fields, which describe the properties of DNA quite well but their computational cost severely limits the number of base pairs and accessible time scales. Coarse-grained models can extend the length and time scales by clustering groups of atoms into single interaction sites. Several coarse-grained DNA models have been developed but few of these are compatible with models for other biomolecules or with common simulation packages. We present a model of DNA using the coarse-grained MARTINI force field that maps roughly four heavy atoms into one interaction site, describes the solvent explicitly and is orders of magnitudes faster than fully atomistic force fields. The DNA model is compatible with all other MARTINI models enabling its use in studying a wide range of biomolecular systems.



866-Pos Board B635
Moltemplate a Coarse-Grained Model Assembly Tool
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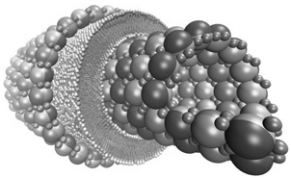
Moltemplate, an open-source program intended for building large scale coarse-grained models, has been developed by our group to facilitate the speed and ease by which such models could be constructed. Although coarse-grained models have long been considered as an indispensable tool in the investigation of biopolymer dynamics and assembly, the actual process of constructing such models is often arduous and impeded by the fact that complex and unconventional force fields must be implemented. Until now, no software has existed for building general coarse-grained biomolecules, and as a result, the use of such models remained relatively inaccessible. Here, we represent a general molecule-builder program, Moltemplate, which together with the LAMMPS simulation program, will hopefully bridge the current gap and bring coarse-grained simulations to a wider audience. As an demonstration of its functionality, we would like to represent its use in the investigation of the nucleation of amyloid fibrils. We have found that context-induced effects (such as alternative folding of the monomer) can have profound consequences on the assembled product (such as the morphology, growth-potential and stability of the aggregate). Other examples, such the stability of membrane proteins, and the growth of microtubules will be discussed.



867-Pos Board B636
Fatty Acid Aggregates Simulated using Constant pH Molecular Dynamics with a Coarse-Grained Model
W.F. Drew Bennett[1], Serena Donnini[2], Gerrit Groenhof[3], D. Peter Tieleman[1].
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Fatty acids are crucial biomolecules, important for lipid metabolism, signaling, models for protocell membranes, soaps, industrial applications, and drug delivery. Oleic acid has complex phase behavior with respect to the protonation state of the carboxylic head group, which depends on the pH of the solution. Oils form at low pHs, vesicles at intermediate pHs, and micelles at high pHs. We use constant pH molecular dynamics with the MARTINI coarse-grained model to investigate oleic acid aggregates at different pH conditions. We determine titration curves for the oleic acid monomers in different aggregates, and observe a shift in the microscopic pKa. In agreement with experimental results, the pKa of a monomer in bulk water is ca. 4 and shifts to ca. 5.5 in a small micelle and ca. 8-9 in a fatty acid bilayer. There is strong anti-cooperative protonation behavior between monomers within an aggregate. This work presents a proof of concept for using constant pH simulations with the MARTINI model, and provides a physiochemical basis for the phase behavior of fatty acids in different aggregate environments.

868-Pos Board B637
Thermodynamics of Oleic Acid Aggregation from Coarse-Grained Molecular Dynamics Simulations
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Known for its health benefits in olive oil, oleic acid is a long chain fatty acid with a cis-9 double bond in its hydrocarbon tail. Oleic acid self-aggregates in a pH-dependent manner as micelles, vesicles, and oil in aqueous solution and is considered a candidate for drug delivery. Despite oleic acid's apparent chemical simplicity, the chemistry underlying oleic acid self-aggregation is not