2174-Pos Board B144
Counterion Release Stabilizes Multi-Shell Structures Of Virus Coat Proteins
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Under conditions of low ionic strength and a pH between about 3.5 and 5.0, solutions of purified coat proteins of cowpea chlorotic mottle virus (CCMV) form spherical multi-shell structures in the absence of viral RNA. The native protein shell, which has an outer diameter of about 28 nm and is built up from 180 coat proteins, forms the inner shell and is surrounded by one or two larger concentric shells. We show that counterion release is the main force stabilizing these multi-shell structures, arguing that this compensates for the outer shells not being able to adopt their smaller optimal radius of curvature. This explains why the structures are only stable at low enough ionic strengths and why we never see the larger outer shells separately in solution. The inner surfaces of the shells are positively charged over a large range of pH values, with most of the positive charge residing on the last 10 nm of the N-terminus side of the protein, which sticks out into the interior. Our calculations show that the multi-shell structures are only stable when the outer surface of the shells is negatively charged, which is above a pH of about 3.5. The fact that we do not see multi-shells at high pH (>5.0) is explained by looking at the stability of the pentamers and hexamers of protein dimers, the building blocks of the shells. Although we focus on CCMV multi-shells, structures of this kind should arise generally in any situation where an attraction between concentric spherical (or cylindrical) shells competes with a preferred spontaneous curvature.

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Nanorheology of viscoelastic shells: Application to viral capsids
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We study the microrheology of nanoparticle shells [A.D. Dinsmore et al., Science 298, 1006 (2002)] and viral capsids [I.L. Ivanovska et al., Proc. Natl. Acad. Sci. U.S.A. 101, 7600 (2004)] by computing the mechanical response function and thermal fluctuation spectrum of a viscoelastic spherical shell that is permeable to the surrounding solvent.
We determine analytically the coupled dynamics of bending and compression modes of the viscoelastic shell coupled to solvent flows inside, outside, and through the porous viral capsid. From this calculation, we identify fundamental length and time scales in the system, and compute the finite-frequency response of the shell to pinching forces applied at antipodal points on it.
This calculation determines the mechanical response of a viral capsid to an AFM-based nanoindentation study. Using these calculations, one can interpret such studies in terms of elastic and dissipative response of the viral capsid to bending and compressional deformations and thereby gain new information regarding the internal deformations of individual capsomers under stress, providing insight into their intermolecular and intramolecular interactions. As an example we study the mechanical effect of a simple allosteric transition in the capsomers.
The frequency-dependent mechanics of complex, viscoelastic and possibly porous spherical shells is not only application to viruses, but also may lead to new measurements of colloidosomes, nanoparticle shells, and lipid vesicles including those that contain pore-forming proteins.

2176-Pos Board B146
Charting the Structure and Energetics of Packaged DNA in Bacteriophages
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Many bacterial viruses resort to pressure in order to infect bacteria, e.g., lambda phage stores its dsDNA genome at surprisingly high pressure and then uses this pressure to drive delivery of the genome. We report on a biophysical interrogation of the DNA configuration and pressure in lambda phage by combining structural and thermodynamic measurements with theoretical modeling. Changes in DNA organization in the capsid are monitored using solution small angle x-ray scattering (SAXS). We vary the DNA-DNA repulsion and DNA bending contributions to the capsid pressure by changing salt concentrations and packaged length, and augment SAXS data with osmotic stress measurements to elicit the evolving structure and energetics of the packaged DNA.
References
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2177-Pos Board B147
Modeling DNA Condensation Phenomena by Coarse-Gained Models:
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Packaging inside Bacteriophages and Compaction inside Bacteria.
The presence of polyvalent cations such as spermine and spermidine in DNA solutions leads to the formation of DNA condensates. This phenomenon has been experimentally observed for DNA confined inside bacteriophages and upon its release into bacterial cells. It has been shown that the topology of DNA in condensates depends not only on the concentration of polycations but also on the presence of small proteins that induce DNA binding such as HU and IHF (Sarkar, 2007, Nuc. Acids Res. 35, 951). In the absence of these proteins the morphology of DNA condensates resembles toroidal structures, whereas the presence of these proteins leads to the formation of rod-like conformations. In this study we present simulations of DNA condensation using a coarse-grained model of DNA under attractive conditions. The first group of simulations describes the condensation of DNA upon its packaging inside bacteriophages lambda and P4. Both systems reveal formation of toroidal condensates inside the capsids. We also show that the forces required to pack the genomes in the presence of polyamines are significantly lower than those observed under repulsive conditions (in the absence of polycations). In the second group of simulations we characterize the effect of binding proteins (modeled by randomly introducing flexible sites along DNA) on the morphology of free (unconfined) DNA condensates. The results show that in the absence of binding proteins the fraction of rod-like structures is 48%. With the flexible sites introduced it becomes 74%. The simulations semi-quantitatively reproduce the experimental data, which supports the proposed model of the role of binding proteins. The formation of toroidal and rod-like condensates in the presence of polyvalent cations and binding proteins also strongly backs the push-pull mechanism of genome injection from bacteriophages inside bacterial cells.

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Deconstructing Viral Shells To Understand Its Building Blocks
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Bacteriophages are known to carry their highly compressed genome under pressure in nanometer sized protein containers (capsids). f29 is a double-stranded DNA *Bacillus subtilis* phage whose capsids are prolate icosahedrons elongated along a 5-fold symmetry axis. The prohead is an assembly intermediate that is made by a reduced number of structural components. To withstand the considerable internal stresses, the prohead combines unexpected strength and resilience despite the fact that only weak protein-protein interactions are keeping the capsids structure together. Here we use Scanning Force Microscopy to study the mechanical properties of shell proteins as a function of their position with in the prohead. While gently probing the capsid, causing small deformations, we observe changes in the local elasticity revealing pentameric structures. When we break the shells in a controlled fashion we find that the capsids fracture along well-defined lines. The observed fracture lines are analyzed and classified according to the known monomer organization from the recently solved pseudoatomic structure. We found that the mechanically coherent building block of the protein shell is a trimer of monomers, organized according to the triangulation net of the icosahedron. Moreover, we find that the interactions between proteins in the equatorial belt are nearly twice weaker than the interactions within the icosahedral end-caps.

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Study Of Mechanical Properties Of Bacteriophage T7
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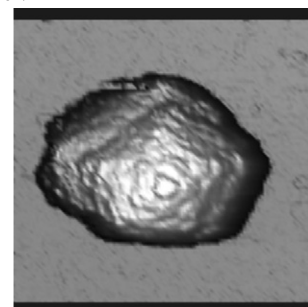
Bacteriophage T7 belongs to the Podoviridae family and is the genus representative enclosing the related variant previously known as phage T3. It contains a 40 kb dsDNA genome and the mature head has icosahedral symmetry, presenting a diameter of 50 nm and a thickness wall of 2.5 nm. By using Atomic Force Microscopy in buffer conditions we have imaged T7 mature capsids and