than AA models. Specifically, knowledge-based potentials are parameterized with regards to both the structure of the AA model and experimentally-derived information. In this case, the CG model has initially been parameterized to reproduce the dissociation constant of 20-bp DNA and the disordered C-terminus of histone 1 (CH1), which form complex coacervates with different internal order as a function of the phosphorylation of CH1 and salt concentration. We will use our CG model to provide insights into the internal structure of the CH1/DNA coacervates, as well as to consider the effects of DNA sequence on coacervate formation. This model could also serve as a basis for integrative modeling, which would allow additional experimental information to be incorporated.

1108-Pos

Repackaging DNA: From Nucleosome Core Particles to Protamine Loops

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The transmission of hereditary information is crucial for the continuation of life. To pass DNA on to the next generation, sperm cells must repackage DNA to create a compact, hydrodynamic sperm head. In some organisms, repackaging occurs by the direct replacement of nucleosome core particles (NCP) with protamine-induced loops. To measure the real-time dynamics of this direct replacement pathway, we use an in vitro tethered particle motion (TPM) assay. In this assay, we tether a polystyrene particle to a glass coverslip using DNA and track the motion of the tethered particle. We then add histones and monitor the change in the motion of bead. If the DNA tether folds, we expect the bead's motion to become constrained. Our original hypothesis was that as NCPs are replaced by protamine, DNA would unfold due to the loss of histone interactions. Then, the DNA would refold as protamine loops the DNA. However, preliminary TPM data show that the motion of the particle does not increase when protamine is added, which suggests that protamine compacts the DNA without unfolding. This finding suggests a new pathway that may yield insight into the repackaging process crucial for reproduction.

1109-Pos

Protamine Folds DNA into a Flower Shape before Forming Toroids

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To engineer large DNA nanostructures, we need to be able to fold DNA to macromolecular levels. One protein of interest is protamine, which drives the almost crystalline-level compaction of the entire sperm genome. Specifically, multiple protamine molecules bind the DNA, looping it into a series of toroids. These toroids then stack in the sperm nucleus to produce a small, hydrodynamic sperm cell that can efficiently travel to the oocyte. In this study, our goal is to identify the pathway for how protamine forms DNA toroids. There are three possible models for toroid formation: 1) Sequential stack, in which subsequent loops stack on top of one another; 2) sequential loops-on-a-string, in which loops form adjacent to one another before collapsing into a toroid; and 3) all-loops-at-once, in which all loops form simultaneously before collapsing into a toroid. To distinguish between models, we employ a combination of atomic force microscopy (AFM) and tethered particle motion (TPM) experiments. AFM enables direct visualization of folded states, while TPM enables real-time measurement of the folding dynamics of individual DNA molecules. Using AFM, we observe folded structures that have 1, 2, 3, or more loops, which would be the case in the sequential loops-on-a-string model. However, structures with multiple loops have a common center, similar to a flower-shape, prompting us to suggest a new model for toroid formation that involves flower-shaped intermediates. TPM data distinguishes multiple folded states as well that coincide with the 1, 2, 3, or more folded loops. Interestingly, these states are reversible. We therefore conclude that toroid nucleation occurs via a sequence of reversible flower intermediates with an increasing number of loops. These results might be applied to fold DNA origami structures, enabling the design of larger and more complex DNA nanostructures.

Posters: Membrane Physical Chemistry II

1110-Pos

Membranes with Decreased Deformability to Study the Kinetics of Fusion Intermediates

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While the initial protein activation steps involved in influenza membrane fusion have been relatively well resolved, the subsequent lipid rearrangements are much more challenging to study. This is because the formation of lipid intermediates is faster than protein activation and thus masked in kinetic measurements of intact virus. To unmask these intermediates, we have developed methods that utilize target membranes with decreased deformability. By using supported lipid bilayers on silica nanoparticles of a defined diameter we are able to alter the deformability of the target membrane without changing its lipid composition. In conjunction with single-virus fusion kinetics, this allows us to examine the effect of membrane deformability on the kinetics of influenza membrane fusion. Our results show that decreasing target membrane deformability does indeed slow lipid mixing between virus and target. Further extensions to this platform then allow stepwise dissection of how membrane mechanical properties affect influenza membrane fusion.

1111-Pos

Alpha-Helical Membrane Protein Folding in "Mixed" and "Ideal" Bicelles

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Lipid-detergent bicelles are often used in membrane protein studies as an alternative to micelles. The ideal bicelle model contains a segregated lipid core surrounded by a detergent rim, and their morphologies depend on the ratio of lipid to detergent (q-ratio). There are several reports that the most widely used bicelle, containing 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine and 1,2-dihexanoyl-*sn*-glycero-3-phosphocholine, forms ideally mixed micelles at q-ratios below 0.5. To date, almost all membrane protein studies using isotropic bicelles, particularly solution NMR spectroscopy, have relied on q-ratios of $\sim$ 0.3 due to favorable tumbling properties. Designing bicelle mixtures with segregated lipid and detergent across a broad range of q-ratios is, therefore, of high interest for membrane protein applications. We investigated common bicelle mixtures with q-ratios of 0.0-1.0 and measured the short diameter, L, with SAXS. The diameter was previously shown to correspond with the mixing behavior reported by SANS and molecular dynamics simulations, with L equal to two lipid lengths in a lipid-segregated bicelle. All alkyl-chain lipid and detergent combinations with phosphocholine-like head groups form mixed micelles up to $\sim$ q-ratio = 0.5. Bicelles containing bulky moieties at detergent alkyl tails and head groups were additionally investigated, which we hypothesize will increase segregation between lipid and detergent components at q ratios less than 0.5. The mixtures most promising for ideal bicelle morphologies at low q-ratios were then used to investigate protein fold and backbone dynamics of a polytopic alpha-helical transmembrane protein using continuous-wave EPR and solution NMR spectroscopy. Our results suggest that lipid-protein interactions influence protein fold distinct from detergent-protein interactions.

1112-Pos

Order Parameter Analysis of Lipids Organization in the Presence of ATP

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Adenosine triphosphate (ATP) is an essential component which provides the energy needed in biological interaction in the vicinity of lipid membranes. In this regard, we investigate on the C-D bond order parameter components of phospholipid in presence of ATP for various temperatures obtained by deuterium nuclear magnetic resonance (^{2}H NMR). In addition, simulations were done using a mean-torque potential model to determine the alignment field, which shows the orientational tendency of each carbon segment. We find that the presence of ATP changes the order parameter component as well as the alignment field. These results also indicate that ATP increases membrane order, which results in a stronger alignment field. When increasing temperature, the order parameter goes down because of increasing entropy. These results suggest that the stronger alignment field could influence ion-transport through membranes, which has applications in many biological processes. However, to determine the influence that carbon position and temperature have on this alignment field, more theoretical work is needed.

1113-Pos

Nanodomains Persist to much Higher Temperatures than Large Scale Phase Separation in Giant Plasma Membrane Vesicles and Can Respond Differently to Alterations of Plasma Membrane Lipid Composition

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