Using a combination of all-atom and coarse-grained molecular dynamics simulations to interpret a range of x-ray scattering experiments, we aim to understand the role of membrane deformation in the action of the Parkinson's Disease protein, α-Synuclein. Our simulation results have led to the hypothesis that αS flattens curved membranes by screening the repulsive interactions between negatively charged, acidic headgroups, thereby reducing the effective area per headgroup and relieving the inherent positive curvature of the lipids on the outer leaflet of synaptic vesicles. We hope to address the question of whether αS influences a membrane's mechanical properties as a route to evaluating this hypothesis. Additionally, we aim to understand the role of αS in recruiting sub-domains of positively charged lipids. A second, smaller peptide (the CRAC motif from gp41) is also studied in an effort to build the computational tools necessary for matching the x-ray data that is used for calculating a membrane's material properties.

2528-Pos

Effects of Subphase on Collapse Behavior of Lung Surfactant

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The phase behavior of binary fluids next to interfaces can be complex. If one fluid has a more favored interaction with the interface the fluids can phase separate in some interfacial region extending into the bulk. Using neutron and x-ray reflectivity, we show phase separation of water/glycerol mixtures next to lipid monolayer interfaces. The glycerol forms a thin layer ten angstroms deep underneath the monolayer. This non-equillibrium interfacial phase separation greatly impacts the mechanical properties of the lipid monolayer. Moreover, the thermodynamic driving force for this de-mixing is complex. Usually such de-mixing is observed when two miscible fluids have significantly different surface tensions at a given interface. However glycerol and water are miscible and have nearly identical surface tensions at the air/water interface. Our work probes what surface tension and interfacial free energy mean in the setting of more complex interfaces. The preference partitioning of glycerol to the interface affects the collapse behavior of the lipid film and has implications on the collapse mechanism of lung surfactant which sits atop an alveolar lining fluid enriched in sugar biopolymers.

2529-Pos

Oxygen Diffusion Through Lung Surfactant Layers

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Pulmonary surfactant, a lipid-protein complex covering the air-liquid interface of alveoli, is essential for preventing alveolar collapse at the end of expiration. To do so, surfactant reduces surface tension by forming a surface-active interfacial film, which has to be crossed by oxygen to reach the pulmonary epithelium and the capillary. The effect of the presence of the pulmonary surfactant layer in oxygen diffusion has not been properly evaluated.
Here we have developed a special setup using luminescent Rutenium-containing organo-metallic oxygen sensors to measure oxygen diffusion rates through capillary water layers containing different concentrations of pulmonary surfactant lipid or lipid-protein preparations.
The potential role of surfactant and the structure of surfactant membrane network in terms of facilitating oxygen diffusion through the air-water respiratory interface will be discussed.

2530-Pos

Molecular Organization of the Tear Film Lipid Layer

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Purpose. To describe the molecular organization of the anterior lipid layer of the tear film.
Methods. Artificial tear fluid lipid layers (ATLL) were deposited on the air-water interface and their physico-chemical behavior was compared to egg-yolk phosphatidylcholine (eggPC) monolayers by using Langmuir-film balance techniques, X-ray diffraction, atomic force microscopy, and Brewster angle microscopy. These experimental approaches were complemented by *in silico* molecular level simulations.
Results. In contrast to eggPC monolayers compression isotherms of the ATLL suggested that at higher surface pressures the ATLL films were no longer monolayers. ATLL films had a lower compressibility compared to eggPC lipid films. At π=20 mN/m both samples or part of the samples were in the condensed phase. Brewster angle microscopy suggested that in the case of ATLL a clear phase separation was observed. Atomic force microscopy preformed at π=20 mN/m showed only a smooth surface for eggPC, whereas for ATLL lipoprotein-like particles were protruding from the otherwise smooth lipid film. Computer simulations on eggPC and ATLL yielded a detailed picture of the atomic level organization of eggPC and ATLL residing on the air-water interface and supported the experimental findings.
Conclusions. Here we provide detailed structural analysis of eggPC and ATLL films deposited on the air-water interface. The results are discussed in the context of *in vivo* function of the tear fluid.

2531-Pos

Molecular Scale Texture and Topological Defects in Lipid Membranes: A New Liquid Crystalline Phase

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Lipid membranes are self-organizing structures that define intercellular and intracellular interfaces in biological systems. Grazing incidence x-ray diffraction (GIXD), provides a sensitive probe of the local, molecular structure and packing of lipid molecules within single membranes. For example, diffraction clearly establishes that dipalmitoyl-phosphatidylcholine (DPPC) membrane leaflets are always coupled across the bilayer, and that even when leaflets are deposited independently the membrane rapidly self-organizes so that opposing lipid tails scatter as one entity. Variation in the azimuthal tilt direction of the lipid tails was required to reproduce the diffraction data indicating an orientational texture of lipid molecules and smectic domains formation identical to larger scale textures observed in many 2-D liquid crystalline systems, but at a molecular scale.
A similar phenomenon is also observed when proteins bind to membrane receptors. The interplay between lipids and proteins is complex: lipids can influence the structure and function of membrane proteins and at the same time proteins can impact lipid organization. In this example, lipid monolayers at the air-water interface containing the ganglioside GM1 were studied in the absence and presence of cholera toxin. At low surface pressures, protein binding perturbed the lipid order such that the molecules were no longer close packed, creating topological defects and lipid-protein domains with orientational texture. This new lipid phase may be a mechanism for toxin penetration and potentially has far broader implications in biological signaling.

2532-Pos

Calculation of Interleaflet Domain Coupling in Mixed Lipid Bilayers

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The coupling between the physical states of the two leaflets (monolayers) of a lipid bilayer is a subject of current interest in relation to both the biology of lipid rafts and the physics of model membranes capable of liquid-liquid phase separation. In these model systems there is experimental evidence of a large coupling which maintains micron-scale registry between domains in the two leaflets. Nevertheless, the mechanism of this coupling has been unclear. We have performed a mean-field calculation with molecular detail to evaluate the contribution to this coupling due only to lipid tail interdigitation. By comparing the free energies of symmetric and asymmetric lipid compositions, we obtain a coupling strength of 0.2 kT per square nanometer. This is enough to account for micron-scale domain registry and is in favorable agreement with a recent estimate from a coarse-grained molecular dynamics simulation. Our result supports the hypothesis that lipid interdigitation is the dominant mechanism for interleaflet domain coupling in model membranes capable of liquid-liquid phase separation.

2533-Pos

Assembly of Lipid Bilayers in Large Scaffold Arrays

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