Experimental studies of anionic membranes have generated several new and interesting information on their behavior under different pH, salt concentration and temperature conditions. However, good microscopic models is still lacking. We propose a generalization of the statistical model for neutral lipids to include the effect of the ionic charges. The ionization state of the lipid polar headgroup depends on the salt concentration, so one may have either dissociated (charged) or associated (neutral) gel/fluid phases, as well as semi-dissociated phases. The model order parameter, specific heat and conductivity are compared with experimental data of an aqueous dispersion of the phospholipid DMPG (dimyristoyl phosphatidylglycerol).

2366-Pos Board B336

Biophysical Characterization Of Phosphatidyl Alcohols In Model Membranes- Effects Of Headgroup Size

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The polymorphic phase behavior of different phospholipids depends strongly on fine details of their head group and backbone structures. Studies of phospholipid head group modification offers an attractive strategy in elucidating how structural elements of the head group effect membrane properties. We are investigating phosphatidyl alcohols with saturated fatty acyl chains and their interactions with phospholipids and sterols. Molecules of interest are dipalmitoyl glycerophospholipids with methanol, ethanol, propanol and butanol as different headgroups. These molecules can be formed from e.g., corresponding phosphatidylcholines due to the transphosphatidylation activity of phospholipase D. Phosphatidyl ethanol is of physiological relevance since it is increasingly formed in cells of chronic alcoholics. Thermodynamic properties such as phase transition temperatures, heat capacity of transitions and transition cooperativity have been studied with high sensitivity differential scanning calorimetry (DSC). The miscibility and effects of cholesterol on mixtures of these negatively charged phospholipids with high Tm and low Tm phospholipids have been determined using DSC, and with fluorescence spectroscopy using domain-selective lipid probes. The relative acyl-chain order in the bilayer membranes has been assessed using steady-state DPH anisotropy. We will report on the phase behavior of these molecules in simple and more complex bilayer systems. The formation, by the dipalmitoyl phosphatidyl alcohols, of sterol-enriched or ordered domains in fluid bilayer membranes will also be determined. Comparison of the properties of these phosphatidyl alcohols with molecules having closely related structures will help in understanding the relationships between the chemical structures, physical properties and functional properties of the phospholipid molecules in model as well as biological membranes.

2367-Pos Board B337

Measurements of Electrostatic Interactions between Charged Membranes

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Neighboring lipid membranes experience attractive and repulsive forces. The attractive (van der Waals) force is due to induced change fluctuations and it acts even between neutral membranes. Repulsive forces arise from the tendency of lipids to stay hydrated and can include electrostatic interactions due to accumulation of membrane surface charge. When the attractive vdW force is balanced by repulsive forces, an equilibrium spacing between lamellae is established, as measured by X-ray scattering. This is often the case for neutral membranes. By contrast, lipid bilayers made entirely of charged lipid species such as the negatively charge phosphatidylserine (PS) swell indefinitely (‘‘unbind’’) in the absence of salt indicating the dominance of electrostatic repulsion. To measure the strength of electrostatic interactions in solution, we manipulate membrane charge in two simple ways: by adsorbing ‘‘sticky’’ ions such as bromide onto neutral phosphatidylcholine lipids, and by mixing-in charged lipid species. We will present results and discuss in what conditions membrane electrostatics can lead to unbinding.

2368-Pos Board B338

The Role of Sedimentation and Osmotic Stress in the Regulation of Surface Drag for GUVs Moving in an Electric Field

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Giant unilamellar vesicles (GUVs) suffer variations in shape when exposed to changes in osmotic stress. These shape variations should alter their drag properties when moving close to a surface by inducing a change in the lubrication drag between the surface and the vesicle due to an excess surface area. Using POPC vesicles labeled with NBD-PE we study the influence that osmotic pressure and sedimentation conditions produce on the dynamics of vesicles moving under the influence of a lateral electric field. As a result we find that vesicles in the 5 - 15 μm size range reach a higher terminal velocity in hypotonic compared to hypertonic conditions. This difference decreases for larger diameters. Confocal fluorescence microscopy is used to measure the shape of the vesicles for different osmotic conditions in order to relate the deformability of the vesicle to the terminal velocities. Additionally, we obtain preliminary measurements on the thickness of the water layer that separates the vesicles from the glass surface, which determines the lubricating drag force. For GUVs that remain mobile this distance ranges between 0.5-3 μm. Variations in the drag conditions are studied using finite element simulations through a 3-D boundary integral method which models the approach of the vesicle to the glass surface. Through this method we study the vesicle deformability, and the limiting value of the water thickness. We relate these results to the movement of the vesicles due to an applied constant force. The theoretical and experimental results are compared using the dimensionless Bond and capillary numbers.

2369-Pos Board B339

Interaction of Buffers with Lipid Membranes

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Common buffers including Tris, MES, and MOPS are used to control the pH values of aqueous solutions. The pH, in turn, determines the charged (protonation) state of macromolecules such as proteins, lipids, and DNA. We have investigated the effect of common buffers on the charged state on lipid aggregates. Immersed in water, common lipids often form multilamellar structures. The extremely uniform interlamellar spacings (measurable by X-ray scattering) depend critically on the chemical nature (composition) of the solvent, including the presence of buffers. Multilamellar structures shrink or expand (swell) depending on how interlamellar forces are modified. We present measurements on the modification of lipid interactions by buffers and discuss specific buffer effects that go beyond the non-specific effect of pH.

2370-Pos Board B340

Lipid Gymnastics: Complete Acyl Chain Reversal in Oxidized Phospholipids: Evidence from Molecular Simulations

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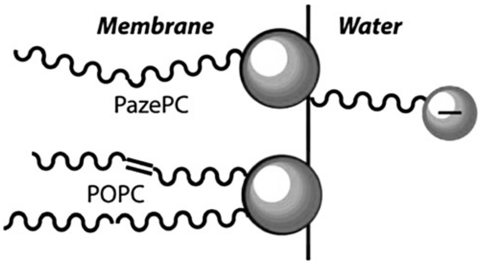
Biological membranes in oxidative environments can contain oxidized phospholipids (OXPLs) with short, polar acyl chains. Two lipid oxidation products of POPC are PoxnoPC and PazePC, which have a carbonyl and an anionic carboxyl group pendant at the end of the short oxidized acyl chain respectively. We have used Molecular Dynamics simulations to investigate the possibility of chain reversal in OXPLs in POPC-OXPL mixtures. The polar azelaoyl chain of PazePC undergoes complete chain reversal without compromising the lipid bilayer integrity at concentrations up to 25% OXPL. The carboxyl group points into the aqueous phase. The carbonyl-containing chain of PoxnoPC is oriented perpendicular to the bilayer normal; and perturbed the lipid packing arrangement more strongly. This work provides molecular evidence of the ‘‘extended lipid conformation’’ in phospholipid membranes. OXPLs are implicated in diseases including cancer and heart disease. The simulations present a clear structural model, using which it will be possible to investigate the interactions of OXPLs with various membrane hosts, ranging from single ions to large proteins. This will ultimately lead to a better understanding of how OXPLs participate in the genesis of diseased states.



2371-Pos Board B341

Headgroup Conformations of Phospholipids from Molecular Dynamics Simulation: Sampling Challenges and Comparison to Experiment

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