X-ray scattering is a promising tool with which to characterize systems of solid-supported membranes. There are many different scattering techniques used in the characterization, but all suffer from a necessarily low electron density contrast between the membrane and the water medium in which it must exist. Labeling membranes with a high-contrast scatterer such as gold is a promising avenue to solve this problem. In this work, silicon-supported membranes of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) were prepared by both standard Langmuir-Blodgett deposition and fusion of vesicles onto the substrate surface. Membranes are characterized using specular x-ray reflectometry, and modeled to fit physical systems. One percent by count 1,2-dipalmitoyl-sn-glycero-phosphoethanolamine (DPPE) with a gold tag attached was then added to both systems. Gold labeled membranes were then characterized and modeled. The effect of gold labeling is shown to characteristically change the membrane density profile in addition to enhancing density contrast between the membrane and the water medium.

1475-Pos

Analysis of the Structure and Interaction in Two-Dimensional Assemblies of Tobacco Mosaic Viruses on Model Lipid Membranes

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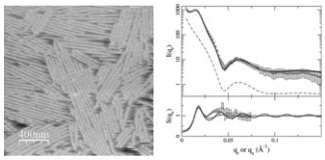
We created two-dimensional (2D) assemblies of tobacco mosaic viruses (TMVs) and characterized their structures using Atomic Force Microscopy (AFM) and X-ray scattering. The TMVs were adsorbed on an oppositely charged, fluid lipid monolayer supported by a solid substrate and submerged in a buffer solution. The lipid monolayer confined the viral particles within a plane, while providing them with lateral mobility so that overall the TMV assembly behaved like a 2D liquid. The inter-particle interaction is controlled by the chemical condition in the buffer. The degree of structural orders observed varied, depending on both the inter-particle interaction and the lateral mobility of the particles. Quantitative analysis of the X-ray scattering data provides information on the nature of the interaction between TMVs as well as possible membrane deformation due to the contact with TMVs. This study provides the proof-of-concept that X-ray scattering may be used to study the structure of membrane associated proteins in substrate-supported single bilayer under near-native conditions.



1476-Pos

Structure and Water Permeability of Fully Hydrated Diphytanoylpc

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Diphytanoylphosphatidylcholine (DPhPC) is a branched chain lipid often used for model membrane studies, including peptide/lipid interactions, model ion channels and lipid raft studies. This work reports results of volume measurements, water permeability measurements P_f, X-ray scattering from oriented samples, and x-ray and neutron scattering from unilamellar vesicles at T=30 °C. The volume/lipid was $V_L = 1427 \pm 1$ Å^3. The area/lipid was found to be 83 ± 1 Å^2 when only x-ray data were used in the H2 model analysis (Klauda et al., Biophys. J. 2006) and $A = 80.3 \pm 1$ Å^2 when both x-ray and neutron data were combined with the SDP model analysis (Kucerka et al., Biophys. J. 2008). P_f was measured to be $7.04 \pm 0.97 \times 10^{-3}$ cm/sec, which is considerably smaller than predicted by the recently proposed 3-slab model (Nagle et al., J. Gen. Physiol. 2008). This suggests that water flow through the branched chain region becomes the rate limiting step instead of the entry of water through the interfacial region when the chains are not branched. The DPhPC head-head thickness (D_{HH}= 36.1 Å), the bending modulus (K_C=$6.4 \pm 1.5 \times 10^{-21}$J) and the Hamaker parameter (H=4.5×10^{-21}J) were similar to the linear chain lipid DOPC. Even though DPhPC does not occur in mammalian cell membranes, these similarities are consistent with DPhPC bilayers being an appropriate model for many cell membrane studies. This work was supported by grants from National Institutes of Health (GM44976, JFN,STN,) and (DK43944,JCM,MZ).

1477-Pos

Osmotic Membrane Deformation Revealed by Solid-State ^{2}H NMR and Small-Angle X-Ray Scattering

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Phospholipid membranes are implicated in cellular homeostasis together with a multitude of key biological functions. Many regulatory functions are known to be mediated through protein-lipid interactions. An important feature of pressure-sensitive membrane proteins (mechanosensitive channels, rhodopsin) is that their activation is coupled to membrane tension and curvature elastic stress [1,2]. Solid-state ^{2}H NMR and small-angle X-ray scattering (SAXS) studies of bilayer ensembles of phospholipids under osmotic stress enable membrane structural deformation to be determined. Here we highlight the results from a combined NMR and SAXS approach utilizing pressure-based force techniques that control membrane structure [3] and tension [1].Our ^{2}H NMR results using both osmotic pressure (PEG osmolyte) and gravimetric pressure (low water concentration) techniques show that the segmental order parameters (S_{CD}) of liquid-crystalline DMPC approach very large values $\approx$0.35 at $\approx$30 °C. These correspond to $\approx$20% change in bilayer structural properties (cross-sectional area per lipid and acyl chain thickness) versusthefully hydrated membrane. The two stresses are thermodynamically equivalent because the change in chemical potential when transferring water from the interlamellar space to the bulk water phase corresponds to the induced pressure. A simple theoretical framework based on a unified thermodynamic description is developed. It is shown that the gating threshold for mechanosensitive channels may be shifted to higher or lower values due to lipid-mediated control of channel properties. These findings demonstrate the applicability of solid-state ^{2}H NMR spectroscopy and SAXS together with membrane stress techniques for investigating the mechanism of pressure sensitivity of membrane proteins. [1] S.I. Sukharev *et al*. (2001) *Biophys. J.***81**, 917-936. [2] A.V. Botelho *et al*. (2006) *Biophys. J.***91**, 4464-4477. [3] H.I. Petrache, M.F. Brown. (2007) *Methods in Membrane Lipids*, Humana Press, 339-351.

1478-Pos

A Modified Lipid Force Field for Charmm: Development and Application to Single-Celled Organism Membranes

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Biological membranes form a barrier to protect the cell from its environment and selectively control the entrance/exit of small molecules. Molecular simulations of these biological membranes require an accurate lipid force field (a major component of the membrane). Previously, extensive *ab initio* quantum mechanical (QM) calculations have been used to improve the aliphatic portion of the CHARMM27 lipid force field. Although this was a significant improvement, the lipid head group required additional modifications to agree with experimental lipid bilayer deuterium order parameters (S_{CD}) and solvation free energies. Therefore, we modified the atomic charges in the carbonyl-glycerol region and fit dihedral energy terms to high-level QM calculations and/or experiment. Molecular dynamics (MD) simulations with this new force field, referred to as CHARMM36 (C36), resulted in a significant improvement to the S_{CD}'s and water hydration for DPPC lipid bilayers. The calculated electrostatic profile and lipid bilayer surface tension decreased significantly. Consequently, the C36 force field resulted in excellent surface areas per lipid (and other properties) with NPT simulations, which is a significant improvement from the C27r force field that required constant area simulations (NPAT) to prevent some bilayers from laterally condensing. MD simulations of other pure lipid bilayers and monolayers also agreed favorably with experimental densities, monolayer surface tensions, and S_{CD}'s. The success of the C36 force field allowed for the study of complex lipid membranes in single-celled organisms. Model membranes were developed and simulated for yeast (six phospholipids, cholesterol, and 25-hydroxysterol) and Chlamydia (five unbranched lipids, a branced lipid, and cholesterol). These membranes are currently being used to study intracellular sterol transport and a porin protein that induces an immune response.

1479-Pos

Calculation of Partition Coefficients of Chain Anchors in Liquid-Ordered and Liquid-Disordered Phases in Model Lipid Bilayers

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We calculate partition coefficients of various chain anchors in liquid-ordered and liquid-disordered phases utilizing a theoretical model of a bilayer membrane containing cholesterol, dipalmitoylphophatidylcholine (DPPC), and dioleoylphosphatidylcholine (DOPC). The model qualitatively reproduces experimentally observed phase diagrams of this ternary system [R. Elliott,