# Membrane Structure II

**2562-Pos Board B332**
**Structural Properties of Water at Interfaces**
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The properties of water molecules at the interface of lipid bilayers are different compared to the properties of bulk water. For example, in bulk water each molecule is hydrogen bonded with four neighboring water molecules on average, whereas this number is changed at the interface. The structure of water next to lipids was studied previously using IR spectroscopy. It was proposed that a mixture model of water (in which lower density domains of water molecules form an ordered hydrogen bonding network and higher density domains of water form a less ordered network) can explain the observed behavior of the IR spectrum. Since water hydrogen-bonded network can be described by tetrahedral geometry, it can be measured by its tetrahedricity. To study the tetrahedricity of water, we outline the procedure for calculating a code in C programming language. We plan to study the tetrahedricity of bulk water and at the interface of a model graphene/water surface to understand the influence of interface on the water hydrogen bonding network.

**2563-Pos Board B333**
**Lateral Pressure Profile in a Lipid Membrane with Curvature: Analytical Expression**
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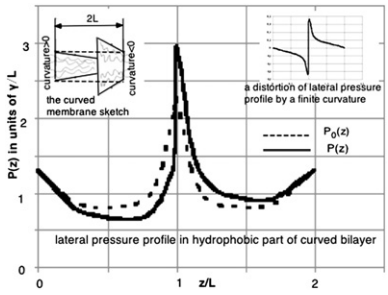
Analytic expression for the lateral pressure distribution in a curved lipid bilayer is derived: $P(z)=P_0(z)+ (a(z)-a_0)dP(z)/da_0$ , as function of the depth $z$ across bilayer, using the flexible strings model of lipid chains developed earlier [1]. $P_0(z)$ is flat bilayer lateral pressure profile [1], $a(z)$ and $a_0$ is area/per lipid in the curved and flat bilayer respectively. In the figure the plots confine to the hydrophobic part of each monolayer. Solid line is lateral pressure profile in a spherical vesicle of thickness 15 Å and curvature radius 1000 Å. Dashed line is the pressure profile in a flat bilayer of the same thickness. $Z=0,2L$ mark the neutral surfaces between headgroups and tails (see left sketch), where flat membrane's area per lipid is conserved. Right insert shows a symmetry breaking distortion of the pressure profile caused by curvature. Hence, distinctly from the flat bilayer, the lateral pressure profile in vesicle is asymmetric with respect to the monolayers interface, as was found in [2] using molecular dynamics.




**References:**
[1] S.I. Mukhin and S.V. Baoukina, Phys. Rev. **E71**, 061918 (2005).
[2] O.H. Samuli Ollila et al., Phys. Rev. Lett. **102**, 078101 (2009).

**2564-Pos Board B334**
**Role of Membrane Tension on Physical Properties of DOPC Lipid Bilayer**
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Mechanical stimuli trigger a wide range of cellular and biochemical processes in the cell. However the underlying molecular mechanisms of this triggering process are not well established. Numerous studies have demonstrated that in many cases mechanochemical signal conversion originates at the cell membrane. In the present study, a series of systematic molecular dynamics simulations were performed to characterize the changes in dioleoylphosphatidylcholine (DOPC) lipid bilayer properties in response to the membrane tension. All simulations were carried out using NAMD program and CHARMM36 force field. Our studies show that membrane tension causes changes in membrane properties such as area per lipid, volume, membrane thickness, lateral diffusion and dipole potential. The results also indicate that the lateral diffusion of lipid molecules is anomalous in nature due to the non-exponential distribution of waiting times. The simulation results were compared with experimental data obtained from fluorescence spectroscopy experiments using fluorescent lipid tracers and dipole-potential sensitive fluorescent probes.

**2565-Pos Board B335**
**Simulations of PEGylated and Tethered Lipid Bilayers**
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Lipid bilayer structures with PEGylated headgroups are highly important for drug delivery and nanotechnology. Here, we study mixtures of DOPC (1,2-Dioleoyl-sn-glycero-3-phosphocholine) bilayers and PEGylated DOPCs at various concentration ratios fully hydrated using the MARTINI coarse-grained force field. We show that external conditions like applying a surface tension allows us to switch from a micellar configuration to a bilayer. We characterize the structures using various radial distribution functions as well as the radius of gyration of PEGylated DOPC. Our results show that under suitable condition, lipid bilayer structure can be transformed and manipulated. We also address systems where the ends of the PEGs are grafted to a surface to form a tethered bilayer. Different grafting densities and tether lengths are studied. Preliminary comparisons to experimental data show that we can obtain realistic structures.

**2566-Pos Board B336**
**Structural Correlations and Thermodynamics of the Gel Phase in Lipid Bilayers**
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We simulate biological membranes using the course grained MARTINI approach. Two dimensional distribution functions show that the gel phase is a well ordered hexagonal lattice. The transition from fluid to gel undergoes an intermediary phase with significant radial and angular correlations. Long range structural correlation along the lattice vectors show that the peak decay of this long lived pre-gel phase is exponential. We also show that the radial distributions of both gel and intermediary phase have sixfold anisotropy and that the angular correlations of the lattice in the gel phase quickly goes to a constant, concurrent with the results for a thermally perturbed hexagonal lattice. The pre-gel phase exhibit angular correlations that decay slowly to a constant. Furthermore we calculate the heat capacity and heat of formation of these two transitions via a slow simulated annealing scheme. We find sharp transitions between these phases and heats of formation close to differential scanning calorimetry data for the main- and pre-transition.

**2567-Pos Board B337**
**Comparison of Orientational Texture in Lipid Bilayers and Langmuir Monolayers**
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In solid ordered domains of lipid bilayers the lipids may have an in-plane orientational order associated with the tilted acyl chains. The variation of this orientation across the sample is denoted the texture. Although biological membrane normally only exist in the fluid phase, the gel phase is present, for instance in skin tissue and during apoptosis.
The texture of monolayers has been investigated previously through the use of mainly Brewster Angle Microscopy (BAM) and AFM. For bilayers we have found that polarized two-photon fluorescence microscopy combined with image analysis is able to provide the orientational texture with single pixel resolution [1]. We have used this method to image the texture of solid ordered domains in lipid bilayers.
In bilayers we typically observe texture patterns with splitting of the domain into 6 subdomains having different orientations. In contrast to monolayers we find a significant variation in the defect structure when going from the center of the domain to the edges. In an attempt to understand texture formation we have systematically compared results from bilayers with the texture of an equivalent monolayer system prepared at different temperatures.
[1] JACS 131(40): p. 14130-14131 (2009)

**2568-Pos Board B338**
**Wide-Field Time Resolved Anisotropy for In-Situ Lipid Phase Dynamics**
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We have developed a new time-resolved fluorescence platform which enables us to follow the molecular orientation and dynamics of a lipid monolayer at the air - water interface. Confocal microscopy is limited in its ability to characterize dynamic orientation changes within cellular membranes. By implementing an all reflective Cassegrain objective we minimize dispersion while eliminating the restriction of collinear excitation. This enables us to unambiguously identify fluorescence probe orientation and dynamic freedom within our membrane model, with the highest available temporal resolution, and without the