preventive vaccine development. Structural, biochemical and biophysical determinations suggest that the membrane-proximal external region (MPER) of glycoprotein 41 may interact with the HIV-1 membrane interface, and induce its destabilization to ensue viral fusion. However, the cholesterol content of the viral membrane (ca. 45 mol %) acts against MPER binding and restructuring activity. Here, using vesicle stability assays, molecular dynamics simulations, atomic force microscopy and NMR structure resolution, we have found that gp41's capacity for destabilizing and provoke merging of the highly rigid viral envelope, actually resides within a sequence connecting the carboxy-terminal MPER section with the N-terminal residues of the transmembrane domain. To determine the potential relevance of this connection as a target for anti-HIV-1 immunogen development, we have sought to generate antibodies against this region by immunizing rabbits with liposome-peptide formulations.

Membrane Structure III

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Critical Stretching and Pores in Bolalipid Membrane from Flexible String Model
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Phase diagram of a bolalipid membrane for critical stretching and pore formation is derived analytically using microscopic flexible strings model [1,2] of monopolar lipid and bolalipid [3] membranes. We use free energy density functional E of the laterally stretched membrane with pore radius R: E = E_0 + ($\pi\perp$2R$\perp$4/2N)$\partial\perp$2Ft(a)/∂a$\perp$2 + P$\pi\perp$2R$\perp$4/Na − PπR$\perp$2+2$\Gamma\pi$R under the applied stretching pressure P and area per lipid a of the self-assembled membrane of N lipids before stretching, and pore linear tension Γ. The hydrophobic part of the lipid chain's free energy Ft was calculated previously for monopolar [1] and bolalipid [2] membranes using self-consistent microscopic model with entropic repulsion between flexible lipid chains. Finding a from the free energy minimum condition: ∂Ft/∂a+γa=0 , with surface tension γ at the hydrophobic-hydrophilic interface, and substituting it into ∂2Ft(a)/∂a2 we find analytic expression for the coefficient in front of R$\perp$4 in the elastic energy. Using E we derive phase diagrams for bolalipid and monopolar lipid membranes and compare their stability, i.e. critical pressures Pc of pore formation. An enhancement of Pc of the bolalipid membrane relative to monopolar lipid bilayer is a consequence of relative suppression of the midmembrane entropy of the membranespanning bolalipid chains with respect to the lipid tails entropy in bilayer midplane region [2]. Consequences of this effect for stability against pores formation of the bolalipid membrane of the archaea cell is investigated.
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Lipid Membranes as Non-Linear Capacitors
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It is commonly assumed that the lipid membrane is an inert capacitor and that macromolecules, like proteins, govern the sophisticated electrical properties of biological membranes. Various authors have shown that the capacitance of pure lipid membranes is a function of voltage due to electrostriction but also piezoelectric properties have been seen biological membranes. Lipid membranes are therefor non-linear capacitors, which can in their own right give rise to currents against the applied electrical field, inductive behavior and electro-mechanical sensitivity. Those features could be essential in the membrane protein coupling and can change the understanding of the electrical properties of biological membranes.

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Monolayer-Bilayer Transformations with Phase Coexistence
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Lateral compression of a lipid monolayer at an air/water interface increases its surface density and reduces surface tension. Reduction of surface tension is possible until a certain threshold, below which the monolayer becomes unstable at the interface and collapses. For homogeneous monolayers, collapse is known to proceed via wrinkling/buckling, followed by folding into bilayers in water. For heterogeneous monolayers with coexisting phases, the mechanism of collapse is not fully understood. The effect of phase separation on monolayer stability and the distribution of phases between the monolayer and bilayers as folds form and grow remain unclear.
We used molecular dynamics simulations to investigate collapse of lipid monolayers with coexisting phases. The coarse-grained force field Martini was employed to achieve large length and time scales. We reproduced liquid-liquid and liquid-solid phase coexistence in monolayers of saturated and unsaturated lipids and cholesterol, and simulated monolayer collapse. The presence of solid domains allowed sustaining lower surface tensions, while the liquid-ordered domains decreased monolayer stability due to spontaneous curvature. Folds formed in the disordered phase in both cases; curved domains shifted nucleation sites towards the phase boundary. The disordered phase was preferentially squeezed-out into bilayers, in agreement with experiments. As a result, the composition and phase fractions were altered in monolayers in equilibrium with bilayers compared to flat monolayers at the same surface tension. Phase behavior of bilayers in turn depended on degree of monolayer compression. The monolayer-bilayer connection was highly enriched in unsaturated lipids. Percolation of solid domains slowed monolayer collapse below the equilibrium tension. The study is important in general for understanding the mechanism of folding of heterogeneous thin films and the role of lateral organizations in biological membranes, and is directly relevant for the function of lung surfactant.

3597-Pos Board B325
Buckling Gel-Phase Membranes is a Way to Measure their Mean Bending Regidity
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The elasticity of lipid membranes can be characterized by two curvature moduli: the mean bending modulus and the Gaussian curvature modulus. Due to the relevance of the mean bending modulus for countless biological processes, considerable effort has been devoted to determine it_both in experiment and in computational studies. The most common computational approach is to measure the power spectrum of shape undulation modes [1]. Unfortunately, this technique is challenging for gel-phase membranes, because their larger modulus renders their fluctuations correspondingly smaller. In contrast, methods that infer a membrane's rigidity from actively bending it yield a signal that becomes stronger as the membrane becomes stiffer. One recently proposed method derives the modulus from the stress-strain relation of a buckled membrane, and it has been shown to provide accurate results for fluid membranes [2,3]. Using a coarse-grained lipid model, we show that this buckling method can also calculate the mean bending modulus of a gel phase membrane. We discuss the efficient implementation of the technique, paying special attention to difficulties that can arise while simulating a membrane in the gel phase. The method also provides insights into the contribution of entropy to the bending modulus, and hence its the temperature dependence.
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Characterisation of Coexisting Liquid Phases in Mixtures of Dipalmitoylphosphatidylcholine and Cholesterol
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Since their introduction, lipid rafts have been considered to be vital for various processes, such as membrane trafficking and signal transduction. While there is growing evidence for their existence and importance, the understanding of their emergence and physical properties is still limited.
Perhaps surprisingly, the understanding of similar issues is limited also in much simpler model systems. One of the most thoroughly studied cases is the binary mixture of dipalmitoylphosphatidylcholine (DPPC) and cholesterol, which despite its simplicity shows a spectrum of phases and their coexistence regions. Even though its phase behaviour is well established, the structural and dynamic details of the nanoscale domains in the coexistence region remain largely unknown.
To shed light on these features, we used atomistic molecular dynamics simulations to consider the phase behaviour of the DPPC-cholesterol system, with a focus on domain properties. Extensive simulations performed at varying temperatures and cholesterol concentrations highlighted that the experimental