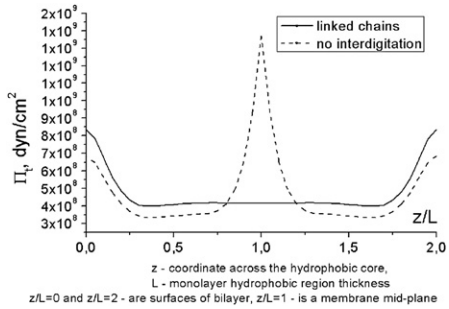
interdigitation free energy increase ΔF_{int} and energy of the hydrophobic mismatch in case of a liquid-condensed domain embedded in the liquid-expanded surrounding during e.g. the liquid-gel phase transition.



3129-Pos Board B176

Multiscale Modeling of supported bilayers

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Supported Lipid Bilayers are an abundant research platform for understanding the behavior of real cell membranes as they allow for additional mechanical stability. However, in computer simulations these systems have been studied only rarely up to now. Recently, we studied systematically the changes that a support induces on a phospholipid bilayer using coarse-grained molecular modeling on different levels.

We characterize the density and pressure profiles as well as the density imbalance inflicted on the membrane by the support. We also determine the diffusion coefficients and characterize the influence of different corrugations of the support. We then determine the free energy of transfer of phospholipids between the proximal (close to the surface) and distal leaflet of a supported membrane using the coarse-grained Martini model. It turns out that there is at equilibrium about a 2-3% higher density in the proximal leaflet.

These results are in favorable agreement with recent data obtained by very large scale modeling using a water free model where flip-flop can be observed directly. We compare results of the free energy of transfer obtained by pulling the lipid across the membrane in different ways. There are small quantitative differences but the overall picture is consistent. We are additionally characterizing the intermediate states which determine the barrier height and therefore the rate of translocation. Simulations in atomistic detail are performed for selected systems in order to confirm the findings. Calculations on unsupported bilayers are used to validate the approach and to determine the barrier to flip-flop in a free membrane.

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Optical Birefringence of Multi-Lamellar Vesicles with Anisotropic Internal Structure

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Multi-lamellar vesicles (MLV) which are shrunk under the osmotic condition can form a small nano-layered structure. When the internal structure of the shrunken MLV(SMLV) is geometrically anisotropic, it has an optically birefringence property; known as form birefringence. When the SMLV is trapped by the optical tweezers with a polarized laser beam, it can rotate due to the optical birefringence. We characterize the geometrical anisotropy of this internal structure using the relation between the rotational motion and the optical birefringence. We also present a simple model to describe the anisotropic internal structure of SMLV, where the layered structure is parameterized with the thickness of each lipid bi-layer and the internal distance between the next bi-layers.

3131-Pos Board B178

Nonlinear Deformations of Bilayer Lipid Membranes

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Novel continuum models that describe the equilibrium configurations of planar lipid bilayers will be presented. The models are derived within the nonlinear theory for smectic A liquid crystals proposed by Stewart (IW Stewart 2007 Contin. Mech. Thermodyn. 18:343) in which the usual director and unit layer normal do not always necessarily coincide. The total energy of lipid bilayers consists of an elastic splay term, smectic layer bending and compression terms, a coupling term between the director and layer normal, a surface tension term, and a surface anchoring term. Nonlinear equilibrium equations are obtained by using variational methods and are then solved by analytical and numerical methods. The solutions illustrate the nonlinear deformations of lipid bilayers including the misalignment of lipid molecules at their interface with other media such as, for example, proteins and surface substrates.

3132-Pos Board B179

Orientational Order and Raft Interactions in Lipid Bilayers

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Model and reconstituted membranes undergo a mixing-demixing phase transition, and, at low temperatures, the membrane is often a two-dimensional emulsion of liquid ordered and liquid disordered phases. This phase separation may be important for many functions of cellular membranes, including vesicle trafficking and signaling, and it has been implicated in a number of human diseases. We describe here the effects of orientational order (tilt, nematic, or hexatic) in one of the low-temperature phases on the behavior of the two-dimensional emulsion. We found that the orientational order in the continuous component of the emulsion can lead to the formation of companion singularities in the order parameter around the inclusions of isotropic liquid disordered phase. The orientational order parameter and strong anchoring boundary conditions also give rise to long-range interactions between the inclusions. The interaction is attractive at large separations and is repulsive at short separations. This interaction stabilizes the emulsion and leads to the formation of inclusion dimers. The sizes of the dimers depend only on the type of the orientational order and the sizes of the inclusions; hence, our calculation of this size can be used to test for the presence of a hidden order parameter in liquid ordered phases. The behavior in the presence of strong thermal fluctuations will be discussed as well.

3133-Pos Board B180

Line Tension Of Membrane Domains Calculated From Chemical Interactions Betweem Lipids And Elastic Splay And Tilt

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Model is developed to calculate the line tension of a domain in bilayer lipid membrane from both the chemical interactions between lipid molecules and the elastic deformations of the membrane. Two-component lipid bilayer is used to display the essential physics that determines line tension, without being obscured by complexities of the multi-component bilayer. Means to expand the approach to multi-component system has been formulated. The domain is assumed to be in thermodynamic equilibrium with the surround. Chemical interactions are incorporated by using regular solution theory, mean field approximation. Whenever a height mismatch exists at the boundary between the domain and the surround, the membrane deforms so as to prevent exposure of hydrophobic surfaces to water. The deformation energy is calculated by assuming that deformations occur through splay and tilt. The calculated line tension can be written as a sum of ''mechanical'' and ''chemical'' terms; each term is implicitly dependent on the other. For height mismatch of only a few Angstroms, line tension is accurately determined from the chemical interactions between lipids alone. For greater height mismatch, both chemical interactions and elastic deformations contribute. The calculated line tension is a function of temperature. Differences in spontaneous curvatures of the membrane lipid components lowers the effective critical temperature for domain formation. Below the critical temperature, the characteristic thickness of the transitional zone between the phases is several nanometers; it rapidly increases as the critical point is approached. If line tension and compositions of domains and surround are known for one temperature, they can be calculated over the entire temperature range. The model therefore allows values of line tension and domain composition that is experimentally measured at one temperature to be theoretically extended to a large range.

3134-Pos Board B181

Lamellar-Hexagonal Phase Transition Kinetics Depend Strongly on Degree of Saturation

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Phase transition temperatures of lipid-water systems have long been known to exhibit a strong dependence on the rate of heating or cooling. The difference between the phase transition temperatures seen on heating and cooling is

known as the hysteresis. Using an optical technique, we have examined the hysteresis for two lipids, SOPE (1-Stearoyl-2-Oleoyl-sn-Glycero-3-Phosphoethanolamine) and DSPE (1,2-Distearoyl-sn-Glycero-3-Phosphoethanolamine. SOPE contains a saturated tail and an unsaturated tail, while in DSPE both tails are saturated. We find that the hysteresis exhibits a power law dependence on the temperature ramping rate and that the hysteresis is markedly reduced for the completely saturated lipid DSPE as compared to the mono-unsaturated lipid SOPE. In turn, the hysteresis of SOPE is markedly reduced compared to that of DOPE, a lipid with two mono-unsaturated tails.

3135-Pos Board B182

Preferential Interaction of α-tocopherol with PUFA-containing Lipids Characterized by Isothermal Titration Calorimetry

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It is becoming generally accepted that membranes laterally segregate into patches (domains) of different lipid composition to provide the environment necessary for the function of a resident protein. Liquid ordered (l_o) lipid rafts enriched in saturated sphingolipids and cholesterol are the best known example. Much less studied are liquid disordered (l_d) domains rich in polyunsaturated phospholipids and depleted in cholesterol, the antithesis of rafts. They are the focus of our research. We hypothesize that α-tocopherol (vitamin E), a lipid-soluble antioxidant found in low concentration in plasma membranes, has preferential affinity for polyunsaturated fatty acid (PUFA)-containing phospholipids in these l_d non-raft regions. In this manner protection of the lipid species most vulnerable to peroxidation due to their multiple double carbon bonds, would be optimized. To test this hypothesis we utilize isothermal titration calorimetry (ITC) to assay the partitioning of α-tocopherol between large unilamellar vesicles (LUV) and methyl-β-cyclodextrin (cyd), a water-soluble molecule with a hydrophobic cavity that binds small hydrophobic molecules. The approach emulates one that has successfully been applied to measure the binding of cholesterol and the results of preliminary experiments have shown that α-tocopherol can be bound by cyd. Partition coefficients K_X measured for α-tocopherol as a function of phospholipid unsaturation are presented and compared with values measured for cholesterol that, in contrast to our proposal for α-tocopherol, has poor affinity for PUFA.

3136-Pos Board B183

The Effect of *Trans* Unsaturation on Molecular Organization in a Phospholipid Membrane

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Despite recognition that the ingestion of *trans* fatty acids (TFA) formed during the partial hydrogenation of vegetable oils may unfavorably affect biochemical function, the impact on the conformation of the molecules into which they incorporate is unknown. We synthesized analogs of 1-elaidoyl-2-stearoylphosphatidylcholine (*t*18:1-18:0PC) and 1-oleoyl-2-stearoylphosphatidylcholine (*c*18:1-18:0PC) with a perdeuterated 18:0 *sn*-2 chain and employed solid state ^{2}H NMR, complemented by computer simulations, to compare molecular organization in a model membrane containing a single ''manmade'' *trans* or ''natural'' *cis* double bond. Moment analysis of the ^{2}H NMR spectra recorded as a function of temperature showed that the chain melting temperature for the *trans* isomer (31.5 °C) is depressed compared to the *cis* isomer (7 °C), reflecting an ability to pack more favorably in the gel state, an interpretation supported by molecular modeling. The calculated intra-molecular van der Waals' attraction between acyl chains is greater for *t*18:1 than *c*18:1 acid because the *trans* chain adopts a $t^-s^-\Delta s^-t^-$ conformation, as opposed to $t^-s^-\Delta s^-g^-$ in a *cis* chain, around the double bond. The average order parameters evaluated for the perdeuterated *sn*-2 chain of *t*18:1-18:0PC and *c*18:1-18:0PC in the liquid crystalline phase coincide within <5%, a result that was reproduced in molecular dynamics (MD) simulations. The values for the average order parameter are 20% below the equivalent saturated PC (18:0-18:0 PC), which is attributed to the increased disorder in the hydrophobic core arising from differences in chain packing. We now have synthesized analogs with a perdeuterated *t*18:1 and *c*18:1 *sn*-1 chain to directly probe the conformational organization of *trans* vs. *cis* chain. (Supported by ACS, PRF 43281-AC7.)

3137-Pos Board B184

Scaffolded Vesicles as a Model Membrane System

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Biological cell membranes are complex systems that consist primarily of a phospholipid bilayer, into which cholesterol, proteins etc. may be integrated. Due to the complexity of biological cell membranes, it is desirable to develop model membrane systems that can be more easily studied. Scaffolded vesicles are an example of such a system. A scaffolded vesicle model membrane system offers a number of advantages with respect to other model systems. By using a porous material as the scaffold, one can achieve an aqueous environment on both sides of the model membrane. This allows for the study of membrane transport processes. The scaffolds porosity may also allow one to more easily integrate transmembrane proteins into the bilayer. Importantly, such a system would remain accessible to both electrochemical and surface analytical techniques. Using FTIR-ATR spectroscopy, the orientation of 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) coated on the porous scaffold (as a 70:30 DMPC:cholesterol bilayer) will be determined. Proteins may then be incorporated into the bilayer of the scaffolded model membrane system for study.

3138-Pos Board B185

Mechanical Effects of Peripherally Binding Proteins on Membrane Tethers

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Our understanding of cell membrane remodeling by proteins has been informed largely by observations of membrane tubulation by proteins in vitro and in vivo. Structural and spectroscopic studies have revealed some important details of the interactions between these proteins and lipids. However, a quantitative description of membrane curvature sensing and generation by proteins, which would guide assessment of the roles of specific proteins and evaluation of hypothesized mechanisms of action, is currently lacking.

We are studying membrane curvature sensing and generation by purified proteins using a fluorescence microscopy-based biomimetic curvature gradient manipulation system, the properties of which are described by membrane elasticity theory. Using tethers of controllable curvature pulled from giant vesicles, we monitor protein partitioning between vesicle and tether, and the effects of proteins on tether properties. These measurements direct our assessment and development of statistical mechanical models that clarify the parameters responsible for protein sensing and control of membrane curvature. Our quantitative framework is used with varying membrane composition and solution conditions to reveal subtle differences between various proteins in their membrane restructuring and curvature propensities.

3139-Pos Board B186

Modeling Morphogenesis of Outer Segments of Vertebrate Photoreceptor Cells

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The vertebrate eye contains two main types of photoreceptor cells: rods and cones. The outer segment of the rod cells are cylindrical in shape and contain 500-1000 pancake-shaped structures stacked on top of each other, ensheathed within a plasma membrane. Each individual pancake can be thought of as an individual sac with an enclosing membrane, a structure known as a vesicle. The shape of these vesicles is very important since misshaping of the vesicles can lead to loss of eyesight. We will discuss how the quasi-equilibrium shapes of these vesicles could be determined by membrane energetics, and will introduce a Metropolis algorithm to obtain thermodynamically stable vesicle shapes.

Interfacial Protein-Lipid Interactions II

3140-Pos Board B187

Pulmonary Surfactant Protein C Reduces the Size of Liquid Ordered Domains in a Ternary Membrane Model System

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Surfactant protein C (SP-C) is the smallest pulmonary surfactant protein and is required for the formation and stability of surface-active films at the air-liquid interface in the lung. The protein consists of a hydrophobic transmembrane α-helix and a cationic N-terminal segment, which contains two palmitoylated cysteines. In the present work, we compared the effect of native palmitoylated and recombinant non-palmitoylated versions of full length SP-C on the liquid ordered (lo)/liquid disordered (ld) phase coexistence in a ternary membrane model system consisting of DPPC, DOPC and cholesterol. This model has