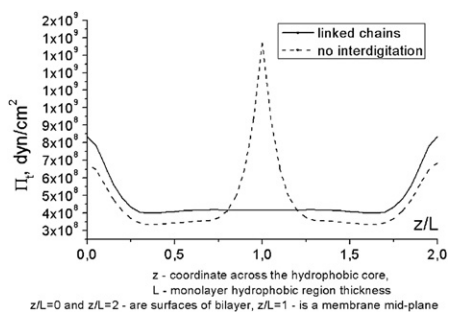


interdigitation free energy increase ΔF_{int} and energy of the hydrophobic mismatch in case of a liquid-condensed domain embedded in the liquid-expanded surrounding during e.g. the liquid-gel phase transition.



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.

3130-Pos Board B177

Optical Birefringence of Multi-Lamellar Vesicles with Anisotropic Internal Structure

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¹Department of Physics, Pusan National University, Busan, Republic of Korea, ²Materials Department, Univ. of California, Santa Barbara, CA, USA. 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

Oriental 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 Between 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