deformations in the metabolic pathways are conducted by the related proteins. However, we believe that such membrane deformations can be caused by controlling the physical properties of the membrane without the aid of proteins. In this context we demonstrate the deformations of vesicle by controlling the spontaneous curvature of lipids.
First, we focused on the lipids with negative spontaneous curvature (NL: DPPE and DPhPC). The binary vesicles composed of NL and lipids with zero spontaneous curvature (ZL: DOPC and DPPC) show a phase separation between NL rich domains and ZL rich matrix under the immiscibility temperature. When the two phase separating vesicles are contacted using micropipettes, they adhere each other through the domain rich in NL.
Second, we have investigated the effects of the lipids with positive spontaneous curvature (PL: DHPC) on the shape of vesicles. The binary vesicles composed of PL and ZL form spherical shape in one-phase region. By decreasing the temperature, the binary vesicles show a burst and then form a single pore on the vesicle. There are three types of pores, simple circular, rolled-rim and wrinkle-rim, depending on the ratio of PL to ZL. The pore closes with increase the temperature and finally vesicles return to the spherical shape again. We discuss this shape deformation of vesicles by calculating time development equation of the membrane free energy.
We believe that the control of the spontaneous curvature of lipids is a key to realize the model metabolic pathways without proteins.

3468-Pos
A Biomolecular Photodiode for Imaging of Cell Membrane Potential
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Despite the recognized importance of electrical signals in certain biological systems, there has been limited success in the creation of a reliable voltage sensor for imaging of such activity. Using standard molecular biology techniques, we have created a biomolecular photodiode consisting of a membrane-bound cytochrome c protein fused with a GFP (green fluorescent protein) variant. A similar photodiode assembly has been shown to produce unidirectional photocurrent in vitro with the cytochrome acting as an acceptor of excited state electrons from the FP donor upon excitation with visible light. Electron transfer between the cytochrome and the FP is a highly voltage dependent process. By embedding this assembly in the plasma membrane of living cells, it is subjected to the same electric potential as the membrane. As the membrane potential of the cell changes, as in an action potential, the extent of electron transfer is expected to vary significantly, resulting in a change in fluorescence intensity of the FP donor. As this is a very fast process with high sensitivity to changes in electric potential, the biophotodiode has potential to form a robust sensor of electrical activity in cells. The feasibility of the sensor is investigated in several ways, including modeling, electrophysiology, and direct application of current to purified membrane fragments.

3469-Pos
Sub-Diffusion and Super-Diffusion of Hydration Water Molecules at Biological Interfaces
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The structure and dynamics of hydration water at the surface of biomolecules (e.g., proteins and lipids in biological membranes) are fundamental for their stability and functioning. Due to the interactions at the surface of a solvated biological membrane, the dynamics of the hydration waters and that of the membrane molecules are to some degree correlated. In spite of previous efforts, little is known about the time and length scale of these correlations. Here, we report on a 0.1 microsecond all-atom molecular dynamics simulation study aimed at investigating the dynamics of the hydration water at the interface of a dimyristoylphosphatidylcholine (DMPC) lipid bilayer. We find that, mainly due to hydrogen bonding with the lipid bilayer, the mean-square displacement of the interfacial water has four well defined dynamical regimes, with characteristic power law (t^n) time (t) dependence: (1) ballistic, for $t < 10$ fs, with $n=2$; (2) sub-diffusive, for 0.2 ps $< t <$ 20 ps, with $n<1$; (3) super-diffusive, for 0.1 ns $< t <$ 1 ns, with $1<n<2$; and (4) Fickian diffusion, for $t >$ 10 ns, with $n=1$. The super-diffusive regime (characterized by a self intermediate scattering function with compressed exponential relaxation) of the hydration water molecules has not been observed before, and possibly determines the length and time scales of the correlation between the dynamics of water and lipid membrane. Furthermore, the water-lipid interactions give rise to an average liquid-like structure of the interfacial water molecules on a length scale corresponding to the average lipid-lipid separation, and the relaxation time of this structure is an order of magnitude larger than what is expected from the self motion of the water.
Computer time was generously provided by the University of Missouri Bioinformatics Consortium.

3470-Pos
Two-Dimensional Continuum Percolation Threshold as a Function of the Radius of the Diffusing Particles
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Lateral diffusion in the plasma membrane is obstructed by proteins bound to the cytoskeleton. The most important parameter describing diffusion in the presence of immobile obstacles is the percolation threshold, where long-range conducting paths disappear and the long-range diffusion coefficient therefore goes to zero. The thresholds are well-known for point diffusing particles on various lattices or the continuum. But for diffusing particles of nonzero radius, the threshold depends on the excluded area, not just the obstacle concentration. For the triangular lattice, the threshold is known to be highly sensitive to the size of the diffusing particle [Saxton, Biophys J 64 (1993) 1053], but lattice calculations give very low resolution. Here high-resolution results are obtained for circular obstacles on the continuum. Random obstacle configurations are generated by Brownian dynamics or Monte Carlo methods, and tested for percolation by examining bond percolation on the Voronoi diagram of the obstacles. The percolation threshold is expressed as the diameter of the largest diffusing particle that can cross a set of obstacles at a prescribed number density. For the simplest case, random overlapping obstacles, the analytical solution is known and the Monte Carlo results agree with it quantitatively. When the obstacles are disks with a $1/r^{12}$ repulsion, the percolating diameter is around 10% lower than for overlapping obstacles. Disks with a $1/r^{6}$ or $1/r^{18}$ repulsion behave similarly. The results are used to find the thresholds for lipids, and for proteins of various diameters. (Supported by NIH grant GM038133)

3471-Pos
Comparison of Lipid Monolayers and Bilayers by Comparative Molecular Dynamics Simulations of a Lipid-Like Dye Molecule
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Using p-polarized internal reflection fluorescence microscopy in monolayer membrane systems, Livanec and Dunn have demonstrated that the order of dipalmitoylphosphatidylcholine (DPPC) lipid molecules decrease as the surface pressure increases (Livanec and Dunn (2008) Langmuir 24 (24), 14066-14073). Although monolayer experiments provide more convenient control of membrane properties such as surface pressure, temperature, and lipid compositions, bilayers can offer a more dependable representation of a true biological membrane. This raises the question whether monolayer membranes can be used to study bilayer membranes. In order to explore the correspondence between monolayer and bilayer membranes, molecular dynamics (MD) simulations with lipid reporter dye molecule BODIPY-PC in a DPPC explicit membrane were performed. The correspondence was measured in different surface pressures: high pressure (40 mN/m), normal pressure (25 mN/m), and low pressure (3 mN/m). Each pressure system consisted of 5 bilayer and 5 monolayer systems, totaling up to 30 different simulations. Each simulation ran for 3 ns of equilibration and 47 ns production. Using trajectories, BODIPY-PC molecule's orientation was characterized in terms of tilt, azimuthal, and rotation angles. The calculations were compared between bilayer and monolayer systems to examine structural similarities. In addition, non-bonded energies (or the enthalpic contribution) of the BODIPY-PC molecule in different pressure systems were compared in order to address the driving force governing tilting of the dye molecule in different pressures. The calculated tilt, azimuthal, and rotation angles suggest that monolayer and bilayer systems yield quite similar results. The energy calculations demonstrate that entropy dominates the tilting of a dye molecule in low and normal pressure whereas enthalpy plays a higher role in tilting of a dye molecule in high pressure.

3472-Pos
Membrane Interactions in Ionic Solutions
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Because of complicated molecular dynamics, calculations of membrane interactions require more complicated models than straightforward electrostatics. The net intermembrane forces measured experimentally by x-ray scattering and osmostic stress must first be decomposed into various components including pure electrostatics, van der Waals, and a less understood hydration force. In addition, in most situations, an entropically generated force is required to account for the repulsive effect of membrane fluctuations (Helfrich force). Another challenge is to corroborate the experimental findings with already calculated results for particular setups. Situations in which ions are excluded from the vicinity of the membrane introduce new complications in the model. We theoretically explore to what extent we can explain these results by calculations of electrostatic interactions in ionic solutions using a Poisson-Boltzmann approach.