Intramolecular excimer formation of 1,3-di(1-pyrenyl)propane (Py-3-Py), and fluorescence polarization of 1,6-diphenyl1,3,5-hexatriene(DPH) were used to investigate the effect of chlorhexidine digulconate (CHX) on the bulk fluidity of outer membranes (OPG) isolated from cultured *Porphyromonas gingivalis* and multilamellar vesicles were prepared with total lipids (OPGTL) extracted from OPG and prepared with mixture (PL) of DPPE and DPPC. The fluorescence polarization of *n*-(9-anthroyloxy)stearic acid (*n*-AS) were used to examined the effect of CHX on the rotational mobility of the surface and interior region of membrane lipid bilayers. CHX decreased the mobility of the surface region of bilayers but the drug increased the mobility of the interior region of membrane lipid bilayers.

These indicate that CHX increased both the lateral and rotational mobilities of probes in OPG, OPGTL and PL bilayers. Selective quenching of Py-3-Py and DPH by TNBS was utilized to examine transbilayer fluidity asymmetry of OPG, OPGTL and PL lipid bilayers. CHX had a greater fluidizing effect on the inner monolayers as compared to the outer monolayer of OPG, OPGTL and PL lipid bilayers. The sensitivities to the increasing effect of fluidity differed according to these membrane lipid bilayers in the descending order of OPG, PL and OPGTL. CHX increased the rotational mobility of the hydrocarbon interior of OPG, OPGTL and PL but decreased the mobility of membrane interface of OPG, OPGTL and PL. The sensitivities to the increasing effects of CHX on the rotational mobility were in proportion to the located depths of the probes in descending order, as follows: 16-AP, 12-AS, 9-AS and 6-AS. The disordering or ordering effects of CHX on the membrane lipids might be responsible for some, but not all of its bateriostatic and bactericidal actions.

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Performance of C36 Lipid Force Field in Pure and Mixed Lipid Bilayer Systems at Different Temperatures

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A lipid membrane modifies its composition in response to environmental changes. Acyl chain length, ratio of saturation/unsaturation, and head group type affect how the composition of the lipid bilayer changes. The aim of this work is to examine the performance of the C36 lipid force field in pure and mixed lipid bilayer systems at different temperatures. We have performed molecular dynamics (MD) simulations of thirty-four lipid systems with ten different fatty acids and five different head groups. Nine additional systems have been simulated at slightly higher temperatures. To examine the changes of mixed lipid bilayer properties, we have simulated twenty lipid systems with pure POPC, pure DOPC, pure DPPC, mixtures of DOPC and DPPC, and mixtures of DOPC, DPPC, and POPC. These systems were simulated at four different temperatures: 283K, 293K, 303K, and 313K. The ratios of lipids in mixed bilayer systems differ according to their temperatures. We performed three independent runs for each system at each temperature to improve the conformational sampling and the statistics of the results. We will present per-lipid surface areas (SAs) and deuterium order parameters (S_{cd}) with different head groups, different acyl chain length, and different levels of chain unsaturation at a given temperature. We will also present the influence of temperature and extent of mixture on the SAs and S_{cd}.

439-Pos Board B225

Quantifying the Diffusion of Membrane Proteins and Peptides in Lipid Bilayers

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Membrane proteins play a key role in cellular processes, e.g. ion transport into and out of the cell as well as signal transduction between cells. Protein diffusion in lipid membranes is important in this regard, since the kinetics of most protein interactions inside the membrane are diffusion limited.

Protein diffusion can be investigated accurately with dual-focus fluorescence correlation spectroscopy (2f-FCS). In the present study, we measured the diffusion of lipids and the SNARE protein Synaptobrevin-2 in free-standing lipid bilayers (Black Lipid Membranes, BLM) and investigated the dependence of the diffusion coefficient on mono- and divalent ions.

Diffusion of proteins and peptides within lipid bilayers is described by the Saffman-Delbrück model. It predicts a logarithmic dependence of the protein's diffusion coefficient on its hydrodynamic radius. In recent publications, however, this has been both challenged and supported.

To test the validity of the Saffman-Delbrück model, we reconstituted proteins of different size into the lipid bilayer, e.g. the SNARE protein Syntaxin, the potassium channel KcsA and the chloride channel EcClC. We found that the Saffman-Delbrück model is only applicable for proteins with a significantly larger hydrodynamic radius compared to the lipids. The diffusion of proteins in the size range of the lipids, however, is better described with a Stokes-Einstein-like model, where the protein's diffusion coefficient is inversely proportional to its hydrodynamic radius.

440-Pos Board B226

Probing Macromolecular Interactions through the Modulation of Hydration Dynamics at the Lipid Membrane Interfaces by Overhauser Dynamic Nuclear Polarization

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Hydration water at molecular interfaces is a sensitively responsive media that is critically coupled to molecular interactions and their associated functions. We study the interactions between lipid membranes and macromolecules (e.g. proteins and polymers) by an ultra-sensitive technique, ^{1}H Overhauser Dynamic Nuclear Polarization (ODNP), through the modulation of translational hydration dynamics at molecular interfaces. It relies on selectively amplified ^{1}H-NMR signals within 10~20Å distance of localized spin labels by r^{-3}-distance dependence of dipolar interaction between electrons and water protons. This powerful approach provides the capability to probe hydration dynamics in deeply buried as well as solvent-exposed molecular interfaces, and enables to explore a wide range of molecular interactions at lipid membrane interfaces with *sensitivity* and *site-specificity* under ambient conditions.

Here we present two examples to illustrate that the underlying functions of membrane-active polymers and membrane proteins are strongly mediated through *interfacial hydration dynamics*. Despite poloxamers, amphiphilic triblock copolymers, are employed as a membrane sealant or permeabilizer, the molecular basis behind their functions is unclear. (*collaboration: Jia-Yu Wang, Ka Yee Lee; University of Chicago*) We found poloxamers present vastly different functions to hydration diffusivity in the lipid membranes, depending on their hydrophobicities and architectures. Using this approach, we study the interaction interface of membrane-bound α-synuclein, the protein that is critically related to the Parkinson's disease. (*collaboration: Jobin Varkey, Ralf Langen; University of Southern California*) Our results confirm α-synuclein forms α-helix upon membrane binding, whereas its C-terminus remains unstructured. Remarkably, we found α-synuclein can form a large twist as the extended α-helix proceeds to the C-terminus. These findings showcase the strength of ODNP to unravel the biophysical functions of macromolecules upon their interactions with lipid membranes through the sensitive detection of modulated hydration dynamics at interaction interfaces.

441-Pos Board B227

Optical Manipulation of Nano-Scale Vesicles

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Naturally occurring lipid vesicles are the most commonly used carriers inside living organisms. To understand vesicle transport and delivery, for example in the synaptic region, and to develop efficient drug-delivery-containers, it is highly desirable to be able to optically control individual vesicles and to measure the distances they travel or the forces exerted on them by the cellular machinery. By using an optimized optical trapping assay in combination with simultaneous confocal microscopy we optical trapped individual nano-scale vesicles with diameters down to 50 nm in 3D using a focused laser beam. The size of vesicles smaller than the diffraction limit was obtained by quantitative confocal fluorescence imaging. A high refractive index sucrose core caused efficient scattering and refraction of the laser light. This allowed for back focal plane detection of the vesicle position in 3D by using a quadrant photodiode, thus providing ~10 μs temporal and nanometer spatial resolution. We also performed the force calibration using an image based method. Finally, as a proof of principle, we demonstrate how to use an optically trapped vesicle to probe the interaction between a ligand and its substrate.