restriction imposed by a supporting substrate. We investigate miscibility transition of ternary lipid mixture, DPPC / DOPC/ Cholesterol, using a combination of fluorescence imaging and time-resolved fluorescence anisotropy. The technique affords unprecedented dynamic characterization for lipid orientation, self-assembly, and dynamic freedom as the monolayer is forced from the liquid to the gel phase. We demonstrate the novelty and applicability of this device by contrasting the time-resolved fluorescence signal of three different lipid probes: 1-palmitoyl-2-{6-[(7-nitro-2-1,3-benzoxadiazol-4-yl)amino] hexanoyl}-sn-glycero-3-phosphocholine (NBD-PC), 5-butyl-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene-3-nonanoic acid (BIODIPY), and 1,1'-dioctadecyl-3,3,3',3'-tetramethylindocarbocyanine perchlorate (Dil) which show dramatically different orientation and dynamic freedom when bound to the lipid layer, over a range of lipid phases. Using this technique we can resolve highly dynamic processes such as the insertion of peptide and proteins into the lipid membrane.

2569-Pos Board B339

Electrostatic Effects on Model Bilayer Stability and Structure

James M. Marr, Zachary D. Schultz.
University of Notre Dame, Notre Dame, IN, USA.

Cellular membranes consist largely of phospholipids, making phospholipids important players for cell processes and cell-cell interactions. Electrostatics are postulated to control structure and function in lipid bilayers. While the effects are largely acknowledged, the mechanisms underlying electrostatic mediated processes are less clear. We have utilized Raman spectroscopy, surface-enhanced Raman scattering (SERS), laser transmission spectroscopy (LTS) and atomic force microscopy (AFM) to monitor the structure and chemical interactions that occur in the classic 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC) and 1,2-dipalmitoyl-*sn*-glycero-3-phospho-L-serine (DPPS) model system. Specifically, we are exploring the stability of these model bilayers in response to Ca^{2+} addition. Our results suggest that electrostatic and chemical interactions induce forces within the bilayer that result in destabilization of vesicles and domain formation in supported bilayer systems.

2570-Pos Board B340

Anomalous Freezing Behavior of Nanoscale Liposomes

Eric J. Spangler[1], Mohamed Laradji[1], P.B. Sunil Kumar[2].
[1]University of Memphis, Memphis, TN, USA, [2]IIT Madras, Chennai, India.

Experiments have shown that the melting transition of small liposomes is broadened when compared to large vesicles or planar membranes [1,2]. Despite their significant biological and biomedical importance, theoretical and computational studies of the phase behavior and structural properties of small liposomes have been limited [3,4]. We present here a systematic computational study of the phase behavior and structural properties of liposomes using a recently developed coarse-grained particle-based model [5]. We particularly focus on the effect of liposome diameter on their thermal and structural properties. Below the melting transition, liposomes are faceted with the gel facets separated by ''grain'' boundaries that are in the fluid phase. In agreement with experiments, we found that the melting transition is significantly broadened as the liposome diameter is decreased and that the heat capacity exhibits two distinct peaks for diameters less than 33 nm, an indication of a decoupling of the melting transition of the two leaflets. This decoupling is clearly demonstrated by the chain order parameters of the two leaflets, which show that the upper leaflet undergoes a melting transition before the inner leaflet. In the gel phase, the lipid tails of the inner leaflet are less ordered than those of the outer leaflet, and the discrepancy between the order parameters of two leaflets increases with decreasing liposomes' diameter. This work is supported by NSF grants (DMR-075547 and EPS-1004083).

[1] R.L. Biltonen and D. Lichtenberg, Chem. Phys. Lipids **64**, 129 (1993)
[2] H. Nagano, T. Najanishi, H. Yao, and K. Ema, Phys. Rev. E **52**, 4244 (1995)
[3] P.V. Ivanova and T. Heimburg, Phys. Rev. E **63**, 041914 (2001)
[4] H.J. Risselada and S.J. Marrink, Soft Matter **5**, 4531 (2009)
[5] J.D. Revalee, M. Laradji, and P.B. Sunil Kumar, J. Chem. Phys. **128**, 035102 (2008)

2571-Pos Board B341

Membrane Structure of Small Unilamellar Vesicles Determined by Small Angle X-Ray Scattering: A Comparison of Full and Local Spectrum Fittings

Ming-Tao Lee[1,2], Wei-Yu Lin[1], Wei-Chin Hung[3].
[1]National Synchrotron Radiation Reasearch Center, Hsinchu, Taiwan,
[2]Department of Physics, National Central University, Jhongli, Taiwan,
[3]Department of Physics, Chinese Military Academy, Fengshan, Taiwan.

We determined the membrane structure of small unilamellar vesicles in aqueous solution by using small angle X-ray scattering. The multi-parameter symmetry and asymmetry models were constructed to fit the full spectrum scattering curve to determine the membrane structure. As a comparison, a simple model with one parameter was used to fit the scattering curve around the second peak to obtain the membrane thickness. We used the model membranes composed of saturated and unsaturated lipids with different chain lengths to prepare small unilamellar vesicles in aqueous solution. The X-ray light source in BL13A and BL23A beam lines of NSRRC and home-made temperature controlled cell with Mylar windows will be applied in the measurements. Consequently, the membrane thicknesses extracted from full and local spectrum fittings are consistent and in agreement with reference papers. However, the parameters determined by full spectrum fittings exist discrepancies in different models except for membrane thickness. The result suggests that one parameter fitting of local spectrum should be a simple, reliable and efficient way to determine membrane thickness of unilamellar vesicles in aqueous solution.

2572-Pos Board B342

Molecular Structure of Phosphatidylglycerol Bilayers: Fluid Phase Lipid Areas and Bilayer Thicknesses as a Function of Temperature

Jianjun Pan[1], **Frederick Heberle**[1], Norbert Kucerka[2],
Stephanie Tristram-Nagle[3], Michelle Szymanski[4], Mary Koepfinger[4],
John Katsaras[1].
[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA, [2]NRC Canadian Neutron Beam Centre, Chalk River, ON, Canada, [3]Carnegie Mellon University, Pittsburgh, PA, USA, [4]Douglass Residential College, Rutgers University, New Brunswick, NJ, USA.

We have determined bilayer structural parameters of commonly used phosphatidylglycerols (PGs) in the fluid phase, by simultaneously analyzing small-angle neutron and X-ray scattering data. We report the temperature dependence of bilayer parameters obtained using the scattering density profile (SDP) model, including the area per lipid and overall bilayer thickness, as well as various intrabilayer structural parameters (e.g. hydrocarbon region thickness). Lipid areas were found to be larger than their neutral phosphatidylcholine (PC) counterparts, which is likely due to electrostatic repulsion of PG headgroups. In general, PG and PC bilayers show a similar response to changes in temperature and chain length, but a differential effect is observed with regard to chain unsaturation: the inclusion of a double bond in a PG lipid results in a smaller change in bilayer area and thickness than for the corresponding PC lipid. The extrapolated molecular area of saturated PG lipids at infinite chain length is similar to that of PC and PE, indicating the pivotal role of the glycerol-carbonyl backbone in shaping the lipid-water interface.

2573-Pos Board B343

The Detailed Scattering Density Profile Model of Pg Bilayers as Determined by Molecular Dynamics Simulations, and Small-Angle Neutron and X-ray Scattering Experiments

Norbert Kucerka[1], Bryan Holland[2], Jianjun Pan[3], Frederick A. Heberle[3],
Chris G. Gray[2], Bruno Tomberli[4], John Katsaras[3].
[1]National Research Council - Chalk River, Chalk River, ON, Canada,
[2]University of Guelph, Guelph, ON, Canada, [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA, [4]Brandon University, Brandon, MB, Canada.

The complex dynamics exhibited by biological membranes are closely correlated to the membrane's structure. Accurate structural data regarding the various membrane components are therefore important in determining specific biomembrane functions. The binding free energy, for example, of Lactoferricin B to mammalian-like membranes (i.e. no net charge) and bacterial-like membranes (i.e net negative charge) has been predicted from molecular dynamics (MD) simulations. However, for the simulation to make any kind of prediction, an accurate structure of the membrane lipids is needed. Area per lipid is often used as the key parameter when assessing the validity of MD simulations. On the other hand, lipid areas obtained from experiment have used models and are thus model dependent. It has therefore been proposed that a better test for validating MD simulations is to compare them to ''raw'' experimental data (e.g. in form of scattering form factors). Experimentally obtained scattering form factors then become the basis for the synergy between experiment and simulation, whereby the simulation results guide the development of more realistic models, and in turn, experimental data aid in the development of more accurate MD force fields.

We combine MD simulations and experiment, both small-angle neutron (SANS) and small-angle X-ray scattering (SAXS), to determine the precise structure of bilayers comprised of bacterial-like (phosphatidylglycerol, PG) lipids. Experiment and simulation are used to develop a one-dimensional scattering density profile (SDP) model suitable for the analysis of the experimental data. The joint refinement of such data (i.e. SANS and SAXS) provides the area per lipid that is then used in the fixed-area simulation. In the final step, the