unsupported bilayers. Recent experiments show that zwitterionic lipid bilayers supported on partially charged, nanoporous silica wafers also do not interact with silica directly. However, in such cases the bilayer is separated from the silica substrate by a relative thicker (~1.5 nm) layer of solvent. We report here results from our MD simulation that reconcile these two seemingly disparate observations. We find that LJ nano-substrates whose porosity and surface hydroxyl density match those of nanoporous silica wafers do not increase the substrate-bilayer distance. Instead, the introduction of partial charge on the LJ substrate increases the substrate-bilayer distance to 1.5 nm. The negative charge on the substrate attracts hydrated ions, creating an electric double layer, which is a sufficient condition to increase the substrate-bilayer distance. While the properties of the bilayer supported on a charged substrate are also different from those of unsupported bilayers, the extent of the perturbation is not as large compared to that induced by uncharged hydroxylated substrates.

**395-Pos Board B175**
**Study of Min Protein-Induced Membrane Waves in vitro**
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In the bacterium Escherichia coli, the proper placement of the division site selection is regulated in part by the pole-to-pole oscillations of Min proteins. In vitro, the oscillation dynamics emerges from the self-organization of MinD, MinE and ATP. However, it is still not clear how the Min proteins affect the E. coli lipid membrane and directly interact with other E. coli proteins. We hypothesized that the spatial oscillations of Min protein systems could play a crucial role in changing lipid membrane dynamics and therefore influence other membrane species indirectly. We developed supported E. coli lipid bilayer platforms in order to systematically explore the underlying mechanism between membrane and Min proteins. We observed spiral membrane waves on fluorescence-labeled E. coli membrane platforms after we introduced unlabeled MinD, MinE and ATP to the membrane. Fluorescence recovery after photobleaching (FRAP) technique was used to study the membrane pattern dynamics. We found that dynamics of the membrane waves had different characteristics from those of the Min protein waves by Kymograph analysis. The simultaneous observation of the labeled Min proteins and the labeled membranes further suggested that the membrane pattern dynamics was directly influenced by the binding concentration gradients of the Min proteins. We will further incorporate some E. coli signaling proteins into the membrane to examine whether their movement or clustering can be influenced by the Min proteins-induced membrane pattern. The result could provide us insights into the long-standing question about the possible function of the E. coli Min protein oscillation phenomenon.
Keywords: Min system, self-organization, supported lipid bilayers, dynamic patterns

**396-Pos Board B176**
**Rapid Assessment of Intracytoplasmic Membranes in Bacteria by Fluorescence Microscopy**
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Intracytoplasmic membranes (ICMs) are known to play an important biological role in bacteria, but many details about these membrane systems remain a mystery. Previously, the primary tool for observing these ICMs was electron microscopy, which limited data collection due to long preparation times and inability to look at dynamic membrane changes. Here we describe a method to rapidly analyze intracytoplasmic membrane structures on a single cell level using fluorescence microscopy and lipophilic dyes on live cells. This allows us to rapidly determine whether or not individual cells possess ICMs. Furthermore we are able to track the growth of multiple single cells over time to elucidate the poorly understood mechanisms by which these membranes are gained or lost with time. Growth conditions also can be altered during imaging to observe how cells immediately react under varying conditions. This technique can be coupled to the use of other fluorescence imaging techniques, such as protein localization via fluorescent protein fusions, or quantitative methods to analyze relative abundance of lipids or proteins. These methods have primarily been applied to methanotropic bacteria, such as *Methylomicrobium alcaliphilum 20z* and *Methylosinus trichosporium OB3b*. Methanotrophs are a type of bacteria that can use single carbon molecules, such as methane, as their sole source of energy and carbon. These methanotrophs produce the membrane bound enzyme, particulate methane monooxygenase (pMMO) which is capable of oxidizing C-H bonds. Our goal is to understand the dynamic relationship between ICMs and pMMO.

**397-Pos Board B177**
**How Reliable are Molecular Dynamics Simulations of Membrane Active Antimicrobial Peptides**
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Membrane-active antimicrobial peptides (AMPs) are challenging to study experimentally, but relatively easy to investigate using molecular dynamics (MD) computer simulations. For this reason, a large number of MD studies of AMPs have been reported over the recent years. Yet relatively little effort has focused on the validity of such simulations. Are these results reliable, and do they agree with what is known experimentally? And how much meaningful information can be obtained? To answer these questions, we demonstrate here some of the requirements and limitations of running MD simulations for several common AMPs: PGLa, melittin, maculatin and BP100. The two most important findings are: (a) Simulation results depend strongly on force field parameters, making experimental verification of the simulations obligatory, and (b) slow orientational and conformational fluctuations mean that much longer sampling timescales (multi-μs) are needed if quantitative agreement between simulation averages and experimental data is to be achieved.

**398-Pos Board B178**
**Dynamic Structural/Amphiphilic "Portrait" of Biomembranes as their Fundamental Property Relevant to Function: Results of Atomistic Simulations**
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Analysis of local dynamic heterogeneities and hydrophobic surface properties of lipid bilayers is an important step toward understanding of the physical processes underlying formation of lipid domains and molecular mechanisms of the so-called ''membrane response'' observed upon binding of external molecules to cell membranes. Here, we used atomistic molecular dynamics simulations to address these problems and study structural/amphiphilic ''portrait'' of a large series of model bilayer membranes (1,2). Rearrangements of membranes upon binding of antimicrobial peptides and association of transmembrane helices were investigated as well (3,4).
It was shown that the water-lipid interface of biomembranes represents a highly dynamic and ''mosaic'' picture, whose parameters depend on the bilayer composition. Formation of such heterogeneities is caused by various intermolecular interactions between lipids, water and ions. Because clustering of the components is determined by a thin balance of differently directed factors, even their minor changes can induce serious rearrangements on the membrane surface. These issues still resist easy experimental characterization.
Probably, these phenomena are indispensable for fast mass/energy transfer near the water/membrane boundary, thus regulating diffusion of molecules in this functionally important area: e.g., approaching of ligands to membrane receptors, delivery of proteins to their sites of insertion into membrane, and so on. Putative role of local heterogeneities and collective phenomena in lipid/water systems is discussed.
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**399-Pos Board B179**
**Monte Carlo Simulations of Phase-Separated Membranes**
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In multi-component lipid mixtures, macro-domains can be directly observed with light microscopy, but nano-domains cannot. Monte-Carlo simulations of liquid-disordered + liquid-ordered phase separation, using a competing-interactions model, can simulate various types of phase morphologies including nano-domains. These simulations capture a more realistic picture of nano-domains as irregular clusters rather than smooth, round disks. On a curved vesicle, when line tension and the competing interaction of bending energy are of similar magnitude, modulated phase patterns occur Current work focuses on studying the various morphologies when competing interactions of line tension, bending energy, and dipole-dipole repulsion form nano-domains.