of mono- and divalent cations. Furthermore, the glycerol moiety of the PG headgroup has a complex conformational space in aqueous media, because of the presence of vicinal hydroxyl groups that are capable of of stabilizing various conformers through hydrogen bonds (H-bonds).
In this work a novel united-atom force field is constructed for PG lipids as a part of the ongoing development of a large, consistent lipid force field library. The torsional and partial atomic charge parameters were calculated based on high-level ab initio quantum mechanical (QM) calculations with semiempirical molecular mechanics (MM) studies. The Lennard-Jones parameters were taken from the OPLS-UA force field developed by Jorgensen [1]. The QM and MM simulations were combined with experimental thermodynamic data of glycerol as target data for parameter optimization. The parameters were further optimized to reproduce the structural, dynamic and elastic properties of pure DMPG and POPG lipid bilayers.
[1] W. L. Jorgensen, J. Phys. Chem. 1986, *90*, 1276–1284.

820-Pos Board B620
Temperature Modulation of the Life Cycles of Phospholipid Bilayer Electropores
Zachary A. Levine, P. Thomas Vernier.
Molecular-scale details of the mechanism of electric field-driven pore formation in phospholipid bilayers are not well understood, in part because the nanoscopic domain at which individual pore formation occurs is not readily accessible to experimental observation. Analytical and numerical models can help to fill this void. Previous studies using molecular dynamics (MD) simulations defined the stages in the creation and annihilation of an electropore as a function of the externally applied electric field, from the formation of an initial water defect to the restoration of the intact bilayer [1]. Here we vary the temperature at which electropermeabilization occurs, and we extract heat capacity and energy profiles for each system. Results will be compared to and, to the extent possible at this time, reconciled with existing mathematical models of electroporation, presenting a more unified and complete framework for future studies.
[1] Levine, Z. A. and P. T. Vernier. 2010. Life Cycle of an Electropore: Field-Dependent and Field-Independent Steps in Pore Creation and Annihilation. Journal of Membrane Biology 236:27–36.

821-Pos Board B621
Nucleotide Modifications Change tRNA Dynamics and Base Pairing
Christian Blau, Gerrit Groenhof, Helmut Grubmüller.
Modified and unmodified yeast tRNA(Phe) in solution was simulated to understand the effect of nucleotide modifications on the dynamics of tRNA. High performance computing techniques were employed to obtain a ''dynamic picture'' at spacial and time resolutions hardly accessible experimentally for these systems. Local flexibility, secondary and tertiary structure, global rearrangements and movements of the whole tRNA were probed by a microsecond of all atom explicit solvent molecular dynamics simulations.
The results of our simulations give new insight on experimentally observed biological impact of nucleotide modifications. Amongst other results we find that tRNA modification leads to a decrease in secondary structure and tertiary interactions in the anticodon stem loop. Nucleotides U16 and U17 show different orientations when modified to dihydrouridine. Modification of A58 to 1-methyladenosine causes local rearrangements in the elbow region. Implications of our results on external factor binding are discussed.

822-Pos Board B622
Molecular Dynamic Simulations of Blast Waves on Bilayers
Rahul Bhowmik, Richard W. Pastor, **Jeffrey T. Mason**.
Many studies using animal models have shown that blast waves cause injuries to the brain despite the lack of a direct physical impact to the brain or skull. Such injuries are manifested as biochemical, functional, or morphological alterations that result in motor and sensory deficits in addition to behavioral changes. Primary blast due to explosions causes an intense rise of atmospheric pressure, the positive phase, followed by a broader under-pressure, the negative phase. The peak overpressure reaches pressures up to 1724 kPa and the blast wave travels at speeds up to 670 m/s. Because of this high velocity, it is difficult to study the interaction of explosive blast waves with neural tissue in real time. Accordingly, we have performed molecular dynamic (MD) simulations of blast waves on myelin membranes to understand how blast waves interact with neural tissue to cause injury. In our simulations, we have created blast overpressure using a planar wall, which exerts a forces of $-K(x_0 - x)^2$; where K is the spring force constant, and x_0 and x are the starting and final positions of the wall, respectively. The intensity of the overpressure wave is controlled by the spring stiffness (K) and the duration of the wave is controlled by how far the wall moves ($x_0 - x$). Our findings demonstrate that the velocity of the blast wave is more deleterious to membranes than is the blast overpressure. At velocities above 600 m/s the negative phase can cause bilayers containing phospholipid and cholesterol to bifurcate at the bilayer center. Such structural perturbations could result in diffuse axonal injury, which is believed to play a role in the pathology of blast injury.

Emerging Single Molecule Techniques - Fluorescence

823-Pos Board B623
Observation of Protein Adsorption Using a Synthetic Nanopore
David J. Niedzwiecki, Liviu Movileanu.
Using the coulter counter technique with a single nanopore, we probed the non-specific adsorption of bovine serum albumin (BSA) to a silicon-based surface at the single molecule level. A potential bias was applied across a silicon nitride membrane containing a single nanopore that was immersed in KCl solution. Ionic current fluctuations across the nanopore revealed long-lived interactions of BSA with the silicon nitride. The nature of these interactions can be classified into two categories, suggesting that BSA adheres to the nitride surface in two distinct orientations. Knowing how proteins from the blood, like BSA, interact with silicon based materials is of growing importance as these materials are integrated into biosensors and medical devices.
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824-Pos Board B624
Force-Free Three-Dimensional Measurements of DNA Conformations Reveals Its Behavior Close to a Wall
Yuval Garini, Guy Nir, Shlomi Medalion, Yitzhak Rabin, Moshe Lindner.
Using a combined setup of tethered particle motion (TPM) with gold nanobeads and total internal reflection (TIR) illumination, we measured the three dimensional end-to-end distribution of a DNA tethered to a wall. Although the lateral Gaussian distribution is well known and studied, the axial distribution was never measured before.
The planar distribution (parallel to the wall) is found to be Gaussian, with good agreement to both the worm like chain (WLC) model and the commonly sued Gaussian random walk (GRW) model. The axial distribution (perpendicular to the surface) is found to be Rayleigh-like, in agreement with WLC simulations. The distribution that is found with these WLC simulations, however, deviates systematically from the GRW distributions for short DNA strands (less than 3 micrometer).
The WLC simulations reveal that the presence of the wall increases the correlations between the orientations of neighboring segments with respect to free DNA. It can also be interpreted as an entropic repulsion due to rejection of polymer conformations from the wall. This repelling potential might play an important role in the DNA functioning when it is close to the nucleus membrane.

825-Pos Board B625
Tracking Degradations of Single DNA and Protein Molecules in Fluid
Daisuke Onoshima, Noritada Kaji, Manabu Tokeshi, Yoshinobu Baba.
Moving images obtained from optical microscopic studies with single biomolecules, including DNA and proteins, provide amazing insights into physico-chemical fundamentals such as dynamics and kinetics in a particular environment. Previously, the observation of large numbers of individual molecules has been used to detect identifiable individual chemical events or components of a chemical synthesis system. These may offer crucial clues towards intricate molecular mechanisms. Despite this importance, analytical applications still have lagged behind the establishment of theoretical principles. Based on the Michaelis-Menten equation, values for the reaction rate constants have traditionally been calculated from the solution phase reaction kinetics. This procedure is predictably effective for discussing a minimal model of the kinetics. However, most biomolecular interactions are thought to involve multiple steps, typically an initial binding followed by a structural rearrangement. Particular attention should be given to the fractionally-sampled molecular steps. Our analysis, described here, uses a technology to determine the detailed molecular information about interactions between DNA and DNA interactive protein. It uses motion capture technology that was originally developed for recording biomechanical movement onto a digital model. We applied it for motion tracking and position sensing of a single DNA molecule undergoing restriction enzyme digestion in a microfluidic device. Quantum dot and total internal reflection fluorescence microscope were used as a marker and a tracker respectively, which allowed motion capture of DNA during interfacial reactions. With our analysis, an enzymatic degradation time was detected at a single molecule level. It was also possible to calculate the observed catalytic rate constant. As an application case of our tracking measurement, protease activity of trypsin was monitored in real time. The geometrical features of the biological