expenses. To date, most of lattice-based MC simulations of lipid membranes have been carried out on triangular lattices. Previously we have argued [1, 2] that the particular lattice geometry in MC simulations should not matter for reproducing the properties of the membrane at scales larger than the lattice unit, provided that the lipid-lipid interaction parameters are properly rescaled. Still, it remained an open question whether there exists a single conversion factor for all lipid-lipid interaction parameters to achieve identical results on triangular and square lattices, or the different interaction parameters have to be adjusted individually. Here, based on the properties of the Ising model, we demonstrate that one can indeed choose a single numerical coefficient to rescale all lipid-lipid interaction parameters depending on the lattice type, which provides one-to-one correspondence of thermodynamics properties of lipid membranes in lattice-based MC simulations on triangular and square lattices.

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1485-Pos Board B215

Molecular Modeling and Simulations of Reverse Micelles

Gozde Eskici, Paul Axelsen.
Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, PA, USA.

The physiochemical properties of sodium di-2-ethylexylsulfoccinate (AOT) reverse micelles in isooctane have been examined since the 1940s by various spectroscopic methods including NMR, neutron scattering, X-ray scattering, quasi-elastic light scattering, and infrared spectroscopy. Several attempts have also been made to create a computational model of a reverse micelle. However, studies to date leave several important questions unanswered about the size and stability of reverse micelles. To address the questions that remain unanswered about the equilibrium size of a reverse micelle, we have conducted simulations of small AOT reverse micelles in isooctane at constant pressure and temperature. Results show that the shape of a reverse micelle depends on its size, i.e. its surface area to volume ratio, and that the density of water within the reverse micelle is density is significantly less than that of bulk water. These results must be considered when interpreting experimental studies about the equilibrium size of a reverse micelle. These studies lay a foundation for future studies of encapsulated polypeptides and reverse micelles made from surfactants other than AOT.

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Curvature and Lipid Clustering within Asymmetric Biologically Relevant Membrane Models

Heidi Koldsø, Mark S.P. Sansom.
Department of Biochemistry, University of Oxford, Oxford, United Kingdom.

Advances in lipidomics are detailing the compositional and dynamic complexity of cell membranes such as leaflet asymmetry, lipid nanodomains, local curvature, lipid diffusion and lipid composition and distribution. These complexities alter how the membrane interacts with proteins and hence have the potential to control the functional behaviour of proteins and it has become clear that the cell membrane does not only act as a barrier but also plays an important role in controlling the function of proteins such as activation of K^+ channels by 4,5-bisphosphate phosphatidylinositol (PIP2) [1], the regulation of the epidermal growth factor receptor by the glycolipid GM3[2] and cholesterol modulation of G-protein coupled receptors[3]. Previous computational studies of membrane proteins have generally been limited to symmetric single lipid component bilayers. We have developed an approach to create highly complex asymmetric biologically relevant membrane models allowing us to obtain a better understanding of membrane properties and enabling us to explore functionally important protein-lipid interactions. We explore properties of biological relevant membranes such as nano-domain formation of certain lipid types but also more macroscopic properties such as membrane undulation and curvature in relation to lipids types and lipid clustering. Extending the system dimensions to > 100 nm allow us to explore membrane dynamics on length scales comparable with experimental ones. The simulations indicate stabilization of curved areas by lipid nano-domains and a tight correlation between lipid species and curvature. We will also explore protein properties such as oligomerisation of e.g. signalling receptors in an ''in vivo in silico'' approach.

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Multiscale Modeling of Four Component Lipid Mixtures: Coarse Grained and United Atom Simulations Reveal Trends in Phase Separation

David G. Ackerman, Gerald W. Feigenson.
Cornell University, Ithaca, NY, USA.

The cell plasma membrane is often modeled using three-component mixtures containing a high melting lipid, a low melting lipid and cholesterol. These ternary mixtures exhibit either nanoscopoic or macroscopic liquid-liquid phase coexistence. An additional patterned phase morphology can exist in four component systems which combine a high melting lipid, cholesterol, a nanodomain-inducing low melting lipid and a macrodomain-inducing low melting lipid. The molecular-level details governing these different phase morphologies are not yet known. Here, we utilize molecular dynamics simulations to analyze how phase separation evolves in a four component mixture. We present data for 11 mixtures at a fixed composition of (16:0,16:0)-pc/(18:2,18:2)-pc/(16:0,18:2)-pc/Cholesterol (DPPC/DLiPC/PLiPC/Chol), where PLiPC is incrementally replaced by DLiPC from one simulation to the next. Each simulation was run to equilibrium over 25 μs using the Martini coarse grained forcefield and was then converted to united atom and run for a further 100 ns. We investigate trends in domain size, composition, interleaflet coupling and properties of the domain interface as a function of replacement of PLiPC by DLiPC.

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Molecular Insights into Electroporation and Electrotransfer through Model Cell Membranes

Marina Kasimova[1,2], Lucie Delemotte[3,4], Andraz Polak[1,5], Damijan Miklavcic[5], Maura Casciola[1,6], Francesca Apollonio[6], Marie Breton[7], Luis Mir[7], Alexey Shaytan[2], Konstantin Shaitan[2], **Mounir Tarek**[1].
[1]CNRS- University of Lorraine, Nancy, France, [2]Biological Faculty, Moscow State University, Moscow, Russian Federation, [3]Temple University, Philadelphia, PA, USA, [4]CNRS - University of Lorraine, Nancy, France, [5]Electrical Engeneering, University of Ljubljana, Ljubljana, Slovenia, [6]Department of Information Engineering, Electronics and Telecommunications, University La Sapienza, Rome, Italy, [7]Vectorology and Anticancerous therapeutics, CNRS- Institut Gustave Roussy, Paris- Villejuif, France.

membranes are permeabilized. Under specific conditions, EP may be reversible, in which case membranes and cells recover their initial state when the applied field is turned off. Due to the availability of corresponding electronic devices, early studies have involved applying electric pulses of microsecond duration. Under such conditions, low magnitude pulses (~few hundreds of V/cm) were required to achieve reversible EP. More recently, devices have emerged where pulses in the kV/cm magnitude range can reach the nanosecond time scale. In such a case, high magnitude pulses (~few hundreds of kV/cm) induce reversible electroporation not only of the plasma membrane but also of the membrane of internal organelles. As it enables the uptake of molecules that usually display poor transmembrane crossing abilities, EP is widely used in biomedicine and biotechnology to enhance the transport of drugs, molecular probes or else nucleic acids, a technique also known as electropermeabilization.

Atomistic simulations in general and molecular dynamics (MD) simulations in particular, have proven to be effective for providing insights into both the structure and the dynamics of model lipid membranes in general. Recent studies have shown that the method is suitable for investigating the electroporation phenomena. Several MD simulations have hence been conducted in order to model the effect of electric fields on membranes, providing perhaps the most complete molecular model of the electroporation process of lipid bilayers. Here we extend these investigations to study both the modulation of electroporation thresholds by lipid composition, and the characteristics of the pores formed under a variety of conditions matching experimental protocols. We explore also ions and large molecules conducting properties of these pores and show exquisite agreement with experiments.