Membrane Physical Chemistry II

2525-Pos Board B217

Interaction Profiles of Amino Acid Side-Chain Analog Pairs within Membrane Environments

Vahid Mirjalili, Michael Feig.
Michigan State University, East Lansing, MI, USA.

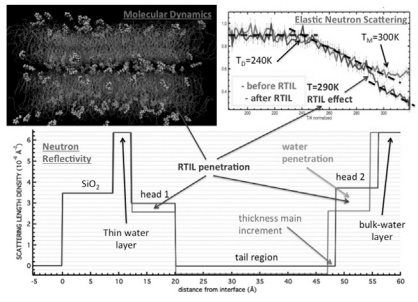
The energetics of amino acid insertion into membranes has been studied extensively but relatively little is known about the association energetics of amino acids within biological membranes. Here, interactions between pairs of four amino acid analog (Asn, Ser, Phe, and Val) in the membrane environment are described from umbrella sampling molecular dynamics simulations. Association interaction free energy profiles as a function of bilayer insertion depth are presented and the physical characteristics of contact pairs are described. The results provide detailed insight into amino acid interactions within membrane environments with implications in the understanding of how membrane-bound peptides and proteins interact and for the association of transmembrane helices. Furthermore, the quantitative energy profiles presented here serve as a benchmark for the parameterization of more simplified models such as coarse-grained models or implicit models of membrane bilayers.

2526-Pos Board B218

Room-Temperature Ionic Liquids Interacting with a Phospholipid Bilayer: A Comprehensive Neutron Scattering and Molecular Dynamics Study

Antonio Benedetto[1,2], Miguel A. Gonzalez[3], Pietro Ballone[4].
[1]School of Physics, University College Dublin, Dublin, Ireland, [2]School of Medical Sciences, The University of Sydney, Sydney, Australia, [3]Institut Laue Langevin (ILL), Grenoble, France, [4]Istituto Italiano di Tecnologia, Roma, Italy.

Recent experiments have shown that Room-Temperature Ionic Liquids (RTIL) can be incorporated into phospholipid bilayers, undermining their stability. Those results have important implications concerning the toxicity of RTILs, but could also point to biotechnological applications. However, the experiments available up to now, provide limited access to the microscopic details on the RTIL-phospholipid interaction. Neutron Scattering (NS) and Molecular Dynamics (MD), instead, represent powerful tools for characterizing both the structure and dynamical properties at the microscopic level. Here we present a comprehensive NS and MD study on phospholipid bilayers in contact with water solution of prototypical RTILs, e.g. [bmim][Cl], [bmim][PF6], and [bmim][NTf2]. Neutron diffraction and reflectivity allow us to determine the changes in the membrane structure when different RTILs are added, while the dynamical properties have been determined by quasi-elastic neutron scattering. MD has been performed on the same systems using Gromacs. NS has been performed at ILL (France), ISIS (UK), and NIST (USA) large-scale facilities, whereas the MD on the supercomputer ICHEC (Ireland). Experimental results and MD predictions agree with each other, and provide a wealth of microscopic information on the RTIL-phospholipid interaction.



2527-Pos Board B219

The Distributions and Orientations of Retinoids in Retinal Membranes Studied with All-Atom Molecular Dynamics Simulations

Jinju Lu[1], Igor Vorobyov[1], Toby W. Allen[1,2].
[1]Department of Chemistry, University of California, Davis, Davis, CA, USA, [2]School of Applied Sciences & Health Innovations Research Institute, RMIT University, Melbourne, Australia.

Understanding the transport of retinoids in lipid bilayers is essential to describe the binding to photoreceptors or retinoid-binding proteins involved in the visual cycle. Utilizing all-atom molecular simulations, we demonstrate how 11-cis retinal, all-trans retinal and all-trans retinol distribute and orient in lipid bilayers with different levels of unsaturation, head group and the presence of cholesterol, characteristic of retinal membranes. We have found that all-trans retinol is more depleted in the membrane core (with a substantially lower density relative to retinal) and less flexible in its orientation (with a more parallel alignment to the membrane normal) than its retinal counterpart. We shall discuss how these results pertain to the vision cycle. In particular, the restricted distribution of retinol may assist the removal of all-trans retinol from the rod outer segment(ROS) membranes by facilitating its binding to certain retinoid-binding proteins. On the other hand, the higher accessibility of the membrane core to all-trans retinal and its flexible orientation may assist its release from bleached photoreceptors. Furthermore, we demonstrate that the presence of cholesterol increases the concentration of 11-cis retinal in the membrane core and will explain how this is consistent with the roles of plasma and disk membranes in the retinoid cycle.

2528-Pos Board B220

Correlations of Specific Ionic Effects using Ion Channels and Surface Charge Measurements

Torri C. Roark[1,2], Oscar Teijido Hermida[2], Tatiana K. Rostovtseva[2], Philip A. Gurnev[2,3], Horia I. Petrache[1], Sergey M. Bezrukov[2].
[1]Department of Physics, Indiana University Purdue University Indianapolis, Indianapolis, IN, USA, [2]NIH/NICHD, Bethesda, MD, USA, [3]Department of Physics, University of Massachusetts, Amherst, MA, USA.

Specific ionic effects, as captured in the Hofmeister series, have been observed in many biological phenomena including protein folding and aggregation and lipid bilayer interactions. Previously we have shown that the Hofmeister effect is present in the activity of gramicidin A channels. In particular, measurements of channel open lifetime and conductance in potassium salts clearly show the existence of two distinct ionic classes which could be identified as kosmotropic and chaotropic. To further investigate this behavior, we have measured the zeta potential of diphytanoyl phosphatidylcholine (DPhPC) liposomes in salt solutions. We observe that anions alter the surface charge of the liposomes depending on the classification of the anion as kosmotropic or chaotropic. Chaotropic anions (SCN^-, ClO_4^-) decrease the surface charge of the liposomes while kosmotropic anions (Cl^-, $H_2PO_4^-$, SO_4^{2-}) have the opposite effect. These results correlate with our previous studies of cation conductance through gramicidin A channels adding new insight into ionic interactions at the lipid-water interface.

2529-Pos Board B221

Molecular Competition between Large and Small Polyethylene-Glycols (PEGs) Partitioning into OMPC Porin Channels

M. Alphan Aksoyoglu[1], Philip Gurnev[1,2], V. Adrian Parsegian[1].
[1]Physics, University of Massachusetts, Amherst, MA, USA, [2]PPB/NICHD/NIH, Bethesda, MD, USA.

Molecular crowding by polyethylene glycols (PEGs) has been employed in a wide range of inquiries into molecular structure and dynamics. Investigating the partitioning of crowded polymers into biological nanopores reveals properties also seen in, e.g., DNA ejection and compaction into viral capsids, as well as in facilitated molecule transport. Capitalizing on our previous work on the partitioning of binary PEG mixtures into the benchmark Alpha-Hemolysin nanopore, we have now studied partitioning of mono- and polydisperse polymer solutions into comparably sized, yet differently structured, diffusion channels. We find that in the presence of large non-partitioning PEG 3400, the small, otherwise equipartitioning PEG 200 partitions disproportionately. Specifically, with 15% PEG 3400, an added 15% PEG 200 reduces channel conductance by 65% (compared with channel conductance in polymer-free solutions), while 15% PEG 200 alone reduces channel conductance by only 45%. We employed open-channel noise analysis to investigate channel diffusion properties of individual polymers, and to compare them with their properties in bulk water solution. In this way we demonstrate and quantify crowding-assisted transport through nanopores in mixed-polymer systems.

2530-Pos Board B222

Charging the Quantum Capacitance of Graphene with a Single Biological Ion Channel

Peter J. Burke.
EECS, University of California, Irvine, Irvine, CA, USA.

Here, we report graphene-based field-effect transistors combined with supported lipid bilayers as a platform for measuring, for the first time, individual ion channel activity. We show that the supported lipid bilayers uniformly coat the single layer graphene surface, acting as a biomimetic barrier that insulates (both electrically and chemically) the graphene from the electrolyte environment. The Dirac point of the graphene FETs is not affected by changes in the solution pH or KCl concentration after it is covered by SLBs. Upon introduction of pore-forming membrane proteins such as alamethicin and gramicidin