Molecular dynamics study of vesicle deformation mechanisms

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[1] Materials, Physics, and Molecular, Cellular and Developmental Biology Departments, University of California, Santa Barbara, CA, USA
[2] National Resource for Automated Molecular Microscopy, Department of Cell Biology, The Scripps Research Institute, La Jolla, CA, USA.

Recently, we have reported block liposomes (BLs), a new vesicle phase formed in mixtures of MVLBG2, DOPC and water (A. Zidovska et al., *Submitted*, 2007). MVLBG2 is a newly synthesized highly charged (16+) lipid (K. Ewert et al., *JACS,* 2006) with giant dendrimer-like headgroup therefore having a headgroup area several times larger than DOPC. The nature of the headgroup leads to a conical shape of the molecule resulting into high spontaneous membrane curvature, when incorporated into lipid bilayer. Therefore, in combination with zero-curvature DOPC, the system exhibits a rich phase diagram revealing novel vesicle morphologies. We carried out structural studies of this phase with differential contrast microscopy (DIC) and cryo transmission electron microscopy (cryo-TEM). At the micron scale DIC reveals a new phase consisting of uniform bone-like vesicles which is present in a narrow composition range. This novel morphology persists down to the nanometer scale. Cryo-TEM reveals a population of nanotubes which are capped by spherical unilammelar vesicles with diameters of few hundred nm and a surprising new morphology of lipid nanorods (fibers) resulting from a spontaneous topological transition from tubes to nanorods. In this work we investigate the contribution of spontaneous curvature and membrane charge to the formation of BLs. By comparing with a system of matching membrane charge density but zero spontaneous curvature and by screening the charge of MVLBG2 but keeping the curvature constant, we were able to identify both, spontaneous curvature and membrane charge, as critical parameters for BLs-formation. The effect of salt and pH on the shape evolution of the BLs was also carefully studied.

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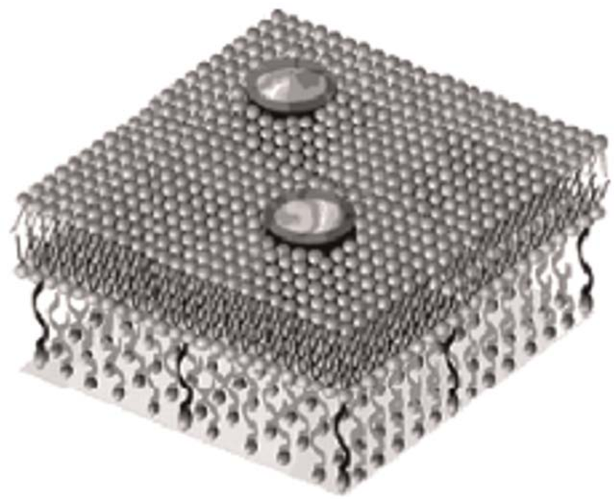
1022-Plat Tethered Bilayer Lipid Membranes: a versatile Model Membrane Platform

Ingo Koeper, Inga Vockenroth, Ann Falk, Lifang Niu
Max Planck Institute for Polymer Research, Mainz, Germany.

Tethered layer lipid membranes (tBLM) have been develloped in the past years to a versatile platform that can mimick essential features of a biological membrane. A tBLM consists of a lipid bilayer, where the inner leaflet is covalentely attatched to a solid support via a spacer unit. Thus, they provide a stable and insulating system, that can be used to study various membrane related processes. We have used tBLMs to study the functional incorporation of ion channels as well as to monitor the interaction of antimicrobial peptides and other proteins with the lipid bilayer. The stuctural properties of the membrane have been analzed in detail by Neutron Scattering. The results allow for an optimization of the molecular architecture.

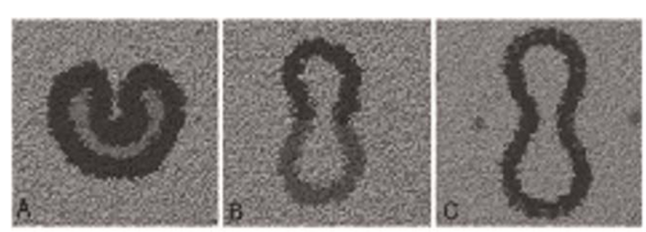
Experimental results obtained by Surface Plasmon Resonance and Impedance Spectroscopy on the function of the ion channels and the interaction pathways of the peptides will be presented.



1023-Plat Molecular Dynamics Study Of Vesicle Deformation Mechanisms

Albert J. Markvoort, Peter Spijker, Rutger A. van Santen, Peter A.J. Hilbers
Technische Universiteit Endhoven, Eindhoven, The Netherlands.

Lipid bilayer membranes are known to form various structures like large sheets or vesicles. When both bilayer leaflets have equal composition, membranes preferentially form flat sheets or spherical vesicles. However, vesicles with a wide variety of shapes, including ellipsoids, discoids, pear-shaped, cup-shaped and budded vesicles, have been shown experimentally. Such shapes were predicted theoretically from energy minimization of continuous sheets as well. We show, using coarse-grained molecular dynamics simulations, how relatively small asymmetry in composition between the two leaflets may result in spontaneously curved bilayers and all these vesicle shapes. Three types of bilayer asymmetry are considered. Firstly, the situation where the headgroup-solvent interaction and thus the lipid packing alters due to a change in pH or ion-concentration of the vesicle interior/exterior (A). Secondly, where asymmetry arises from phase separation of two lipid types (B). And thirdly, where asymmetry arises from growth of one of the bilayer leaflets by incorporation of additional lipids from the solvent (C).



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