BP 21: Membranes and Vesicles II

Time: Tuesday 14:00–16:00 Location: ZEU 250

BP 21.1 Tue 14:00 ZEU 250

Interactions of Radical Oxygen Species with Phosphatidylcholine Monolayers and Liposomes — •Andreas Gröning[1], Heiko Ahrens[1], Frank Lawrenz[1], Thomas Ortmann[1], Gerald Brezesinski[2], Fritz Scholz[3], Doris Vollmer[4], and Christiane A. Helm[1] — [1]Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]MPI KGF, 14476 Potsdam, Germany — [3]Inst. f. Biochemie, Uni Greifswald, 17487 Greifswald — [4]MPIP, 55128 Mainz, Germany

During times of environmental stress (e.g., UV or heat exposure), levels of reactive oxygen species (ROS) can increase. This may result in significant damage to cell structures. Here we focus on the effect of hydroxyl radicals (produced by Fenton reaction) on model membranes.

For DPPC monolayers at the air/water interface a decrease in the lateral pressure is used as a measure of the efficiency of the radical attack. Combining isotherms, X-ray diffraction and IRRAS we find a partial cleavage of the head group leading to a reduced head group size with negative charge. X-ray reflectivity demonstrates Fe^{2+} binding to the head group, fluorescence microscopy immediate nucleation of new domains in the condensed phase.

The radicals destroy DMPC liposomes, only fragments remain as is observed with confocal microscopy. Differential scanning calorimetry shows that an increasing radical concentration causes a shift of the alkyl chain melting transition to higher temperatures.

Summarising, both monolayers and liposomes solidify on exposure to ROS, consistent with a common molecular mechanism.

BP 21.2 Tue 14:15 ZEU 250

The complexity of membrane domain formation. — •Djurre H de Jong[1], Siewert J Marrink[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Germany — [2]Molecular Dynamics Group, University of Groningen, The Netherlands

Living cells are enveloped by the plasma membrane (PM): a thin layer consisting of a complex mixture of lipids and proteins. Rather than being a "shopping bag" keeping together the cell content, the PM plays an active and diverse role in the functioning of the cell. A fascinating aspect of the PM is the formation of transient, lateral domains, consisting of both lipids and proteins.

The time and length scales at which these membrane domains occur make them difficult to study, both experimentally (too small, too transient) or with simulations of full atomistic detail (too large, too long timescales). Here we use coarse grain molecular dynamics (CGMD) simulations, applying the Martini force field, to gain insight in the dynamics involved. Previously we have used this model to study the partitioning of membrane proteins between different domains in model bilayers and the influence of specific proteins and minor lipid species on the formation of domains. Here we quantify the energetic contributions to phase separation that different variation in system composition have. To this aim we combined the long timescales achieved with the Martini force field with the ability to sample non-physical states using sophisticated free energy sampling methods implemented in the software packages PLUMED and Gromacs.

BP 21.3 Tue 14:30 ZEU 250

Molecular Requirements for Raft Formation in a Lipid/Cholesterol System — •Davit Hakobyan and Andreas Heuer — WWU Münster, Institut für Physikalische Chemie, Münster, Germany

Recent comparison of the MARTINI coarse-grained (CG) bilayer system with an equivalent atomistic system comprised of DPPC, unsaturated dilinoleyl phosphatidylcholine (DUPC) lipids and cholesterol (CHOL) showed very good agreement on the phase separation phenomena [1]. Here the properties of CG lipids and CHOL are systematically varied to study the molecular requirements for the raft formation. The DUPC lipid is assimilated to DPPC lipid by modifying the angles, the angle force constants as well as the bead types of the chains. It turns out that the unmixing is largely driven by van der Waals interactions between DPPC - CHOL/DPPC pairs and is nearly independent of the entropy of the DUPC chains. On the other hand reduction of the angle force constant of DPPC chains by 60 % keeps the system mixed suggesting that the entropic contribution of DPPC chains is important for the unmixing. By substituting the CHOL with shorter and stiffer DPPC-like molecules one observes unmixing similar to DPPC/DUPC/CHOL system which suggests the rigid and flat structure of CHOL to play a key role in raft formation. With a stiffened last bead of CHOL the order of DPPC/CHOL domain significantly increases indicating that the conformational entropy of CHOL is important to prohibit the gelation [2]. 1. Hakobyan, Heuer, J. Phys. Chem. B, 2013, 117, 3841. 2. Hakobyan, Heuer, PLOS ONE, In Press.

BP 21.4 Tue 14:45 ZEU 250

Domain formation in a membrane coupled to an actin network — •Sina Sadeghi[1], Alf Honigmann[2], Christian Eggeling[2], and Richard Vink[1] — [1]Institute of Theoretical Physics, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Department of NanoBiophotonics, Göttingen, Germany

Lateral heterogeneity of the plasma membrane is receiving much attention. In contrast to model membranes which exhibit phase separation below a certain temperature, biological membranes typically do not phase separate. One hypothesis is that the cytoskeleton network on the cytoplasmic side of the cell membrane prevents phase separation. This motivates the study of pattern formation in membranes in the presence of an actin network. To this end, a series of experiments were performed on a supported membrane that was bound to an actin network via certain cross linker lipids (pinning sites). These experiments show that the lipid domain pattern that arises is strongly affected by the interaction of the pinning site with the surrounding diffusing lipids. In the present work, we propose an extended (Ising) model to rationalize these findings. Our model includes the effects of the membrane curvature on the lipid organization. To be precise, we modelled the elastic properties of the membrane using the Helfrich expansion, and assumed a coupling between the lipid domains and the local membrane curvature. Using computer simulation, we find that this coupling is crucial in order to reproduce the experimental results, especially for the case where the pinning sites have a small affinity for saturated lipids.

BP 21.5 Tue 15:00 ZEU 250

Probing the influence of soluble domains on the diffusion of peripheral membrane proteins — •Gernot Guigas and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Diffusion coefficients of membrane proteins are commonly assumed to be well predicted by the Saffman-Delbrück relation. The latter describes proteins as single membrane-spanning cylinders, i.e. effects of bulky extra-membrane domains and spatial protein interactions at crowded conditions are neglected. However, these quantities potentially play an important role for the survival of parasites of the trypanosome family in the bloodstream of mammals. To evade antibody recognition by the host's immune system, trypanosomes exchange their complete, very dense surface coat of bulky GPI-anchored glycoprotein VSG by a genetic variant within few minutes. Diffusion plays a crucial role for an efficient exchange of the dense VSG coat. We have used coarse-grained membrane simulations to study the diffusion properties of VSG and similar peripheral membrane proteins at crowded conditions. Both protein packing density and the size of the soluble domain have a strong influence on protein mobility. Diffusion coefficients are reduced by almost an order of magnitude when the VSG surface area fraction reaches physiological values of 30% and more. Enlarging the extra-membrane domain results in a similar reduction of VSG's diffusional mobility.

BP 21.6 Tue 15:15 ZEU 250

Translocation of amphiphilic polymers through lipid bilayer membranes - balanced hydrophobicity versus polarization — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

We discuss adsorption and passive translocation of amphiphilic polymers such as random copolymers [1] through a self-assembled lipid bilayer membrane. By using the bond fluctuation model with explicit solvent [2] we consider copolymers of hydrophilic and hydrophobic sites under variation of the fraction, H, of hydrophobic sites and

chain length. Our results indicate a point of balanced hydrophobicity, $H_L = 0.6$, where a slight excess of hydrophobic monomers compensates an additional insertion barrier due to the self-organized packing of the bilayer. Translocation events of shorter polymers through the membrane can be observed close to the balanced condition $H = H_L$. For longer chains, translocations are suppressed due to the "polarization" of the amphiphilic molecules with respect to the interface. Close to the point of balanced hydrophobicity, the polymer induces dynamic and static perturbations in the bilayer and increased permeability with respect to solvent. We give a more general outlook on how to design membrane active polymers with a desired emphasis on either translocation or permeabilization on the onset of balanced hydrophobicity.

[1] T. Goda, Y. Goto, und K. Ishihara, Biomaterials, 31, 2380 (2010).
[2] J.-U. Sommer, M. Werner, und V. A. Baulin, Europhys. Lett., 98, 18003 (2012)

BP 21.7 Tue 15:30 ZEU 250

Asymmetric phospholipid: lipopolysaccharide bilayers; a Gram-negative bacterial outer membrane mimic — •Maximilian Skoda[1], Luke Clifton[1], Emma Daulton[1], Arwel Hughes[1], Anton Le Brun[2], Jeremy Lakey[3], and Stephen Holt[2] — [1]ISIS, STFC, Harwell, UK — [2]Bragg Institute, ANSTO, Kirrawee DC,Australia — [3]Institute for Cell and Molecular Biosciences, Newcastle University, Newcastle upon Tyne, UK

The Gram-negative bacterial outer membrane (OM) is a complex and highly asymmetric biological barrier but the small size of bacteria has hindered advances in in-vivo examination of membrane dynamics. Thus, model OMs, amenable to physical study, are important sources of data. Here, we present data from asymmetric bilayers which emulate the OM and are formed by a simple two-step approach. LB deposition of phosphatidylcholine on an SiO2 surface formed the inner leaflet and Langmuir-Schaefer deposition of either Lipid A or Escherichia coli rough lipopolysaccharides (LPS) the outer one. The membranes were examined using neutron reflectometry (NR). NR data showed that in all cases the initial deposition asymmetry was mostly maintained for more than 16 h. This stability enabled the sizes of the headgroups and bilayer roughness of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine and Lipid A, Rc- and Ra-LPS to be clearly resolved. This shows that rough LPS can be manipulated like phospholipids and used to fabricate advanced asymmetric bacterial membrane models using well-known bilayer deposition techniques. Such models will enable OM dynamics and interactions to be studied under in-vivo like conditions.

BP 21.8 Tue 15:45 ZEU 250

Water-mediated forces at hydrophilic and hydrophobic surfaces — •Matej Kanduc[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Free University Berlin, D-14195 Berlin, Germany — [2]Institut Laue-Langevin, Grenoble, France

Using all-atom molecular dynamics simulations, we study water-mediated interactions between surfaces of various polarities in order to elucidate the relation between the repulsive hydration and attractive hydrophobic forces. We find that the hydration forces are oscillatory in the stiffer membranes, whereas monotonically-decaying in softer ones and they correlate with oscillations in density profiles. Based on the simulations at prescribed chemical potential and the free energy analysis, we determine the "Berg limit" crossover, which delimits the repulsive and attractive regimes. The surface attraction appears as a result of water cavitation, since the liquid water between the membranes becomes metastable with respect to vapor phase. We also show that the attraction repulsion regimes highly correlate with the formation and breaking of overall hydrogen bonds upon bringing the surfaces in close-contact state.