# **BP 19: Biological Membranes II**

Time: Tuesday 14:00–15:15

Lipid Bilayer Membranes

Poly(*N*-isopropylacrylamide)

## Location: ZEU 260

## BP 19.1 Tue 14:00 ZEU 260 on Multistimuli-Responsive Copolymer Cushions —

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To mimic the native environment of a lipid bilayer in respect to the extracellular matrix or intracellular structures, we pursue the approach to use a thin polymer film as bilayer cushion support in order to prevent transmembrane proteins from pinning to the support. With the aim to actively tune transmembrane protein mobility, we first studied the characteristics of a bilayer membrane formed on a stimuli-responsive polymer cushion. Swelling characteristics of thin films of poly(Nisopropylacrylamid-co-carboxyacrylamid) were probed by ellipsometry and quartz crystal microbalance (QCM) and found to switch in thickness between 15 nm and 150 nm depending on monomer composition, pH and temperature. The mobility of lipid bilayer on top of the cushions, as analyzed by fluorescence recovery after photobleaching (FRAP), yielded higher lipid diffusion coefficients ((6.3 - 9.6)  $\mu m^2 s^{-1}$ ) in comparison to solid glass supports ((3.0 - 5.9)  $\mu m^2 s^{-1}$ ) independent of the swelling state of the polymer cushion. This finding revealed a very weak coupling of the lipid bilayer with the polymer cushion. Further, focus of interest is set on the impact of the tunable frictional drag between transmembrane adhesion receptors (integrins) and cushion support, which is expected to influence mobility, activation, and receptor clustering.

BP 19.2 Tue 14:15 ZEU 260

Lipid bilayers interacting with polymer chains — •MARCO WERNER<sup>1,2</sup> and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden, Germany — <sup>2</sup>Technische Universität Dresden - Institut für Theoretische Physik

We apply the bond fluctuation model [I. Carmesin and K. Kremer, Macromol. 21, 2819 (1988)], a lattice-based Monte Carlo method, to study amphiphile bilayers and their interactions with polymers. Hydrophobic interactions are induced by explicit solvent. This allows us to simulate self assembling planar bilayers, vesicles and hydrophobic polymers avoiding artificial freezing effects. We focus on the spectrum of effects which arise when bringing together fluctuating bilayers and flexible polymers of various compositions and hydrophobic interactions. Particular effects like translocation of polymers through membranes [T. Goda, Y. Goto and K. Ishihara, Biomaterials 31, 2380 (2010)] and changes in membrane-permeability [A.L. Lynch, R. Chen, P.J. Dominowski, E.Y. Shalaev, R.J. Yancey Jr. and N.K.H. Slater, Biomaterials 31, 2380 (2010)] have been observed experimentally and might become relevant for drug delivery and cell reprogramming. In our simulations we use the local permeability of the membrane as a measure for the perturbation due to interacting polymers. We found that homopolymers with moderate hydrophobicity get weakly adsorbed hence inducing larger fluctuations. This enhances the permeability for solvent locally. On the other hand, strongly hydrophobic chains are trapped in the hydrophobic layer where they act as stoppers for permeating solvent.

#### BP 19.3 Tue 14:30 ZEU 260

Surface viscosity and intermonolayer friction in a soft, solvent-free model of lipid bilayers — •MARTIN HÖMBERG and MARCUS MÜLLER — Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany

In coarse-grained models of lipid bilayers one integrates out several microscopic degrees of freedom so that the study of membranes comprising thousands of lipids becomes feasible in computer simulations. Thermodynamical, structural, and mechanical properties of biological bilayers can be accurately reproduced in these models. However, the coarse-graining also eliminates degrees of freedom that should appear in the coarse-grained dynamics as dissipation and thermal noise. Hence, the coarse-grained and the actual dynamics may differ severely.

Here we employ a solvent-free, coarse-grained model to analyze two dynamical quantities: the surface viscosity and the intermonolayer friction. We compare the surface viscosity obtained within a Green-Kubo approach with the one obtained from reverse NEMD simulations. The measurement of the intermonolayer friction differs from experiments and simulations with an explicit solvent, therefore we are using a modified version of the SL-theory of the dynamics of bilayer undulations and another Green-Kubo approach for obtaining it.

Finally, we discuss how to map our bead-spring model onto a twodimensional model of coupled monolayers where the lipids are represented by point particles. The interactions and the thermostat are tuned so that it reproduces the RDF and the structure factor, but more importantly also the surface viscosity and the intermonolayer friction.

#### BP 19.4 Tue 14:45 ZEU 260

**Chemical oscillations in cell membranes** — •CHRIS HÄNDEL<sup>1</sup>, UNDINE DIETRICH<sup>2</sup>, SERGIO ALONSO<sup>3</sup>, MARKUS BÄR<sup>4</sup>, and JOSEF KÄS<sup>5</sup> — <sup>1</sup>Division of Soft Matter Physics, University of Leipzig, Germany — <sup>2</sup>Division of Soft Matter Physics, University of Leipzig, Germany — <sup>3</sup>Physikalisch-Technische Bundesanstalt, Berlin, Germany — <sup>4</sup>Physikalisch-Technische Bundesanstalt, Berlin, Germany — <sup>5</sup>Division of Soft Matter Physics, University of Leipzig, Germany

The MARCKS protein is an actin filament cross-linking protein which has relevant functions in different organisms. It is located at the plasma membrane and interacts via electrostatic forces with PIP2 containing cell membranes. In a model membrane, designed by a mixed DPPC/PIP2- monolayer, the binding of MARCKS peptide to the membrane increases the lateral pressure. The unbinding dynamics modulated by PKC generates a reaction-diffusion system. This leads to oscillations of the lateral pressure which can be attributed to changes in the liquid condensed domain size. An adequate and sensitive tool for monitoring these oscillations is the Langmuir trough technique combined with a film balance. The present work confirms the theoretical calculations of this reaction-diffusion system by using model membranes. These calculations describe the dynamic distribution of acidic lipids in response to cytosolic proteins and regulating enzymes. We obtained oscillations in lateral pressure and analyzed the images of the domains depending on the lateral pressure. Furthermore, our results indicate that the oscillations correlate with changes in shape and size of the domains.

BP 19.5 Tue 15:00 ZEU 260 Minimalistic model for bilayer membranes hydrophobic inclusions: application to membrane fusion — GIOVANNI MARELLI<sup>1</sup>, JELGER RISSELADA<sup>2</sup>, and •MARCUS MUELLER<sup>1</sup> — <sup>1</sup>Insitut für theoretische Physik Frederich Hund Platz 1 37077 Goettingen — <sup>2</sup>Max Planck Institute for Biophysical Chemistry, Fassberg 11 37077 Göttingen

We develop a coarse-grained solvent free model to study the interactions of a hydrophobic inclusion with a lipid membrane. For different sets of system's parameters we have calculated the mechanical properties of the self-assembled structures (eg., bending rigidity and line tension of a pore) as well as the phase behavior (lamellar vs inverted hexagonal morphology). We propose two alternative methods to describe a hydrophobic inclusion: a rigid cylinder or a collection of tightly coupled particles and place it in the hydrophobic shell of the membrane. The inclusion induces in the membrane a local ordering of the lipids (e.g. packing effects) and a long-range distortion of the membrane thickness. The surface tension induced by the protein induce pore formation at a certain distance away from its center and the superposition of many proteins result in a stable pore and we present the local pressure profile. This is a first step towards studying the role of the proteins in the fusion process and to understand how their radius and surface tension can select different fusion pathways.