BP 6: Posters: Membranes and vesicles

Time: Monday 17:30–19:30 Location: P3

BP 6.1 Mon 17:30 P3

Modeling vesicular transport in Chromaffin cells — •Daungruthai Jarukanont — university of Kassel, Kassel, Germany

In cell communications, the transport of vesicles is essential for storage and release of chemical messenger molecules. Here, we demonstrate that the statistical analysis of electrophysiological measurements viewed as a time series of spikes permits to determine the equation of motion governing vesicle transport. We perform amperometric measurements of Chromaffin cells for inter-release events interval analysis. Histogram of most recording follow Inverse-Gaussian distribution which can be connected to Brownian motion of particles with a drift term. Therefore we model the vesicles as diffusive particles with external force in membrane direction. Their motion follow over-damped Langevin equation with constant drift velocity, and their density evolve by the corresponding Fokker-Planck equation. The simulations are able to reproduce our and others published experiments in good agreement.

BP 6.2 Mon 17:30 P3

Lipid bilayers on microporous substrates — •Theresa Kaufeld[1], Claudia Steinem[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut - Biophysik, Georg-August Univesität Göttingen — [2]Institut für organische und biomolekulare Chemie, Georg-August Universität Göttingen

We have designed microporous substrates with individually addressable arrays of micrometer-sized apertures for a combination of electrical experiments and fluorescence microscopy, which are also suitable for other techniques such as mechanical manipulation of lipid bilayers. An integrated electrode facilitates access for microscope objectives. We characterized the substrates in terms of surface roughness and pore geometry by SEM and AFM. We then used impedance spectroscopy to characterize the substrate electrically with and without the integrated electrode and measured a resistance in the kilo-Ohm range, which is clearly distinguishable from the Giga-Ohm seal we found with pore-spanning lipid bilayers. Solvent-free lipid bilayers were formed by GUV spreading and imaged with fluorescence microscopy. Electric experiments using alamethicin as a test ion channel showed single-channel resolution.

BP 6.3 Mon 17:30 P3

α-Synuclein insertion into supported lipid bilayer as seen by in situ X-ray reflectivity — •Hendrik Hähl[1], Isabelle Möller[1], Irena Kiesel[2], Dorinel Verdes[1], Christian Sternemann[2], and Stefan Seeger[1] — [1]Institute of Physical Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich — [2]Fakultät Physik/DELTA, TU Dortmund, D-44221 Dortmund

α-Synuclein (αS) is a small 140 residues protein, which is unstructured in its cytosolic form and folds into α-helices upon insertion into the cell membrane. The protein is closely related to the Parkinson disease (PD) via the appearance of aggregates in neuronal cells, which consist mainly of missfolded αS. Yet, neither the normal function of αS nor its role in the pathogenesis of the disease is fully understood. Both seems to be associated with the interaction with the membrane. In its membrane bound form the protein may cause disruption or permeabilization of the membrane. Especially variants appearing in early-onset forms of PD show an increased propensity to membrane destabilization. Here, we applied in situ X-ray reflectivity at high beam energy to monitor the structural changes of supported lipid bilayers upon inclusion of αS and thus aim at a better understanding of the membrane interaction of αS. By comparison with the evolution of a blank bilayer, the wild type form as well as the highly toxic variant E57K were found to intrude deeply into the lipid head groups of the bilayer. Moreover, an observed decrease in the bilayer's thickness due to the protein insertion shows the protein's ability to force a remodeling of the membrane.

BP 6.4 Mon 17:30 P3

Hydration repulsion between membranes and polar surfaces: simulation approaches versus continuum theories — •Matej Kanduc[1], Alexander Schlaich[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Free University Berlin, D-14195 Berlin, Germany — [2]Institut Laue-Langevin, Grenoble, France

A computer all-atom simulation approach for the study of the hydration repulsion between lipid membranes and polar surfaces is presented. We show the main results on repulsive hydration pressures, interaction thermodynamics, and interaction mechanisms. We have a close look at the influence of the experimental boundary conditions on the repulsion mechanisms due to the unfavorable overlap of interfacial water layers. To this end, we analyze several water order parameters in simulations of interacting polar surfaces and compare the results to the predictions of continuum theories.

BP 6.5 Mon 17:30 P3

Coarse-grained simulations of membranes interacting with amyloid fibril forming peptides — •André Kesser and Friederike Schmid — Johannes Gutenberg-Universität Mainz, Mainz

We are developing a generic coarse-grained model to investigate nucleation of amyloid peptides in the presence of lipid membranes. To this end, we combine a simple lipid membrane model developed in our group with a peptide model proposed by S. Auer and coworkers, which is derived from the popular tube model. Both peptides and lipids are represented by linear stiff chains connected by beads, with additional angular potentials, non-bonded Lennard-Jones type interactions and (in the case of peptides) additional hydrogen bonds. Currently we are building a c++ based Software to investigate these models by Monte Carlo and Molecular Dynamics simulations. We describe the model and present first results.

BP 6.6 Mon 17:30 P3

Infrared mapping of membrane proteins with 30 nm lateral resolution — Iban Amenabar[1], •Elmar Hassan Hubrich[2], Joachim Heberle[2], and Rainer Hillenbrand[1] — [1]CIC nanoGUNE Consolider, 20018 Donostia-San Sebastián, Spain — [2]Experimental Molecular Biophysics, Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

Infrared spectroscopy is a common technique to study proteins. However, the diffraction limit prevents resolution on the nanometer scale. Using Fourier transform infrared nanospectroscopy (nano-FTIR), we were able to measure membrane proteins with a lateral resolution of 30 nm.

Nano-FTIR combines scattering-type scanning near-field optical microscopy (s-SNOM) and Fourier transform infrared spectroscopy (FTIR). A metalized tip of an atomic force microscope (AFM) is illuminated with a broadband infrared laser and the backscattered light is analyzed by a Fourier transform infrared spectrometer.

BP 6.7 Mon 17:30 P3

Time-resolved electron tomography reveals how the plasma membrane is reshaped during endocytosis — •Martin Schorb[1], Wanda Kukulski[1,2], Marko Kaksonen[2], and John AG Briggs[1,2] — [1]Structural and Computational Biology Unit, EMBL, Meyerhofstr. 1, 69117 Heidelberg — [2]Cell biology and Biophysics Unit, EMBL, Meyerhofstr. 1, 69117 Heidelberg

Endocytosis is a highly dynamic process that requires a precise temporal and spatial orchestration of multi-component protein modules in order to collect cargo, invaginate the plasma membrane and eventually form an endocytic transport vesicle. Using different pairs of endocytic proteins tagged with GFP and RFP, which act at different stages during endocytosis, we were able to label specific timepoints during the process. By then applying a correlative fluorescence and electron tomography (ET) method, we located specific intermediate stages in 211 individual endocytic budding events, and reconstructed them in 3D. This dataset provides description of plasma membrane (PM) morphology during the transitions from a plane membrane to tubular invagination, through formation of a constricted neck followed by scission of a vesicle. At each timepoint the presence or absence of key protein players is known. This represents a comprehensive, spatiotemporal description of the plasma membrane topology during endocytosis. A multi-parameter analysis of the membrane profile shapes provides quantitative information about how protein modules of the endocytic machinery coordinate the changes in membrane morphology required for vesicle budding in vivo.

BP 6.8 Mon 17:30 P3

Investigation of DPPC-Membranes in the gel phase and

its phase transition in Molecular Dynamics Simulations — •Bartosz Kowalik[1], Alexander Schlaich[1], Emanuel Schneck[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut Laue-Langevin, 6 Rue Jules Horowitz, 38000 Grenoble, France

Membranes in gel phases and melting transitions to the liquid phase have become a topic of increasing interest recently. Experiments and computer simulations have revealed sharp phase transitions in many physical quantities, which still are not completely understood. In our work, we investigate such a membrane consisting of dipalmitoylphosphatidylcholine (DPPC) that forms a lipid bilayer in an aqueous surrounding. We perform Molecular Dynamics Simulations, which allow us to look into atomistic detail of such systems.

We examine in detail the thermodynamic phase transition. Also, we investigate the differences in structure, energy and order parameters, especially we present a framework to derive the bending rigidities of membranes from Molecular Dynamics Simulations.

BP 6.9 Mon 17:30 P3

The role of ions in the Hydration Interaction between polar surfaces — •Alexander Schlaich[1], Matej Kanduc[1], Emanuel Schneck[2], and Roland R. Netz[1] — [1]Fachereich Physik, Freie Universität Berlin, Arnimalle 14, 14195 Berlin — [2]Institut Laue-Langevin, 6 Rue Jules Horowitz, 38000 Grenoble, France

Atomistic computer simulations are an essential tool for the study of the hydration repulsion between biological membranes, which becomes the dominating force at nanometer separations, giving rise to membrane stability. However, the study of interaction pressures, interaction thermodynamics, and interaction mechanisms with computer simulations still is a challenging task as the correct chemical potential of water needs to be accounted for.

We present atomistic simulations of simple polar surfaces in water and analyze the influence of ions present in the water slab at prescribed chemical potential, using Thermodynamic Extrapolation, a technique which has become available only recently. At physiological conditions ions play an important role both for structural and physiological behavior of membranes. We also present their influence on dielectric properties of the water confined between the surfaces and check the applicability of continuum theory on the observed effects.

BP 6.10 Mon 17:30 P3

Environmental effects on diffusion in the Trypanosome membrane — Marius Glogger, Andreas Hartel, Markus Engstler, and •Susanne Fenz — University of Würzburg, Biocenter: Zoology I, Würzburg, Germany

Trypanosomes (T. brucei) are the pathogen of sleeping sickness. They exhibit a surface coat of identical variable surface glycoproteins (VSGs) as protection against the innate immune response of the host. This coat is extremely dense, but also highly dynamic. This ambivalent character is in the focus of our research interest. Here, we will present our insights on the effect of the environmental parameters, ambient medium and lipid matrix, on VSG dynamics as measured by Fluorescence Recovery after Photobleaching (FRAP). In order to perform FRAP on endogenously highly motile trypanosomes they have to be immobilized, e.g. embedded in gelatin gels. To probe whether this condition biases the measurements we performed control experiments in model membranes. Surprisingly, neither the absolute diffusion coefficient nor the mobile fraction was affected. We hypothesize that a low viscosity layer of buffer at the trypanosome-gelatine interface served as a lubricant. Thus, it ensured that the observable diffusion was still dominated by frictional dissipation within the membrane and with neighboring variant and invariant membrane proteins. VSGs are anchored to the cell membrane via a glycosylphosphatidylinositol (GPI) moiety. In a second set of experiments we will characterize the fluidity of the lipid matrix both in the inner and outer membrane leaflet and thus define the framework for a holistic interpretation of VSG dynamics.

BP 6.11 Mon 17:30 P3

Strongly hydrogen bonded water in the hydrophobic tail of lipid bilayers — •Marie Tritschel and Stephan Gekle — Biofluid Simulation and Modeling, Universität Bayreuth

Recent vibrational sum frequency experiments [1] detected strongly hydrogen bonded water molecules at lipid interfaces which were tentatively attributed to hydrogen bonds between water molecules and the phosphate group. However, similar features were also detected in lipids without a phosphate group such as DPTAP.

Using molecular dynamics simulation we show that in addition to water phosphate bonds there exists a sizeable amount of water molecules strongly hydrogen bonded to the carbonyl group in the hydrophobic tail of DPPC. The interaction energy of these bonds is approximately twice as high as in bulk water. Since similar carbonyl groups are also present in DPTAP this may explain the experimental observations.

Finally, we show that the interaction energy of a hydrogen bond is similar when the second binding partner is either water or an atom from a neighbouring lipid, whereas it is higher when the water shares its two hydrogen bonds with the same lipid.

[1] M. Bonn, H. J. Bakker, A. Ghosh, S. Yamamoto, M. Sovago, and R. K. Campen; **132** *J. Am. Chem. Soc.* [2010], 14971

BP 6.12 Mon 17:30 P3

Interaction of amphiphilic triblock copolymers with lipid bilayer membranes: Monte-Carlo simulations — •Hauke Rabbel[1,2], Marco Werner[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden - Institute for Theoretical Physics

Amphiphilic ABA triblock copolymers show interesting behaviour in their interactions with lipid membranes. For example PEO-PPO-PEO, also known under the trademark Pluronics, have found applications in pharmaceutical contexts both as membrane sealents and permeabilizers. Despite their applications, the nature of the interaction with cellular membranes is not yet fully understood. Here we study the interactions of different types of ABA triblock copolymers with lipid bilayer membranes using the bond fluctuation model with explicit solvent[1,2]. We consider polymers with different A- and B-block lengths under variation of the relative hydrophobicities of the constituents. The results indicate that the surface active behaviour of ABA triblock copolymers adsorbed at lipid membranes can be understood by their hydrophilic-lipophilic balance, as supported by recent experimental observations[3]. Triblock copolymers with purely hydrophilic A-blocks and a well chosen hydrophobicity of the B-blocks may find use as membrane-active agents, when fixed in a membrane spanning conformation.

[1] I.Carmesin and K.Kremer, Macromolecules 1988, 21, 2819-2823
[2] M. Werner, J.-U. Sommer, V.A. Baulin, Soft Matter 2012, 8, 11714
[3] Wang, Marks, Lee, Biomacromolecules 2012, 13, 2616-2623