BP 38: Membranes and Vesicles I

Time: Wednesday 9:30–13:00 Location: HÜL 386

Invited Talk BP 38.1 Wed 9:30 HÜL 386

Simulations move toward the understanding of protein-mediated membrane fusion — •Herre Jelger Risselada — Dept of Theoretical Physics, Georg-August University, Göttingen, Germany — Leibniz Inst. of Surface Modification, Leipzig, Germany

Membrane fusion is fundamental for the cycle of life. From the start (sperm fusion), into being (synaptic fusion and intra cellular fusion reactions), toward a possible end (viral infections). Over the last three decennia the process of membrane fusion has been intensively studied by experiments but also by theory. As a matter of fact, theory –at the time in the form of continuum elastic models– has played a dominant role in envisioning the lipidic fusion reaction and its formed intermediates. These insights have lead to the popular stalk-pore hypothesis which still governs our view on membrane fusion up to today. The role of fusion proteins herein was initially confined to bringing the membranes into close apposition by exerting mechanical force to overcome the activation energy barrier. The subsequently formed transition states were considered to be exclusively lipidic. Recent molecular dynamics simulations have contributed to the emerging consensus that such simple and clear-cut separation between the role of the fusion proteins and that of the pure lipid membrane misses their close coupling, which turns out to be essential for a quantitative understanding of protein mediated membrane fusion. Here, I will highlight possible strategies which fusion proteins or involved helper proteins may evoke to overcome the free energy barriers of membrane fusion up to the final opening of the fusion pore.

BP 38.2 Wed 10:00 HÜL 386

Carbon nanotubes mediate fusion of lipid vesicles — •Stephanie Linker, Ramachandra Bhaskara, Martin Vögele, Jürgen Köfinger, and Gerhard Hummer — Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Max-von-Laue Straße 3, D-60438 Frankfurt am Main, Germany

The fusion of lipid membranes is opposed by high energetic barriers. In living organisms, complex protein machineries carry out this biologically essential process. Here we show that membrane-spanning carbon nanotubes (CNTs) can trigger spontaneous fusion of small lipid vesicles.

In coarse-grained molecular dynamics simulations, we find that a CNT bridging between two vesicles locally perturbs their lipid structure. Their outer leaflets merge as the CNT pulls lipids out of the membranes, creating an hourglass-shaped fusion intermediate with still intact inner leaflets. As the CNT moves away from its symmetry axis, the inner leaflets merge, forming a pore that completes fusion. CNT-mediated vesicle fusion offers a fresh perspective on a poorly understood process. Possible applications include the design of new fusion agents, e.g., for the targeted delivery of drugs or nucleic acids.

BP 38.3 Wed 10:15 HÜL 386

Shape remodeling vesicles by localized actin polymerization — •Katharina Henneberg[1], Felix Keber[1], Christian Cyron[1], Jan Faix[2], and Andreas Bausch[1] — [1]Technical University of Munich, Munich, Germany — [2]Hannover Medical School, Hannover, Germany

Interactions between the cytoskeleton and the cell membrane are essential for various cellular processes. Here we reconstitute lamellipodia and filopodia like structures in a bottom up approach inside giant unilamellar vesicles (GUVs). We couple the network from the inside to the lipid membrane of GUVs. By the use of different actin binding proteins (ABPs) we control the binding characteristics of actin to the membrane and the network architecture. One of the key players is Arp2/3, which binds via its activator VCA to the vesicle's membrane. The autocatalytic nature of Arp2/3 and the finite volume of the vesicle result in the formation of patches of a dense actin network, which ultimately leads to pronounced membrane deformations. The capping protein (CP) determines thereby the resulting membrane deformations by finetuning the actin network geometry. We are able to model the formation of the localized networks by kinetic equations, a continuum elastic model suffices to describe the resulting membrane shape deformations.

BP 38.4 Wed 10:30 HÜL 386

Distance-Dependent Structures of Interacting Membranes Displaying Synthetic Polymers and Wild-Type Bacterial Lipopolysaccharides — •Ignacio Rodriguez Loureiro[1], Ernesto Scoppola[1], Victoria Latza[1], Luca Bertinetti[1], Aurelio Barbetta[1,2], Giovanna Fragneto[3], and Emanuel Schneck[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Institut de Chimie Séparative de Marcoule, France — [3]Institut Laue-Langevin, Grenoble, France

Polymer brushes are found on the surfaces of important classes of biological membranes, such as lipopolysaccharides on bacterial outer membranes. The latter mediate the interaction with other bacteria and thus influence the physical properties of bacterial biofilms. But interacting polymer brushes are also of technological relevance, for instance in the field of surface lubrication. The interaction between polymer-decorated surfaces is coupled to the distance-dependent conformation of the polymer chains. This problem has been addressed by theory, but accurate experimental data on polymer conformations under confinement are rare. Here, we utilize neutron reflectometry (NR) to determine the distance-dependent structure of interacting lipid membrane surfaces decorated with hydrophilic poly(ethylene glycol) (PEG) brushes. To gain insight into bacterial interactions in biofilms we also investigate the structure of two interacting surfaces formed by wild-type bacterial lipopolysaccharides with strain-specific O-side chains.

BP 38.5 Wed 10:45 HÜL 386

Pure Protein Bilayers and Vesicles from Native Fungal Hydrophobins — Hendrik Hähl[1], Jose Nabor Vargas[1], Alessandra Griffo[2], Päivi Laaksonen[2], Géza Szilvay[3], Michael Lienemann[3], Karin Jacobs[1], Ralf Seemann[1], and •Jean-Baptiste Fleury[1] — [1]Saarland University, 66123 Saarbrücken, Germany — [2]Aalto University, 00076 Aalto, Finland — [3]VTT Technical Research Centre of Finland, 02150 Espoo, Finland

In this study, a microfluidic approach to generate free-standing, protein bilayers and protein vesicles is presented, which are composed solely of the hydrophobin HFBI, which is a small, amphiphilic protein produced by filamentous fungi. The amphiphilicity of the proteins allows them to self-assemble at any hydrophilic/hydrophobic interface in very stable monolayers. These monolayers are used to generate free-standing bilayers. Employing different fluids in a microfluidic setup, the stability of bilayers in both possible orientations (i.e in the hydrophilic or hydrophobic contact situation) is demonstrated. This allows the creation of hydrophobin membranes between either aqueous, oily, or gaseous compartments. These membranes are then used to produce aqueous, oily or gaseous hydrophobin vesicles by means of the microfluidic jetting technique. The resulting lipid-free vesicles are the first example of vesicles only composed of proteins. With the insertion of functioning gramicidin pores, the foundation for employing these vesicles as a new experimental class of encapsulating platform in synthetic biology is laid.

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30 min break

BP 38.6 Wed 11:30 HÜL 386

Measurements of lateral diffusion of phospholipids in the artificial cell membrane using diamond nanomagnetometry — •Farida Shagieva, Ya Wang, Zhiqin Chu, Andrea Zappe, Felipe Favaro de Oliveira, Andrej Denisenko, Amit Finkler, and Jörg Wrachtrup — 3rd Institute of Physics, University of Stuttgart, Stuttgart, Germany

Nuclear magnetic resonance (NMR) spectroscopy is serving as a powerful tool in physics and life sciences, but is limited by macroscopic sample quantities (several micrometers). Most recently, the shallow nitrogen vacancy centres underneath the surface of diamond chip started to be used to perform nanoscale NMR imaging and spectroscopy of nuclear species under ambient conditions [1]. These multifunctional quantum sensors provide the noninvasive methods to not only get the chemical composition of the molecules but also study the system dynamics in the nanoscopic volume above the diamond surface. The incredibly small size of the detection volume allows to study the membrane structure around each biomolecule individually.

Here we demonstrate the measurements of lateral diffusion of phos-

pholipids in artificial vesicles modelling cell membranes on the top of diamond nanopillars through the correlation spectroscopy protocol. Pillar-shaped photonic structures hosting such NV centers enables not only significantly increase the photon flux in comparison to the bulk diamond, but also provide NMR measurements inside the vesicles.

[1] T. Staudacher, F. Shi, S. Pezzagna et al., Science 339, 561 (2013).

BP 38.7 Wed 11:45 HÜL 386

Rupturing the hemi-fission intermediate in membrane fission: roles of tension and dynamin's conformational changes — •Guojie Zhang and Marcus Müller — Institute for Theoretical Physics, Georg-August University, Göttingen, Germany

Membrane fission is a fundamental process in cell, involved in intracellular trafficking, virus infection, etc. It is a collective phenomenon mediated by proteins (mainly dynamin), in which an initially continuous membrane breaks into two topologically independent membranes. So far, however, its underlying molecular mechanism, especially on the specific role of dynamin in fission, is only incompletely understood. Recent experimental and simulation studies concluded that dynamin-mediated fission proceeds via the formation and rupture of a metastable hemi-fission intermediate by dynamin's conformational changes. The latter is a thermally activated process but the transition state is unknown. Here, we employ computer simulation of coarse-grained models of membrane and dynamin, combined with enhanced sampling techniques, to explore: (a) pathways, free-energy barriers, and the concomitant transition states during the rupture of a protein-free hemi-fission state under tension; (b) dynamin's conformational changes, which could lower the free-energy barriers of rupturing the hemi-fission and thus complete membrane fission.

BP 38.8 Wed 12:00 HÜL 386

High-speed single particle tracking on giant unilamellar vesicles — Susann Spindler, •Martin Kaller, and Vahid Sandoghdar — Max Planck Institute for the Science of Light, Erlangen, Germany

Interferometric scattering detection microscopy (iSCAT) is a powerful method for single particle tracking (SPT) experiments. Recently, we reported on the use of iSCAT for visualizing the diffusion of gold nanoparticles (GNPs) as small as 5nm attached to lipids in model membranes with nanometer lateral precision and at up to 1 MHz frame rate [1]. Here, we demonstrate one of the unique capabilities of iSCAT, namely high axial resolution in tracking the displacement of a nanoparticle and present three-dimensional trajectories of GNP-labeled lipids and unlabeled virus-like particles diffusing on a giant unilamellar vesicle (GUV) membrane. We discuss the differences in the observed diffusion behaviour in this system and compare them to our previous studies in supported bilayers [2].

[1] S. Spindler, J. Ehrig, K. König, T. Nowak, M. Piliarik, H. E. Stein, R. W. Taylor, E. Garanger, S. Lecommandoux, I. D. Alves, V. Sandoghdar, J. Phys. D: Appl. Phys. 49 (2016) [2] C.-L. Hsieh, S. Spindler, J. Ehrig, V. Sandoghdar, J. Phys. Chem. B 118 (2014).

BP 38.9 Wed 12:15 HÜL 386

Solid-supported DMPC multilayers containing cholesterol at high hydrostatic pressure — •Göran Surmeier, Michael Paulus, Paul Salmen, Yury Forov, Susanne Dogan, Lukas Tepper, Benedikt Nowak, Metin Tolan, and Julia Nase — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

A phospholipid bilayer is the basic component of cell membranes, which separates the intracellular and extracellular region. Bilayers undergo pressure- and temperature-induced phase transitions. However, they need their high flexibility, which is given in the liquid phase, to fulfill their biological functionalities. Real membranes are highly complex systems that are interstratified by cholesterol and proteins. Adding cholesterol shifts the phase boundaries of phospholipid bilayers. While these phase transitions were already studied in bulk solutions in detail, the behavior of solid-supported membranes at high hydrostatic pressure is widely unknown.

We present an in-situ high pressure X-ray reflectometry study on the structure of solid supported DMPC bi- and multilayers containing cholesterol in different concentrations. The reflectivities were measured at the solid-liquid interface between silicon and an aqueous buffer solution in a high pressure cell employing pressures up to a maximum of 5000 bar. We observed a decrease of the critical pressure and an expansion of the transition area of the liquid-gel phase transition with increasing cholesterol concentrations at 37°C and were able to determine the cholesterol concentration-dependent behavior of the compressibility of gel phase membranes at 20°C.

BP 38.10 Wed 12:30 HÜL 386

Molecular Dynamics Simulations Elucidate the Tight Cohesion between Glycolipid Membranes — Matej Kanduc[1,2], Alexander Schlaich[2], Alex de Vries[3], Juliette Jouhet[4], Eric Maréchal[4], Bruno Demé[5], Roland Netz[2], and •Emanuel Schneck[6] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin (Germany) — [2]Freie Universität Berlin (Germany) — [3]University of Groningen (The Netherlands) — [4]CEA Grenoble (France) — [5]Institut Laue-Langevin, Grenoble (France) — [6]Max Planck Institute of Colloids and Interfaces, Potsdam (Germany)

Membrane systems that naturally occur as densely packed membrane stacks contain high amounts of glycolipids whose saccharide headgroups display multiple small electric dipoles in the form of hydroxyl groups. Experimentally the hydration repulsion between glycolipid membranes is of much shorter range than that between phospholipids whose headgroups carry single large electric dipole due to the zwitterionic charge distribution. Using solvent-explicit Molecular Dynamics simulations and accounting for the water chemical potential, we quantitatively reproduce the experimentally observed, different pressure-versus-distance curves of membrane stacks composed of phospholipids and of the glycolipid digalactosyldiacylglycerol (DGDG). We show that the short-ranged water uptake into the glycolipid membranes is solely driven by the hydrogen-bond balance involved in non-ideal water/sugar mixing. Water structuring effects and lipid configurational perturbations, responsible for the more long-ranged repulsion between phospholipid membranes, are inoperative for the glycolipids.

BP 38.11 Wed 12:45 HÜL 386

DNA-oligomers as model likers for membrane adhesion — •Mohammad Kamal[1], Franck Thibaudau[1], Ana-Sunčana Smith[2], and Kheya Sengupta[1] — [1]Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Aix - Marseille Université-CNRS UMR 7325, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, France — [2]PULS Group, Department of Physics and Cluster of Excellence: EAM, Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, Germany

In the last decade, DNA-linkers have been extensively used as selective glue to tune inter-colloidal interactions with the aim of creating new meta-materials which exploit the versatility of DNA. Here we take a similar approach to use the power of DNA origami to test ideas in the context of model membrane adhesion. We use Reflection Interference Contrast Microscopy (RICM) to quantify the interaction between the membrane of a giant unilamellar vesicle and a supported lipid bilayer employing short DNA sequences as linkers. The linker-length was varied independently of its biding affinity. The linker flexibility was also varied by using either single (ss) or double stranded (ds) DNA. For ds-DNA, the separation (d) between the two interacting membranes is smaller than or equal to the linker length. For corresponding ss-DNA, d is always smaller. The linker-length influences the adhesion strength only at low concentrations, and for a given length, ds-DNA is a more efficient binder than ss-DNA. We also explore the possibility of adhesion induced phase separation using binary-mixtures of linkers. The results are interpreted in terms of a thermodynamic model.