CPP 43: Membranes and Vesicles I (joint session BP/CPP)

Time: Wednesday 9:30–13:00

Location: H 1028

CPP 43.1 Wed 9:30 H 1028 Actin polymerization driving localized membrane deformation — •Remy Kusters¹, Camille Simon¹, Jean-Francois Joanny^{1,2}, Cecile Sykes¹, and Pierre Sens¹ — ¹Institut Curie, Paris, France — ²ESPCI, Paris, France

The actin cytoskeleton is able to exert both pushing and pulling forces on the cell membrane, mediating processes such as cellular motility, endocytosis and cytokinesis. In order to investigate the exclusive role of actin dynamics on membrane deformations, the actin dynamics is reconstituted on the outer surface of a deformable liposome. Depending on the elasticity of the membrane and the forces generated by the actin polymerization, both tubular extrusions (i.e. towards the actin cortex) and localized spike-like protrusions occur along the surface of the liposome. In this talk I present a theoretical model where uniform actin polymerization can drive localized membrane deformations and show how polymerization kinetics and membrane/cortex mechanics impact their size and stability.

CPP 43.2 Wed 9:45 H 1028

Modeling the flat-to-curved transition during clathrinmediated endocytosis — •Felix Frey¹, Delia Bucher², Kem Sochacki³, JUSTIN TARASKA³, STEEVE BOULANT², and ULRICH Schwarz¹ — ¹Institute for Theoretical Physics, Heidelberg University — ²Department of Infectious Diseases, Virology, University Hospital Heidelberg — ³NIH, Bethesda, U.S.A.

Clathrin-mediated endocytosis (CME) is essential for the cellular uptake of nutrients and receptors. Although CME has been studied for decades, the exact sequence of molecular and structural events remains elusive. Two basic models have been suggested for the way CME proceeds. (1) In the constant curvature model, it is assumed that clathrin-coated pits grow with constant curvature, determined by the geometry of clathrin triskelia. (2) In the constant area model, it is assumed that clathrin triskelia first assemble into flat hexagonal arrays that later invaginate with a constant surface area. This second model implicitly assumes that during bending, some hexagons are converted into pentagons. Here, we integrate data sets from correlative electron and light microscopy and quantify the sequence of ultrastructural rearrangements of the clathrin coat during endocytosis in mammalian cells with the help of some simple mathematical growth laws. Our analysis shows that clathrin-coated structures initially grow flat but start to acquire curvature when 70% of the final clathrin content is reached. Hence, our analysis suggests that elements of both suggested models are present and that mechanical and cellular factors will decide about the relative weights of growth versus curvature formation.

CPP 43.3 Wed 10:00 H 1028

Formation and Stabilization of Pores in Bilayer Membranes by Peptide-like Amphiphilic Polymers — •ANKUSH CHECKERVARTY^{1,2}, MARCO WERNER^{1,3}, and JENS UWE SOMMER^{1,2} — ¹Leibniz-Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany — ²Institute of Theoretical Physics, Technische Universitat Dresden, Germany — ³Universitat Rovira i Virgili, Departament dEnginyeria Quimica, Av. Paisos Catalans 26, 43007 Tarragona, Spain

We study pore formation in models of lipid-bilayer membranes interacting with amphiphilic copolymers mimicking anti-microbial peptides using Monte Carlo simulations rationalized by a simple brush-model for the fluid membrane. In our study at least a weak tension on the membrane is required to observe pore-formation induced by the adsorption of flexible amphiphilic copolymers. The copolymers enhance the pore stability by decreasing the line tension due to weak adsorption along the rim of the pore. Pore formation is enhanced with increasing length of copolymers or stronger stretching of the membrane. Both solvent and copolymer permeability increase as the pore becomes stable. Pore-formation proceeds via a meta-stable pore-state according to adiscontinuous phase transition scenario which lead to finite poresizes at once. Our generic model of copolymer-induced pore-formation does not require high polymer concentration at the pores nor any selforganization of the copolymers to open the pore.

CPP 43.4 Wed 10:15 H 1028 Shapes of red blood cell doublets — •Masoud Hoore, DMITRY A. FEDOSOV, and GERHARD GOMPPER — Theoretical Soft Matter and Biophysics, Institute of Complex Systems, Forschungszentrum Juelich GmbH

Red blood cell (RBC) aggregates play an important role in determining blood rheology. RBCs in solution interact attractively to form various shapes of RBC doublets. Here, the attractive interactions can be varied by changing the solution conditions. A systematic numerical study on RBC doublet formation is performed, which takes into account the shear elasticity of the RBC membrane due to the spectrin cytoskeleton, in addition to the bending rigidity. The results are obtained from molecular dynamics simulations of triangulated surfaces considering thermal effects. The phase space of the RBC doublet shapes in a wide range of adhesion strengths, reduced volumes, and shear elasticities is obtained. Experimental images of RBC doublets in different solutions show similar configurations. Furthermore, it is shown that rouleau formation is affected by the doublet structure. It is shown that the shear elasticity of the RBC membrane changes the doublet phases significantly.

 $CPP \ 43.5 \ \ Wed \ 10:30 \ \ H \ 1028$ Conditions of Spontaneous Translocation of Individual Nanotube Porin Through a Phospolipid Bilayer — Yachong Guo^{1,2}, Marco Werner², Ralf Seemann³, Vladimir Baulin², and •Jean-Baptiste Fleury³ — ¹Nanjing University, Nanjing , China — ²Universitat Rovira i Virgili, Tarragona, Spain — ³Saarland Univsersity, Saarbruecken, Germany

Single ultra-short nanotubes can be inserted in cell membrane to be used as a membrane nanosensor or to form artificial ionic channels. Recent studies reported that ultra-short nanotubes can passively be inserted perpendicularly to the lipid bilayer core. After this insertion, it is commonly expected that these ultra-short nanotubes should stay trapped into the lipid bilayer core as its represents a potential well. In contrast to such expectations, we investigate the possible conditions that could lead a single nanotube to translocate spontaneously across a lipid bilayer. We demonstrate that membrane stretching and subnanometer nanotube, are essential to enable this type of translocation, while no translocations are occurring in lipid bilayers under low tension. The proof of this tension-dependent translocation event is obtained by observating directly a single nanotube quitting a highly stretched lipid bilayer. A quantitative analysis of the kinetic pathway associated to this translocation event is measured by using a specially designed microfluidic device combining optical fluorescence microscopy with simultaneous electrophysiological measurements.

 $\label{eq:constraint} CPP \ 43.6 \ \ Wed \ 10:45 \ \ H \ 1028$ Membrane fluctuations of malaria-infected red blood cells — •JULIA JÄGER^{1,2}, BENJAMIN FRÖHLICH³, MOTOMU TANAKA³, MICHAEL LANZER⁴, and ULRICH SCHWARZ^{1,2} — ¹Institut für Theoretische Physik, Universität Heidelberg — ²Bioquant, Universität Heidelberg — ³Institut für Physikalische Chemie, Universität Heidelberg — ⁴Parasitologie, UniversitätsKlinikum Heidelberg

Once inside the body, malaria parasites invade red blood cells in order to hide from the immune system and to digest hemoglobin. Over the course of 48 hours the parasite completely remodels the red blood cell, so that the cell becomes round and stiff and eventually breaks open. One way to monitor this remodeling process is the measurement of the cell membrane's flickering spectrum, which is a standard approach to extract the mechanical properties of cell membranes. In addition to the usual interface Hamiltonian for the membrane, we take into account the connections between the outer lipid bilayer and the spectrin network underlying the plasma membrane, which are known to become increasingly clustered over the course of the infection. We focus on the confinement parameter in the interface Hamiltonian and show how it scales with the number and strength of the connections. Finally, we compare our results with experiments.

15 min. break

Invited Talk CPP 43.7 Wed 11:15 H 1028 Computer simulation of collective phenomena that alter the topology of membranes — •MARCUS MÜLLER — Georg-Auguist-Universität Göttingen, Institut für Theoretische Physik, Göttingen,

Germany

Using computer simulation and self-consistent field theory of coarsegrained models for lipid membranes, we study the free-energy landscape of collective phenomena that alter the topology of lipid membranes. These basic processes - pore formation, fusion and fission often involve time scales of tens of nanometers and milliseconds that are large for atomistic simulation. Frequently, they involve transition states with high curvatures that are difficult to describe by Helfrichlike models. Coarse- grained models can access the relevant time and length scales, allow for a systematic exploration of parameters like the lipid architecture or membrane tension, and they are well suited to study collective phenomena that alter the topology of membranes.

The talk will discuss different computational techniques - Wang-Landau sampling, field-theoretic umbrella sampling, and the string method - to investigate metastable intermediates (like the stalk in the course of membrane fusion) and transition states of pore formation, membrane fusion and fission. Using coarse-grained models, we explore the universal aspects of topology-altering processes in membranes and comment on the extent, to which coarse-grained model capture specific effects of protein-mediated processes.

CPP 43.8 Wed 11:45 H 1028

Formation of Coatless Membrane Vesicles — •SUSANNE LIESE¹, ROSSANA ROJAS¹, EVA WENZEL², CAMILLA RAIBORG², HARALD STENMARK², and ANDREAS CARLSON¹ — ¹University of Oslo, Department of Mathematics — ²Oslo University Hospital, Institute for Cancer Research

The formation of membrane vesicles is an important part of various processes in cell biology. Among others, cells use vesicle formation as an uptake mechanism for controlling their activity and to communicate with other cells through the cargo material that is encapsulated in the membrane vesicle. It all starts with a small initial deformation of the membrane, which subsequently grows and leads to the formation of a vesicle. This dynamic process is induced by membrane associated proteins, which generate forces within the membrane. Membrane compartments inside the cell, such as the endosome, form coatless vesicles but the force generating membrane proteins are not becoming a part of the vesicle. To understand this process, we develop an elastic membrane model to study the biophysical origin of coatless vesicle formation. Our results highlight how elastic membrane parameters and transmembrane proteins determine the shape of the deformed membrane and the equilibrium size distribution of vesicles.

CPP 43.9 Wed 12:00 H 1028

Outperforming nature: synthetic enzyme built from DNA flips lipids of biological membranes at record rates •Alexander Ohmann¹, Chen-Yu Li², Christopher Maffeo², KAREEM AL NAHAS¹, KEVIN N. BAUMANN¹, KERSTIN GÖPFRICH¹ JEJOONG YOO², ULRICH F. KEYSER¹, and ALEKSEI AKSIMENTIEV² ^{- 1}Cavendish Laboratory, University of Cambridge, Cambridge, UK —²University of Illinois at Urbana-Champaign, Champaign, IL, USA Mimicking enzyme function and increasing performance of naturally evolved proteins is one of the most challenging and intriguing aims of nanoscience. Here, we employ DNA nanotechnology to design a synthetic enzyme that substantially outperforms its biological archetypes. Consisting of only eight strands, our DNA nanostructure spontaneously inserts into biological membranes by forming a toroidal pore that connects the membrane's inner and outer leaflets. The membrane insertion catalyzes spontaneous transport of lipid molecules between the bilayer leaflets, rapidly equilibrating the lipid composition. Through a combination of microscopic simulations and single-molecule experiments we find the lipid transport rate catalyzed by the DNA nanostructure to exceed 10^7 molecules per second, which is three orders of magnitude higher than the rate of lipid transport catalyzed by biological enzymes. Furthermore, we show that our DNA-based enzyme can control the composition of human cell membranes, which opens new avenues for applications of membrane-interacting DNA systems in medicine.

CPP 43.10 Wed 12:15 H 1028

Membrane-mediated interactions between inclusions: the role of shape and background curvature $-\bullet$ AFSHIN VAHID¹, ANDELA SARIC², and TIMON IDEMA¹ — ¹TU Delft, Delft, the Netherlands — ²University Collage London (UCL), London, United Kingdom Lipid membranes are vital to cell function. Their combination of fluid and elastic properties allows cells to cope with an out of equilibrium environment. Consequently, membranes exhibit a large variety of shapes, ranging from simple spherical liposomes to complex tubular networks. These shapes are regulated by protein inclusions, that can act both as curvature sensors and curvature inducers. We model the interaction between such inclusions in curved lipid bilayers. We show that in contrast to flat membranes, the inclusions can attract each other and collectively form biologically relevant patterns. For example, we find that even identical inclusions can spontaneously form rings on closed membranes, and those rings again act as curvature sensors. We further demonstrate that the curvature sensing and curvature inducing property of proteins are two sides of the same coin, depending on protein density. In particular, proteins can constrict tubular membranes and facilitate their splitting. This feature was recently observed in mitochondria, and can prevent entanglement with tubes of the ER network also present in the cell.

CPP 43.11 Wed 12:30 H 1028 Membrane curvature and nanobuds generated by lipids with bulky head groups — •APARNA SREEKUMARI and REINHARD LIPOWSKY — Theory and Bio-systems, Max Planck Institute of Colloids and Interfaces Golm, D-14424 Potsdam, Germany

We study the mechanical and curvature-elastic properties of bilayer membranes with compositional asymmetry by molecular simulations. The compositional asymmetry is achieved by inserting lipids with a bulky head group into one leaflet (or monolayer) of the bilayer. As we increase the mole fraction ϕ_1 of the bulky-head lipids, we observe a remarkable evolution of the stress profile across the bilayer and a strong increase in the first moment of this profile. In order to extract the spontaneous curvature from this moment, we also determine the bending rigidity of the bilayer which is found to exhibit a non-monotonic dependence on ϕ_1 . The latter behaviour reflects changes in the mean density of the lipid tails and head groups. The resulting spontaneous curvature is found to be quite large compared to other molecular mechanisms for bilayer asymmetry. The generated curvature leads to the formation of nanobuds, which provide new membrane compartments, in close analogy to cellular budding processes.

 $\label{eq:CPP 43.12} \mbox{ Wed 12:45 } \mbox{ H 1028} \\ \mbox{Formation and phase transitions of vapour deposited phospholipid bilayers on porous silicon substrates — Nicolas Moraga¹, Marcelo Cisternas¹, Diego Diaz¹, Rodrigo Catalan¹, Maria J. Retamal², Tomas P. Corrales³, Mark Busch⁴, Patrick Huber⁴, Marco Soto-Arriaza², and •Ulrich G. Volkmann¹ — ¹Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — ²Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — ³Department of Physics, UTFSM, Valparaiso, Chile — ⁴TUHH, Hamburg, Germany$

Study of phospholipid artificial membranes on solid substrates has become a relevant way to gain insight into the physical behaviour of cell membranes. In this work, porous silicon substrates (pSi) were made using a two-electrode cell to produce different pore diameters. Substrates were characterized with Field Emission Electron Microscopy. The phospholipid (DPPC) was deposited in high vacuum from the gas phase on the pSi. Film thickness was controlled using Very High Resolution Ellipsometry (VHRE). Samples were hydrated in air with ultrapure water to assemble the bilayer. Phase transitions were measured with VHRE and Stray Light Intensity during temperature cycles. AFM was used to study morphological changes of bilayers as a function of temperature. Our results open new ways to hydrate lipid bilayers using pSi with a specific pore diameter. Acknowledgements: Postdoctoral FONDECYT #3160803 (MJR), FONDECYT #1141105 (UGV) and #1171047 (MSA), FONDECYT INICIACION #11160664 (TPC), CONICYT Fellowships (RC, MC) and CONICYT-PIA ACT 1409.