BP 24: Posters: Membranes and vesicles

Time: Tuesday 14:00–16:00 Location: Poster A

BP 24.1 Tue 14:00 Poster A

The crossover from hydration repulsion to cavitation-induced attraction between asymmetric hydrophilic and hydrophobic surfaces — •Matej Kanduc and Roland Netz — Department of Physics, Free University Berlin

Utilizing all-atom molecular dynamics simulations at constant water chemical potential in combination with basic scaling arguments, we study hydration-induced interactions between two overall neutral yet polar planar surfaces with different wetting properties. Whether the water film between the two surfaces is unstable and cavitation gives rise to long-range attraction, depends on the sum of the two individual surface contact angles. Consequently, cavitation-induced attraction also occurs between a hydrophobic surface and a mildly hydrophilic surface. If both surfaces are hydrophilic, hydration repulsion prevails. In between the regimes of cavitation-induced attraction and hydration repulsion we find a narrow range of contact angles where the two surfaces adhere without cavitation. The extent of this regime depends on the inter-surface adhesion properties. Simple scaling laws for the onset of cavitation and the adhesion transition are presented and favorably compared with simulations in a generic phase diagram as a function of the two surface contact angles.

BP 24.2 Tue 14:00 Poster A

Modelling the Red Blood Cell membrane — •Daniel Schmidt[1,2], Udo Seifert[2], and Ana-Sunčana Smith[1] — [1]Inst. f. Theor. Physik and Excellence Cluster "Engineering of Advanced Materials", Universität Erlangen-Nürnberg — [2]II. Inst. f. Theor. Physik, Universität Stuttgart

The outer shell of a Red Blood Cell (RBC) is understood as a flexible membrane with the underlying cytoskeletal network of spectrin fibres. The spectrin network is connected to the membrane at specific junctions of the network. Thereby, the connections between the spectrin network and the membrane open and close stochastically which is actively regulated. In experiments, with advanced microscopic techniques, the membrane spectrum is measured without detailed knowledge about the underlying network.

We model the flexible membrane by the famous Helfrich-Hamiltonian with bending rigidity and membrane tension, whereas the connections to the spectrin network are simple harmonic springs. More precisely, we investigate an almost planar segment of the RBC membrane and the connections open and close stochastically accordingly to the binding affinity. With this model, we look at the experimentally accessible membrane spectrum. Moreover, in a continuum approach, we compare our results to an often used membrane model with a harmonic interaction instead of connections to the spectrin network.

BP 24.3 Tue 14:00 Poster A

Analysis of rheological properties of dense capsule suspensions using boundary element method — Daiki Matsunaga, •Yohsuke Imai, Takami Yamaguchi, and Takuji Ishikawa — 6-6-01, Aramaki Aza Aoba, Aoba ku, Sendai, Japan

A capsule is a liquid drop enclosed by thin, deformable membrane. Biological cells and membrane-bounded drugs can be thought of as capsules. Since it is important to understand the rheology of capsule suspensions such as blood, a number of studies have been conducted to clarify the viscosity of capsule suspensions. However, it is still unknown that how the capsule will change its contribution of viscosity increase, when changing the volume fraction of capsules. We present a numerical analysis of a dense capsule suspension with volume fraction varying from 0 to 30%. In order to speed up the computation of boundary element method, we utilized GPU computing for the simulation. The results show that volume fraction increase leads to an increase in the deformation of the capsule, while reducing the orientation angle with respect to the velocity direction. We also report how these changes in capsule deformations would affect the bulk rheology of the suspension.

BP 24.4 Tue 14:00 Poster A

How perfluorooctanoic acid inserts into a biomimetic model membrane — •Beate-Annette Brüning[1,2], Martin Kreuzer[1,3], and Roland Steitz[1] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Delft University of Technology, Delft, Netherlands — [3]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Perfluorinated compounds are found as biproducts of a wide range of industrial products. Upon entering cellular membranes, the compounds are known to cause developmental and reproductive disorders. We mimick the bioaccumulation in these membranes by inserting the perfluorinated surfactant PFOA into a DMPC phospholipid bilayer. We study changes in the membrane interface structure by X-ray diffraction and neutron reflectometry. We discuss our findings in the light of varying scattering contrasts: taking advantage of the C/F-contrast using X-ray diffraction, we probe the insertion of the perfluorinated surfactant into the phospholipid bilayer interior. We further observe changes in the thickness of the inter-bilayer hydration water layer using neutron reflectivity and H2O/D2O exchange. The combined X-ray and neutron scattering experiment suggests two main effects of PFOA-insertion into the membrane: i) changes in lipid acyl chain ordering combined with bilayer leaflet approximation, ii) 'drying' of the membrane (thinning of hydration water layer). We discuss, how both effects could contribute to a previously observed rigidification of the membrane through the perfluorooctanoic acid [1].

[1] B. Brüning and B. Farago; Perfluorooctanoic acid rigidifies a model lipid membrane; Physical Review E 89, 040702(R) (2014).

BP 24.5 Tue 14:00 Poster A

UV induced Polymerization of Phospholipids at Langmuir Blodgett Through — •Roland Hillmann, Marius Dotter, Sören Grannemann, Lukas Galla, Andy Sischka, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

We investigate the translocation of macromolecules like ssDNA through biological nanopores with Optical Tweezers force mechanics. Therefore Alpha-Hemolysin biopores are integrated into supported bilayer lipid membranes (BLM) or into polymerized lipid-bilayers. This will be accomplished either by the black lipid painting method, or by a liquid-solid Langmuir-Blodgett transfer with subsequent UV light polymerization of the phospholipids containing diacethylene. The high stability of the BLM allows an analyzation by AFM or HIM.

BP 24.6 Tue 14:00 Poster A

Exocytotic activity of living cells imaged with surface plasmon resonance microscopy — Stephan Michael, •Matthias Gerhardt, and Carsten Beta — Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam, Germany

Surface plasmon resonance microscopy allows for imaging of the complex refractive index at gold-liquid interfaces. The complex refractive index of the interface mainly depends on the molecular composition of the samples attached to the gold surface regarding its charge and density. In our case Dictyostelium cells were sedimented onto a gold surface to study the cell-substrate interface. In the region of cell-surface attachment, we observed transient localized events characterized by a step-like change in the complex refractive index at the gold-liquid/cell interface. The duration of such events was found to be within 1-2 sec. In the surface plasmon resonance image, those events mostly appeared as disc-shaped objects with a diameter of about 1-2 um within the region of the cell-substrate interface. While sedimented cells displayed such events spontaneously but rarely, a hypoosmotic shock was found to trigger a significantly higher rate of events. Dictyostelium cells equilibrate their osmolarity by releasing dispensable ions into the extracellular space using their contractile vacuole. Since the area of the observed disc-shaped events was found to be within the size of intracellular vesicles (which have been observed in the same cells using bright field microscopy) we conclude that exocytotic activity of the contractile vacuole can be observed by surface plasmon resonance microscopy.

BP 24.7 Tue 14:00 Poster A

Three-dimensional fluorescence-free tracking of a nanoparticle on a giant unilamellar vesicle — •Susann Spindler, Jens Ehrig, and Vahid Sandoghdar — Max-Planck-Institute for the science of light, Erlangen, Germany

Among the diversity of model membrane systems, giant unilamellar vesicles (GUVs) represent a favourable model system for a cell membrane because of their compatible sizes and shape. Furthermore, GUVs

provide a convenient platform for studying basic membrane phenomena in a model system without the artefacts of a substrate. We report on using interferometric scattering (iSCAT) microscopy as a fluorescence-free technique to study the three-dimensional diffusion of single particles such as virus particles and gold particles attached to lipids on a GUV. iSCAT is based on measuring the interference of the Rayleigh scattering with a reference light beam and allows for high temporal resolution as well as nanometer precision in particle tracking. Moreover, iSCAT provides high-resolution information on the axial displacement of the particle, allowing one to map the curved GUV surface. We compare our observations of lipid diffusion in GUVs with those in supported lipid bilayers [1].

[1] C.-L. Hsieh, S. Spindler, J. Ehrig, and V. Sandoghdar, J. Phys. Chem. B 118 (2014)

BP 24.8 Tue 14:00 Poster A

Direct Measurement of Mechanical Properties of Unsupported Lipid Bilayer under Hydrodynamic Deformation — •Cornelia Walter[1], Michael Hein[1], Ralf Seemann[1,2], and Jean-Baptiste Fleury[1] — [1]Saarland University, Experimental Physics, Saarbruecken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Mechanical properties of lipid membranes like inter-monolayer friction or surface viscosity are important for several biological processes like cell migration, synovial articular motion or cell mechanism in general. The mechanical properties of lipid bilayers were experimentally investigated in detail by Evans and co-workers in the 90's. However, the for these studies vesicles or on supported bilayers were used which question their bio-relevance. Here, we present a new strategy to investigate mechanical properties of free-standing lipid bilayers using hydrodynamic deformation in microfluidic chips.

BP 24.9 Tue 14:00 Poster A

Giant Unilamellar Vesicles as Biological Microreactors — •Anna Lippert[1,2], Navid Bonakdar[1], and Vahid Sandoghdar[1] — [1]Max Planck Institute for the Science of Light , Günther-Scharowsky-Str. 1 D-91058 Erlangen — [2]Friedrich- Alexander Universität Erlangen-Nürnberg, Schloßplatz 4, 91054 Erlangen

The goal of our project is the establishment of a biological microreactor, enabling the production of complex metabolites. As a first simple system we report on our efforts to incorporate the necessary enzymes and transporter proteins to import and convert sucrose into glucose-6-phosphat in a giant unilamellar vesicle (GUV). We aim to use this platform to study confined kinetics, diffusion and transporter activity under controlled conditions.

BP 24.10 Tue 14:00 Poster A

Fabrication of Giant Unilamellar Vesicles — •Hannah Stein[1,2], Susann Spindler[1], and Vahid Sandoghdar[1] — [1]Max Planck Institute for the Science of Light Günther-Scharowsky-Str. 1 D-91058 Erlangen — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg D-91058 Erlangen

Giant Unilamellar Vesicles (GUVs) offer a useful model system for studying fundamental biophysical properties such as lipid diffusion or the interaction of proteins or viruses with membranes. A variety of fabrication methods for GUVs in low ionic solutions already exist, however the formation of giant vesicles under physiological conditions still poses a challenge. We present methods for preparing GUVs in the range of 50-100um diameter in high ionic buffers with different osmolarity using electroformation on ITO covered glasses or lipid swelling on a polymer layer.

BP 24.11 Tue 14:00 Poster A

Comparison of the hydration repulsion between lipid bilayers in MD simulations and experiments. — •Bartosz Kowalik[1], Emanuel Schneck[2], Matej Kanduč[1], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Biomaterials Department, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany

Experiments performed in the last decades gave insight into the nature of the hydration repulsion between lipid membranes. With our Molecular Dynamics Simulations, we want to link the results of the experiments with a theoretical foundation. In particular we investigate the entropic and enthalpic contribution of the interaction between hydrated membranes. We also analyse the structural parameters of the membranes at different hydration levels and discuss our results for both the fluid as well as the gel phase by comparing them to the experimental data.

BP 24.12 Tue 14:00 Poster A

Formation and study of TiN coatings on titanium substrate using plasma immersion ion implantation for applications in biological membranes — Marcelo Cisternas[1,2], Alvaro Henrriquez[1,2], Heman Bhuyan[1,2], Maria Retamal[1,2], Mario Favre[1,2], •Ulrich Volkmann[1,2], Darina Manova[3], Stephan Mandl[3], and Fernando Guzman[4] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]CIEN-UC, Santiago, Chile. — [3]Leibniz-Institut für Oberflächenmodifizierung, Leipzig, Germany — [4]4Depto. De Fisica FCFM, Universidad de Chile, Santiago, Chile

Artificial membranes represent models of the behavior of their biological counterparts. The objectives of this study are the formation and study of a biocompatible environment that serves as a support and ensure stability in phospholipids membranes. In this work was formed and analyzed experimentally a system composed of DPPC / CH / TiN + TiO2 / Ti, where DPPC is the phospholipid previously studied [J. Chem. Phys. 141, 104201 (2014)], chitosan CH , which acts as hydrating matrix for the phospholipid and TiN + TiO2 is the biocompatible surface of titanium Ti. The substrate used was Ti, material widely used in biomedical applications, but requires biocompatible coatings to be used in critical areas like implants. Coatings of titanium nitride (TiN) besides having well known properties of hardness, increase the corrosion resistance and maintain the biocompatibility of titanium.

BP 24.13 Tue 14:00 Poster A

Receptor-mediated wrapping of nanoparticles — •Karandeep Singh, Sabyasachi Dasgupta, Thorsten Auth, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Cargo is internalized by biological cells using different internalization processes, e. g. endocytosis, phagocytosis, and pinocytosis. In all cases, the cargo is inside a carrier that interacts with the membrane. Towards the understanding of these processes, we tackle the internalization of a carrier using a minimalistic model of a spherical nanoparticle with attached ligands, a lipid bilayer membrane, and receptors that mediate the interaction between membrane and nanoparticle.

In our model, we calculate the deformation energy of the fluid membrane using the Helfrich Hamiltonian. The receptors on the membrane bind to the ligands on the nanoparticle, which we take into account using the binding energy and the entropy terms for the free energy of the receptors. For a given fraction of the particle being wrapped by the membrane, we obtain an optimum number of bound receptors at equilibrium. The number of bound receptors depends on the overall receptor density on the membrane, the binding energy gain per receptor, and the area of the membrane that is not bound to the particle. For receptor-mediated adhesion, we find that the transition between unwrapped and completely-wrapped states occurs gradually via partially-wrapped states.

BP 24.14 Tue 14:00 Poster A

Monte-Carlo 2D Model of Bilayer System — •Davit Hakobyan and Andreas Heuer — WWU Münster, Institut für Physikalische Chemie, Münster, Germany

Various Molecular Dynamics (MD) and 2D Monte-Carlo systems were proposed for investigation of the processes in model bilayer systems. Particularly, with help of a relatively simple 2D 3-particle lattice model the phase separation of saturated and unsaturated lipids and cholesterol was demonstrated [Reigada et al. 2008, DOI: 10.1063/1.2817333]. In this lattice model, however, different lipids and cholesterol were only differentiated by the size of the pair-wise interaction and lacked specific properties of lipids and cholesterol.

Here we introduce 2D models of basic bilayer components where their characteristic properties are taken into account. In this model the individual particles of the 2D system present lipids or cholesterol with additional information about the order parameter of the alkyl chain. The free energy of this system is decomposed into separate and carefully chosen entropic and enthalpic parts. The parameters and the balance of entropy and enthalpy for this 2D model were checked against the all-atom MD simulations to certify the adequateness. We further adapt the model to be able to observe phase separation of a ternary system with saturated and unsataurated lipids and cholesterol.

In this way we can systematically explore the range of compositions and molecular properties for which phase separation is possible.

BP 24.15 Tue 14:00 Poster A

Hydration interaction of charged polar surfaces — •Alexander Schlaich[1], Matej Kanduc[1], Emanuel Schneck[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany — [2]Max Planck Institut für Kolloid- und Grenzflächenforschung, D-14476 Potsdam, Germany

We study the hydration interactions between polar surfaces as a model for lipid membranes using atomistic computer simulations at prescribed water chemical potential and analyze interaction pressures, interaction thermodynamics, and interaction mechanisms.

The overlap of interfacial water layers is analyzed via several distinct water order parameters and compared with predictions of simple continuum theories. We further investigate the electrostatic interaction between charged model membrane surfaces in the presence of counter ions and show that continuum models can successfully describe Coulombic interactions. To this end, we also analyze the dielectric properties of the interfacial water and examine the solvation of salt in water under confinement.

BP 24.16 Tue 14:00 Poster A

Numerical simulation of endocytosis - Continuum models of membranes with curvature-inducing molecules — •Sebastian Aland[1], John Lowengrub[2], and Jun Allard[2] — [1]Institut für wissenschaftliches Rechnen, TU Dresden, Germany — [2]Department of mathematics, University of California Irvine, USA

We present new diffuse interface models for the dynamics of inextensible vesicles in a viscous fluid. A new feature of this work is the implementation of the local inextensibility condition by using a local Lagrange multiplier harmonically extended off the interface. To make the method even more robust, we develop a local relaxation scheme that dynamically corrects local stretching/compression errors, thereby preventing their accumulation. We present numerical results that confirm the effectiveness of the proposed models in a test case scenario of vesicles in shear flow. Finally we apply the model to a problem of clathrin-mediated endocytosis. Clathrin proteins attach to the membrane and alter locally its bending stiffness and spontaneous curvature. This process can lead to budding and pinch-off of small vesicles. First numerical simulation results will be shown.