

## BP 19: Posters - Membranes and Vesicles

Time: Monday 17:30–19:30

Location: Poster C

## BP 19.1 Mon 17:30 Poster C

**Three-dimensional lattice Boltzmann simulations of capsules with viscosity contrast** — ●ABDALLAH DADDI-MOUSSA-IDER<sup>1</sup>, BADR KAOU<sup>2,3,1</sup>, and STEPHAN GEKLE<sup>1</sup> — <sup>1</sup>Biofluid Simulation and Modeling, University of Bayreuth, 95440 Bayreuth, Germany — <sup>2</sup>CNRS - University of Technology of Compiègne, UMR 7338 - Biomechanics and Bioengineering, 60200 Compiègne, France — <sup>3</sup>Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany

We study dynamics and deformation of a spherical capsule subjected to shear flow using three-dimensional lattice Boltzmann simulations. The capsule membrane is modeled as a two-dimensional surface exhibiting resistance toward shearing, area dilatation and bending. The two-way coupling, between the fluid and the capsule, is ensured by the immersed boundary method. The viscosity contrast, between the viscosities of the encapsulated and the suspending fluids, is implemented by extending the method proposed in [Kaoui and Harting, Two-dimensional lattice Boltzmann simulations of vesicles with viscosity contrast, *Rheologica Acta* (2015)] to the three-dimensional case. We benchmarked our method against other previous methods in literature and we got perfect agreement for a wide range of the viscosity contrasts. Afterward we studied shape recovery of a capsule, after cessation of the applied shear flow, and we found that deformation decays exponentially with a characteristic time that depends on the membrane elastic properties and on the viscosity contrast.

## BP 19.2 Mon 17:30 Poster C

**Neutron Reflectometry Yields Distance-Dependent Structures of Interacting Lipid Membrane Surfaces Decorated with Hydrophilic Polymers** — ●IGNACIO RODRIGUEZ LOUREIRO<sup>1</sup>, VICTORIA LATZA<sup>1</sup>, AURELIO BARBETTA<sup>1,2</sup>, LUCA BERTINETTI<sup>1</sup>, GIOVANNA FRAGNETO<sup>3</sup>, and EMANUEL SCHNECK<sup>1</sup> — <sup>1</sup>Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — <sup>2</sup>Institut de Chimie Séparative de Marcoule, France — <sup>3</sup>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 to determine the distance-dependent structure of interacting lipid membrane surfaces decorated with hydrophilic poly(ethylene glycol) (PEG) brushes. We also have a look at two interacting lipopolysaccharide surfaces.

## BP 19.3 Mon 17:30 Poster C

**Micropipettes as force sensors in biomechanical studies** — ●CHRISTIAN KREIS, MARCIN MAKOWSKI, QUENTIN MAGDELAINE, and OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

The precise determination of acting forces is fundamentally important for the characterization of mechanical properties of soft matter and biological processes. Optical tweezers and AFM force probes can provide quantitative information on interactions on the micro- and nanoscale. However, these techniques are limited to objects within a certain force and size range. We design micropipette force sensors from glass capillaries and employ these to study the interactions of biological matter with interfaces. The technique enables us to manipulate macroscopic and microscopic objects, with a size range from  $\mu\text{m}$  to mm, while measuring forces in the range from pN to mN. Additionally, it allows for quantitative force-shape and force-deformation correlations, as it is purely based on optical high-resolution (and eventually high-speed) imaging involving image cross-correlation analysis. Thus, we can manipulate single cells, multicellular aggregates, cellular tissues and even macroscopic organisms while tracking simultaneously their dynamical response. Here, we present the technique itself, as well as the force calibration of the micropipettes. Finally, we also provide experimental results on the adhesion of eukaryotic flagella to solid surfaces, the propulsion forces of the microalgae *Chlamydomonas* and the elastic

properties of multicellular *Volvox* colonies.

## BP 19.4 Mon 17:30 Poster C

**AFM Study on Cross-linked Nanodisc Systems** — ●PATRICK PAUL<sup>1</sup>, DENNIS KUBICZEK<sup>2</sup>, NICHOLAS BODENBERGER<sup>2</sup>, FRANK ROSENAU<sup>2</sup>, and KAY-E. GOTTSCHALK<sup>1</sup> — <sup>1</sup>Institute of Experimental Physics, Ulm University, Ulm, Germany — <sup>2</sup>Center for Translational Peptide Research, Ulm University, Ulm, Germany

Nanodiscs offer various possibilities in bio nanotechnology [1]. Embedding different proteins in the lipid double layer functionalize them in a designed way [2]. By adding reactive groups to the membrane scaffold proteins (MSP) crosslinking gets possible between the discs.

We present a study of cross-linked nanodiscs to create arrays of functionalized surfaces. With the help of atomic force microscopy we control and monitor sample preparation.

[1] Bayburt et al., *J Struct Biol.*, 1998 Sep;123(1):37-44.[2] Nath et al., *Biochemistry*, 2007 Feb 27;46(8):2059-69.

## BP 19.5 Mon 17:30 Poster C

**Investigating Phagocytic Particle Uptake into Giant Unilamellar Vesicles using Photonic Force Microscopy** — ●NICOLAS SCHUDELL and ALEXANDER ROHRBACH — Lab for Bio- and Nanophotonics, University of Freiburg

Particle binding and possible particle uptakes are ubiquitous in cell biology starting and controlling a manifold of processes. In particular, the immunological process of phagocytosis, the engulfment of a solid particle by a cell, eliminates debris and pathogens by a yet unknown amount of physical and chemical energy. The complex uptake mechanism and the different forces involved in it are only partly understood. In order to unveil the mechanistic principles, GUVs are used as a simplistic biomimetic model of a cell. They allow to investigate the important role of the lipid membrane during particle uptake. Here, we use a Photonic Force Microscope (PFM), based on optical tweezers and ultrafast 3D tracking, to approach an 1  $\mu\text{m}$  trapped latex bead to an immobilized GUV, until the uptake occurs. The PFM allows quantifying the position fluctuations of the trapped particle during the uptake process in 3D and with nanometer precision. Thereby, we are able to record force and energy profiles, as well as changes in the viscous drag and stiffness of the membrane. A Helfrich energy model for global and local deformation was developed for the comparison with our experimental data.

## BP 19.6 Mon 17:30 Poster C

**Hydrogen bond balance and entropy determine the interaction between glycolipid membranes in plant thylakoids** — MATEJ KANDUČ<sup>1,2</sup>, ●ALEXANDER SCHLAICH<sup>1</sup>, ALEX DE VRIES<sup>3</sup>, BRUNO DEMÉ<sup>4</sup>, ROLAND R. NETZ<sup>1</sup>, and EMANUEL SCHNECK<sup>5</sup> — <sup>1</sup>Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — <sup>2</sup>Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — <sup>3</sup>Groningen Biomolecular Sciences and Biotechnology (GBB) Institute and Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands — <sup>4</sup>Institut Laue-Langevin, Grenoble, France — <sup>5</sup>Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Naturally stacked biological membranes contain high amounts of glycolipids. Swelling experiments with membranes composed of glycolipids from plant thylakoids revealed that the interaction between these membranes is repulsive only at very low hydration. Even in excess water the membranes stay in close contact, which is in contrast to commonly studied phospholipid membranes.

Using solvent-explicit Molecular Dynamics simulations and taking the chemical potential of water into account, we reproduce the experimentally obtained pressure-distance curves of membranes composed of the plant glycolipid DGDG. Our analysis identifies the hydrogen bond balance and entropic contributions as the key determinants of the interaction. Furthermore, we find that even at the swelling limit the opposing membrane surfaces interact directly via hydrogen bonds.

## BP 19.7 Mon 17:30 Poster C

**Combination of MD Simulations with Two-State Kinetic Rate Modeling Elucidates the Chain Melting Transition**

**of Phospholipid Bilayers for Different Hydration Levels** — ●BARTOSZ KOWALIK<sup>1</sup>, THOMAS SCHUBERT<sup>2</sup>, HIROFUMI WADA<sup>3</sup>, MOTOMU TANAKA<sup>2,4</sup>, ROLAND NETZ<sup>1</sup>, and EMANUEL SCHNECK<sup>5</sup> — <sup>1</sup>Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — <sup>2</sup>Institute of Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — <sup>3</sup>Department of Physics, Ritsumeikan University, Kusatsu, 525-8577 Shiga, Japan — <sup>4</sup>Institute for Intergrated Cell-Material Sciences, Kyoto University, 606-8501 Kyoto, Japan — <sup>5</sup>Biomaterials Department, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

The phase behavior of membrane lipids plays an important role in the formation of functional domains in biological membranes and crucially affects molecular transport through lipid layers. We investigate the thermotropic chain melting transition from the ordered gel phase to the disordered fluid phase in membranes composed of DPPC by atomistic molecular dynamics simulations in which the membranes are subject to variable heating rates. We find that the transition is initiated by a localized nucleus and followed by the propagation of the phase boundary. A two-state kinetic rate model allows characterizing the transition state in terms of thermodynamic quantities. The extrapolated equilibrium melting temperature increases with reduced membrane hydration and thus in tendency reproduces the experimentally observed dependence on dehydrating osmotic stress.

BP 19.8 Mon 17:30 Poster C

**Diffusion of membrane-bound ligand-receptor bonds** — ●HENNING STUMPF<sup>1</sup>, DANIEL SCHMIDT<sup>1,2</sup>, and ANA-SUNČANA SMITH<sup>1,3</sup> — <sup>1</sup>PULS Group, Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg — <sup>2</sup>II. Institut für Theoretische Physik, Universität Stuttgart — <sup>3</sup>Division of Physical Chemistry, Institute Ruđer Bošković, Zagreb

Protein-mediated membrane adhesion plays a crucial role for many cell functions. In a biomimetic model system, a ligand-decorated membrane adheres to an opposing membrane representing receptors. Prior to formation of a ligand-receptor bond, both individual binders exhibit a protein-specific mobility. However, the mobility of a ligand-receptor bond is significantly decreased compared to the individual binder mobilities. Thus, a bond is often considered as immobile.

In the current work, we address the mobility of a ligand-receptor construct by analytical and numerical means. We calculate the diffusion constant of a single bond as a function of the diffusion constants of the individual binders, the elastic coupling and the affinity. Furthermore, we analyse the thermal induced displacement of the bond and find that it depends sensitively on membrane-mediated correlations between individual bonds. Moreover, entropic contributions of the unbound ligands and receptors in their respective, and possibly finite, reservoirs allow for a free energy discussion of adhesion domain formation.

BP 19.9 Mon 17:30 Poster C

**Hydration Interaction between phospholipid membranes in the presence of co-solutes** — ●ANIRUDH GUPTA<sup>1</sup>, ALEXANDER SCHLAICH<sup>1</sup>, DAT PHAM<sup>2</sup>, MATEJ KANDUČ<sup>3</sup>, EMANUEL SCHNECK<sup>4</sup>, EMMA SPARR<sup>2</sup>, and ROLAND R. NETZ<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — <sup>2</sup>Physical Chemistry,

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We study the interaction between phospholipid bilayers across water in the presence of co-solutes, namely TMAO (Trimethylamine N-oxide) and urea. We investigate the interaction mechanisms and thermodynamics using atomistic simulations at prescribed water chemical potential. Our interaction pressures successfully reproduce experimental data, unveiling that the membranes become more repulsive due to addition of co-solutes, as also indicated by the experiments. TMAO acts as a stabilizer for proteins while urea acts as a denaturant. It is also well known that TMAO is repelled more from proteins than the urea molecules. Our results also indicate that TMAO molecules are repelled further away from the bilayer than urea; however, the effect of both co-solutes on the membrane interaction is similar.

BP 19.10 Mon 17:30 Poster C

**Stalk Intermediates on the 'Magic' Lipid Mixture** — YIHUI XU and ●TIM SALDITT — Institut für Röntgenphysik, Uni Göttingen, Göttingen

Stalk intermediate structures formed by pure lipid mixtures in hydrated air have already been well studied by many groups. Our group has successfully found a few 'magic' lipid mixtures who can form stalk structures at rather high relative humidities. In order to extend this research to a more biologically relevant condition, we are now trying to immerse these 'magic' mixtures into aqueous solution, and promote the stalks structures using detergent/polymers.

BP 19.11 Mon 17:30 Poster C

**X-ray reflectivity investigation of structure and kinetics of photoswitchable lipid monolayers** — ●KUNTAL CHATTERJEE<sup>1</sup>, BJÖRN HAUSHAHN<sup>1</sup>, CHEN SHEN<sup>1,3</sup>, SVEN FESTERSEN<sup>1</sup>, JONAS WARIAS<sup>1</sup>, BENJAMIN RUNGE<sup>1</sup>, FRANZISKA REISE<sup>4</sup>, THISBE LINDHORST<sup>4</sup>, BEATE KLÖSGEN<sup>3</sup>, OLAF MAGNUSSEN<sup>1,2</sup>, and BRIDGET MURPHY<sup>1,2</sup> — <sup>1</sup>Institute for Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — <sup>2</sup>Ruprecht Heansel Laboratory, University of Kiel, 24098 Kiel, Germany — <sup>3</sup>University of Southern Denmark, 5230 Odense M, Denmark — <sup>4</sup>Otto Diels Institute of Organic Chemistry, University of Kiel, 24118 Kiel, Germany

The mechanical and dynamic properties of phospholipid membranes are of importance for important biological functions, such as switching of embedded proteins. In order to investigate these properties we study model systems in which amphiphilic photoswitchable molecules are integrated into Langmuir films of phospholipids. We have modified glycolipids to contain an azobenzene photoswitch between the chain and the head group and successfully embedded those in a monolayer of dipalmitoylphosphatidylcholine (DPPC). This allows us to reversibly change the azobenzene-glycolipid orientation between trans- and cis-conformation by illumination with UV and blue light. We have followed the structural changes in this model membrane and the switching kinetics of the system with Langmuir isotherms and in situ X-ray reflectivity at the LISA diffractometer P08, PETRA III. This work is funded by SFB 677. The LISA instrument at PETRA III is funded by BMBF 05K13FK2.