BP 18: Membranes and Vesicles I

Time: Wednesday 9:30–12:15 Location: H44

Invited Talk BP 18.1 Wed 9:30 H44

Out-of-equilibrium membrane physics and cellular organelles. — •Pierre Sens — CNRS-ESPCI, Paris, France

Most molecules secreted or internalized by Eukaryotic cells follow well defined routes, the secretory and endocytic pathways, along which they are exposed to a succession of biochemical environments by sequentially visiting different membrane-bound organelles. Molecules internalized by endocytosis move from early to late endosomes before being sorted and carried to their final destination. Molecules synthesized in the endoplasmic reticulum go through the Golgi apparatus, itself divided into cis, medial and trans compartments (called cisternae), where they undergo post-transcriptional maturation and sorting. One fundamental issue underlying the organization and regulation of intracellular transport is whether progression along the transport pathways occurs by exchange between organelles of fixed biochemical identities (via the budding and scission of carrier vesicles), or by the biochemical maturation of the organelles themselves.

In this talk, I will present some aspects of the Physics of out-of-equilibrium membrane system, and discuss their relevance to intracellular transport. I will particularly focus on the dynamical coupling between biochemical maturation and phase separation of membrane components, and its possible relevance for the generation and maintenance of the Golgi apparatus.

BP 18.2 Wed 10:00 H44

Effect of thermal noise on vesicles and capsules in linear flow — •David Abreu and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Fluid vesicles and elastic capsules are micrometer-sized objects, which implies that they are subject to the influence of thermal fluctuations. In particular, their behaviour in linear flow might be affected by these fluctuations. However, most theoretical models and simulations neglect thermal noise, although it plays an important role in experiments [1].

First, we add thermal noise to reduced models of undeformable vesicles and capsules in shear flow and show that thermal effects are relevant under realistic conditions [2]. We analyze the steady states for the different dynamical regimes as well as the vicinity of dynamical transitions (i.e., tank-treading to tumbling) where intermittent behaviour due to noise always occurs.

For deformable vesicles in general flow [3], we show that thermal fluctuations have to be taken into account in order to correctly explain the trembling motion observed experimentally [1]. We recover the experimental phase diagram and analyze the statistical properties of the three steady states (tank-treading, tumbling and trembling), showing that thermal noise is strongly amplified during trembling.

[1] N. J. Zabusky et al., Phys. Fluids 23, 041905 (2011); M. Levant and V. Steinberg, submitted (2012).

[2] D. Abreu and U. Seifert, Phys. Rev. E 86, 010902(R) (2012).

[3] D. Abreu and U. Seifert, in preparation.

BP 18.3 Wed 10:15 H44

Quantitative understanding of the nonspecific vesicle-substrate adhesion — •Daniel Schmidt[1], Udo Seifert[1], and Ana-Sunčana Smith[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart — [2]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg

Phospholipid membranes in cellular and biomimetic systems exhibit significant thermal fluctuations. These fluctuations play an important role in the regulatory mechanisms of the cell recognition process, when a cell binds to another cell membrane or, as in biomimetic systems, to a rigid substrate. The presence of such a substrate is manifested by the emergence of a non-specific potential, the strength of which is coupled to the membrane tension. The latter in turn affects the fluctuations in a fashion that is not fully understood.

Here we develop a procedure for the accurate determination of the membrane tension and the strength of the non-specific potential from experimental data, independent of the choice of the measurable - the membrane shape, the spatial or the temporal correlation functions. We achieve this goal after overcoming the limitations of the typically used, harmonic approximation of the potential. Additionally, we extract the true fluctuations from the apparent ones, which are modified due to the finite temporal and spatial resolution in microscopy. As a result, we obtain the first coherent view of the behavior of the membrane in a vicinity of a substrate, in a system that is of a finite size and away from the unbinding transition.

BP 18.4 Wed 10:30 H44

Curvature as a Mechanism for Biomolecule Localisation in Bacterial Cells — •Lars D. Renner[1,2], Prahathess Eswaramoorthy[3], Kumaran S. Ramamurthi[3], Douglas B. Weibel[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]University of Wisconsin-Madison, Madison, WI, USA — [3]National Cancer Institute, Bethesda, MD, USA

One of the central questions in cell biology is how the temporal and spatial organization of the cell machinery within the cell is established, maintained, and replicated. In Eubacteria, an understanding of the cellular organization of proteins is just beginning to take shape. Recent data suggests that there are geometric cues for the localization of proteins and lipids in bacteria. We found that microdomains of cardiolipin (CL) preferentially localize to regions of large, negative curvature. We use a top-down approach that combines in vivo and in vitro experiments with E. coli and B. subtilis cells. We find that a critical difference in the radius of curvature ΔC (curvature difference between cell poles and midcell) of approx. 0.5 μm^{-1} is required to drive the polar localization of MinD and DivIVA. Our data provides support for curvature as a general mechanism for regulating the spatial organization in bacterial membranes. This research expands our understanding of Eubacterial cell biology and provides insight into the spatial and temporal dynamics of membranes and their role in cell biology.

BP 18.5 Wed 10:45 H44

Shape determines membrane protein cluster formation — Diana Morozova, Matthias Weiss, and •Gernot Guigas — Experimental Physics I, University of Bayreuth

About 30% of all protein species in a cell are membrane proteins. They take part in a multitude of vital cellular processes, e.g. signal and mass transfer at the plasma membrane. In many cases, membrane proteins need to cluster to perform their specific duty. Using mesoscopic simulations, we have studied the influence of protein shape on the clustering ability. We show via the potential of mean force that lipid-mediated interactions between transmembrane proteins depend on two key parameters [1]: the shape of the proteins' hydrophobic domain and their hydrophobic mismatch. Protein interactions can be attractive or repulsive, depending on the characteristic bilayer perturbations induced by the proteins. These findings are compared to results on peripheral membrane proteins that reside only in one leaflet of the membrane [2]. Here, we observe various higher-order structures depending on the size and penetration depth of the protein's hydrophobic moiety. Surprisingly, even clustering across opposing leaflets of a bilayer is observed.

[1] D. Morozova, M. Weiss, and G. Guigas, Soft Matt. 8, 11905 (2012). [2] D. Morozova, G. Guigas, and M. Weiss, PLOS Comp. Biol. 7, e1002067 (2011).

15 min break

BP 18.6 Wed 11:15 H44

Specific binding of chloride ions to lipid vesicles and implications at molecular scale — •Volker Knecht[1] and Benjamin Klasczyk[2] — [1]Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, Hermann-Herder Strasse 3, D-79104 Freiburg — [2]MELAG Medical Technology, D-10829 Berlin

Biological membranes comprised of lipids and proteins are in contact with electrolytes like aqueous NaCl solutions. Based on molecular dynamics (MD) simulations it is widely thought that Na^+ ions specifically bind to POPC bilayers while Cl^- ions merely form a diffuse layer of counterions screening the positive membrane charge due to the Na^+ ions. I will present a comparison of recent data from electrophoresis and isothermal calorimetry experiments indicating that in fact both ion species show very similar affinities. Force field issues with the MD

studies are highlighted by our finding that a widely used simulation setup showing asymmetric affinities of Na^+ and Cl^- ions for POPC bilayers overestimates the effect of NaCl on the electrophoretic mobility of a POPC membrane by an order of magnitude. Implications for previous simulation results on the effect of NaCl on the structure of the membrane and the interfacial water are discussed. Our results suggest that a range of published simulation results on the interaction of NaCl with PC bilayers have to be reconsidered and revised.

BP 18.7 Wed 11:30 H44

Interbilayer repulsion force from coarse-grained simulations — •Yuliya Smirnova[1], Volker Knecht[2], and Marcus Müller[1] — [1]Georg August University, Institute for Theoretical Physics, Göttingen, Germany — [2]University of Freiburg, Institute of Physics, Freiburg, Germany

Using the coarse-grained MARTINI model of POPC lipids and water [1] we study interactions between bilayer membranes with and without external forces applied to the system. Upon dehydration the bilayer structure changes differently: without external forces, the membrane thickness increases; with an external force acting on the center of mass of the bilayers, however, membranes laterally stretch. We find that in both cases the interbilayer forces decay exponentially with slightly different decay lengths and substantially different pre-exponential coefficients. We propose a way to estimate hydration repulsion between lipid bilayers from both simulations and our results for the disjoining pressure are in good agreement with experimental results.

[1] Marrink S.J.; Risselada H.J.; Yefimov S.; Tieleman D.P.; de Vries A.H. J. Chem. Phys. B, 2007, 111, p 7812.

BP 18.8 Wed 11:45 H44

Phase separation in a Lipid/Cholesterol System: Coarse-grained and United-atom Simulations — •Davit Hakobyan and Andreas Heuer — WWU Münster, Institut für Physikalische Chemie, Münster, Germany

The separation of liquid-ordered and liquid-disordered phases of lipids in membranes is a subject of continuous experimental as well as theoretical investigations.

Microscale coarse-grained (CG) and united-atom (UA) simulations are performed to investigate the phase separation of a membrane bilayer for the ternary system of saturated 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and unsaturated 1,2-dilinoleoyl-sn-glycero-3-phosphocholine (DUPC) and cholesterol (CHOL). The results of 9 microsecond UA simulation demonstrate the onset of phase separation and are compared with the results of the corresponding CG system. While sharing the structural features of phase separation in the CG model, the onset of de-mixing for the UA model is nearly two orders of magnitude slower. This factor can be rationalized by the different short-time diffusion constants.

Various system properties such as order parameters, lipid - CHOL and CHOL - CHOL interactions are compared between the UA and the CG models. From the structural perspective the phase separation process appears to be rather similar for both models, which illustrates once more the power of using CG approaches. The results are further extended by analysis of different unsaturated lipids, different CHOL concentrations as well as different UA force fields.

BP 18.9 Wed 12:00 H44

Compatible solutes and their effects on DPPC lipid bilayers: a computer simulation study — •Jens Smiatek[1], Rakesh Kumar Harishchandra[3], Hans-Joachim Galla[3], and Andreas Heuer[2] — [1]Institut für Computerphysik, Universität Stuttgart, Germany — [2]Institut für Physikalische Chemie, WWU Münster, Germany — [3]Institut für Biochemie, WWU Münster, Germany

The influence of compatible solutes on the properties of DPPC lipid bilayers is studied by semi-isotropic constant pressure (NPT) Molecular Dynamics simulations. Our findings indicate an increase of the surface pressure and the solvent accessible surface area in presence of higher hydroxyectoine concentrations. By free energy calculations of a single DPPC molecule in presence of hydroxyectoine, we are able to validate a modified free solvation energy. As a consequence of this effect, we conclude that the underlying reason for the observed increase of the surface pressure is given by a better solubility of the DPPC lipids. These results are also supported by regarding the ratio of the hydrophilic to the hydrophobic solvent accessible surface area.