BP 2: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Monday 9:30–13:00 Location: H 1058

BP 2.1 Mon 9:30 H 1058

PFG-NMR studies of ATP diffusion in PEG-DA hydrogels and aqueous solutions of PEG-DA polymers — •Günter Majer[1] and Alexander Southan[2] — [1]MPI für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Institut für Grenzflächenverfahrenstechnik und Plasmatechnologie IGVP, Universität Stuttgart, Nobelstraße 12, 70569 Stuttgart, Germany

Adenosine triphosphate (ATP) is the major carrier of chemical energy in cells. The diffusion of ATP in hydrogels, which have a structural resemblance to the natural extracellular matrix, is therefore of great importance for understanding many biological processes. A powerful tool to determine the diffusion coefficients of ATP and other solutes directly, i.e. without the need for a fluorescent label and independent of any diffusion-model assumptions, is pulsed field gradient nuclear magnetic resonance (PFG-NMR). We present precise PFG-NMR measurements of ATP diffusion in PEG-DA hydrogels of various mesh sizes as well as in aqueous solutions of PEG-DA polymers, which are not cross-linked to a three-dimensional network. A major result of this work is that the diffusion coefficients are determined by the polymer volume fraction only, regardless of whether the polymers are cross-linked or not. Obviously, the ATP diffusion takes place only in the aqueous regions of the systems, with the volume fraction of the polymers, including a solvating water layer, being blocked for the ATP molecules. This modified obstruction model is most appropriate to correctly describe ATP diffusion in PEG-DA hydrogels.

BP 2.2 Mon 9:45 H 1058

Ion and Molecule Transport Bulk and in Nanopores - a NMR study — •Sarah Schneider and Michael Vogel — TU Darmstadt Institut fuer Festkoerperphysik, Darmstadt, Germany

We analyze ion and molecule transport in aqueous salt solutions confined to nanopores as part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While being highly selective and sensitive, biological ion channels lack the robustness for technological applications. Contrarily silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favorable properties of both fields.

To optimize such pores, it is of strong interest to understand the influence of the confinement on the T-dependent ion and molecule transport inside. We vary the pore parameters systematically and study their effects on the dynamics by NMR. Using ^{1}H and ^{2}H NMR we can selectively investigate water dynamics whereas ^{7}Li and ^{23}Na NMR analyze the local and long-range dynamics of ionic species. Analyzing the local ion and water dynamics reveals a slowdown with increasing salt concentration, which may differ in bulk and confinement due to altered prospensity for crystallization. At a given concentration there is a slowdown in confinement with more heterogenious dynamics. Both can be explained by a slower layer at the pore walls and bulk-like dynamics in the pore center. Field-gradient NMR is applied to measure self-diffusion. The extent of the effect and the relation between short- and long-range dynamics depend on the confinement properties.

BP 2.3 Mon 10:00 H 1058

Fluoridation of hydroxyapatite - time dependence and protective properties — •Thomas Faidt[1], Andreas Friedrichs[1], Christian Zeitz[1], Samuel Grandthyll[1], Michael Hans[2], Matthias Hannig[3], Frank Müller[1], and Karin Jacobs[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Functional Materials, Saarland University, Saarbrücken, Germany — [3]Clinic of Operative Dentistry, Periodontology and Preventive Dentistry, Saarland University Hospital, Homburg, Germany

The application of fluoride containing products to protect tooth enamel from caries is daily practice for many decades. However, to this day little is known about the time dependence of fluoride uptake in hydroxyapatite (HAP) which is the mineral component of human enamel. In our study, we used highly dense HAP pellet samples as a model system for the crystallites of tooth enamel. To investigate the time dependence of the fluoride uptake, samples were exposed to a fluoride solution (NaF, 500 ppm) for different times. XPS depth profiling revealed a saturation behavior both for the overall amount of fluoride taken up by the sample and for the thickness of the formed fluoridated layer. We found that the maximum thickness of the fluoridated layer is about 13 nm. To explore the efficacy of such an ultrathin layer as a protective shield against acid attacks, we used AFM to determine the etching rates of untreated and fluoridated HAP samples. In spite of very low fluoride concentrations in the fluoridated samples, our results show a strong reduction of the etching rate after fluoride treatment.

BP 2.4 Mon 10:15 H 1058

Flexoelectricity in bones — •Fabian Vasquez-Sancho[1,2], Amir Abdollahi[3], Dragan Damjanovic[4], and Gustau Catalan[1,5] — [1]Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalunya — [2]CICIMA, Universidad de Costa Rica, San Jose, Costa Rica — [3]Laboratori de Calcul Numeric, Universitat Politecnica de Catalunya, Barcelona, Catalunya — [4]Ecole Politechnique Federale de Lausanne (EPFL), Lausanne, Switzerland — [5]Institut Catala de Recerca i Estudis Avançats (ICREA), Barcelona, Catalunya

Bones have been known to generate electricity under pressure since Fukada and Yasuda's seminal measurement of bone piezoelectricity in 1957. This piezoelectricity is thought to be essential for bone's self-repair and remodelling properties, and its origin is attributed to the piezoelectricity of collagen (the main structural protein of bones). However, since the discovery of flexoelectricity, it is known that strain gradients can also generate voltages in materials of any symmetry. Here we have detected and quantified the flexoelectricity of bone and bone mineral (hydroxyapatite), and determined that flexoelectricity can account for bone's electrical response to inhomogeneous deformations. In addition, we have used the flexoelectric coefficient of hydroxyapatite to calculate the (flexo)electric fields generated by cracks in bone mineral. Crack-generated electricity has been found to be large enough to be able to induce osteocyte apoptosis and thus initiate the crack-healing process, indicating a central role of flexoelectricity in bone damage repair and remodelling.

Invited Talk BP 2.5 Mon 10:30 H 1058

Light-based tools for investigating cell-ECM and cell-cell interactions — •Aranzazu del Campo — INM-Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany

Cells are able to sense and respond to biochemical and mechanical signals of their microenvironment. Despite impressive progress in the field of mechanotransduction, we still lack precise biophysical tools to dynamically regulate receptors and forces at the cell-ECM and cell-cell interfaces at molecular scale. In this context, novel tools based on phototriggers, light-driven molecular motors and optogenetics will be presented.

15 min. break

BP 2.6 Mon 11:15 H 1058

Quantitative Prediction of Multivalent Ligand-Receptor Binding Affinities for Influenza, Cholera and Anthrax Inhibition — Susanne Liese[1,2] and •Roland R. Netz[1] — [1]Freie Universität Berlin, Fachbereich Physik — [2]University of Oslo, Department of Mathematics

Multivalency achieves strong, yet reversible binding by the simultaneous formation of multiple weak bonds. It is a key interaction principle in biology and promising for the synthesis of high-affinity inhibitors of pathogens. We present a model for the binding affinity of synthetic multivalent ligands onto multivalent receptors consisting of n receptor units arranged on a regular polygon. Ligands consist of a rigid polygonal core to which monovalent ligand units are attached via flexible linker polymers. The calculated binding affinities quantitatively agree with experimental studies for cholera toxin (n=5) and anthrax receptor (n=7) and allow to predict optimal core size and linker length. Maximal binding affinity is achieved for a core that matches the receptor size and for linkers that are slightly longer than the difference between receptor size and core size. We construct an enhancement diagram that quantifies the multivalent binding affinity compared to monovalent ligands. We conclude that multivalent ligands against influenza viral hemagglutinin (n=3), cholera toxin (n=5) and anthrax receptor (n=7) can outperform monovalent ligands only for a monovalent ligand affinity that exceeds a core-size dependent threshold value. Thus multivalent drug design needs to balance core size, linker length as well

as monovalent ligand unit affinity.

BP 2.7 Mon 11:30 H 1058

Are there knots in chromosomes? — Jonathan Siebert[1], Alexey Kivel[1], Tim Stevens[2], Ernest Laue[2], and •Peter Virnau[1] — [1]JGU Mainz, Institut für Physik — [2]Cambridge University, Department of Biochemistry

Recent developments have for the first time allowed the determination of three-dimensional structures of individual chromosomes and genomes in nuclei of single haploid mouse embryonic stem (ES) cells based on Hi-C chromosome conformation contact data. Although these first structures have a relatively low resolution, they provide the first experimental data that can be used to study chromosome and intact genome folding. Here we further analyze these structures and provide the first evidence that G1 phase chromosomes are knotted [1], consistent with the fact that plots of contact probability vs sequence separation show a power law dependence that is intermediate between that of a fractal globule and an equilibrium structure.

[1]J.T. Siebert et al., Are There Knots in Chromosomes?, Polymers 9:8 (2017)

BP 2.8 Mon 11:45 H 1058

Small-angle X-ray scattering on gold nanoparticle-decorated DNA-origami nanostructures — •Kilian Frank[1,2], Caroline Hartl[1], Amelie Heuer-Jungemann[1], Tim Liedl[1], and Bert Nickel[1] — [1]Faculty of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]present address: Georg-August-Universität, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The DNA origami technique is a robust method for positioning guest molecules at the nanoscale, allowing for 3D crystalline assembly from monomeric building blocks. We report on synchrotron small-angle X-ray scattering (SAXS) experiments on DNA origami with guest gold nanoparticles. Geometric models were applied to investigate the particle placement and the lattice parameters of crystalline superstructures. In collaboration with Heinz Amenitsch (TU Graz) the model-free pair distance distribution function (PDDF) from the scattering data was analyzed. The PDDF reveals interparticle distances with nanometer resolution and is thus a valuable tool in the study of DNA-templated particle assemblies. The structure of a DNA-based lattice was confirmed to be rhombohedral with a spacing of 65 nm (T. Zhang, C. Hartl, S. Fischer, K. Frank, P. Nickels, A. Heuer-Jungemann, B. Nickel and T. Liedl. arXiv: 1706.06965). In situ SAXS confirmed previously found melting temperatures of the structures. These results help to optimize future designs of monomeric building blocks regarding lattice type and size.

BP 2.9 Mon 12:00 H 1058

Magnetic collecting of malaria pigment crystals by magnetized thin films — •Szilvia Mucza[1], Tamas Prok[1], Agnes Orban[1], Adrienne Furedi[2], Peter Furjes[2], and Istvan Kezsmarki[1] — [1]Dept. of Physics, Budapest Uni. of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — [2]Inst. of Technical Physics and Materials Science, Centre for Energy Research, HAS, 1121 Budapest, HU

Malaria pigment (hemozoin) crystals are the by-product of the hemoglobin metabolism and are unique indicators of the malaria infection. These micrometer-sized, needle-like, paramagnetic crystals have low crystal symmetry, thus show optical and magnetic anisotropy. Our group has been developing a malaria diagnostic device based on their linear dichroism and we aim to integrate a magnetic prefilter to increase the method's efficiency.

For this reason we started to investigate the behaviour of hemozoin crystals in their liquid suspension under magnetic field. To enhance the magnetic field gradient we designed micron-sized magnetizable periodic structures by lithography, and we observed the behaviour of synthetically prepared hemozoin crystals in liquid over these structures. We explained our observations theoretically, with the modeling of the magnetic properties near the surface of the periodic structure. We performed measurements under flow using an aligned microfluidic system to optimize different geometric parameters of magnetic structures.

BP 2.10 Mon 12:15 H 1058

Fibers and glasses: the complex behavior of protein droplets — •Louise Jawerth[1,2], Elisabeth Fischer-Friedrich[3], Suropriya Saha[1], Anthony Hyman[2], and Frank Jülicher[1] — [1]MPI for the Physics of Complex Systems. Dresden — [2]MPI of Molecular Cell Biology and Genetics, Dresden — [3]Biotec, TU Dresden

Liquid-like protein droplets are intracellular compartments that segregate material without the use of a physical barrier such as a membrane. Such compartments are important in a wide array of biological processes ranging from embryonic development to pathological fiber formation during neurodegenerative disease. The existence of many of these compartments has been known for decades; however, only recently has it become clear that these compartments exhibit liquid-like properties. In this talk, I will discuss our efforts to characterize and quantify these new materials in vitro. I will preset our recent work on quantifying the mechanical properties of these droplets using a combination of active and passive microrheology. We find that these droplets are not simple liquids, but become increasingly elastic as the droplets age. This appears to be a universal behavior shared by many protein varieties that form droplets. Furthermore, this and other characteristics are strikingly similar to behaviors observed in glass-like materials suggesting that protein droplets are in fact not simple liquids but, rather, a type of glass.

BP 2.11 Mon 12:30 H 1058

Light-driven biomolecule electrophoresis by asymmetric photochemistry — •Michael Kiess, Friederike Möller, and Dieter Braun — LMU Munich, Amalienstrasse 54, 80799 München, Germany

Ion and pH gradients across membranes are widespread in biology and are decisive for cell metabolism and signal transmission. We recreate such gradients in bulk water by local photolysis of photodissociable compounds. Focused light creates a non-equilibrium between photoproducts of different charges. Similar to pattern formation in biology, the differential diffusion of the photoproducts generates a radial electric field on a micrometer scale. Charged biomolecules move in this field through electrophoresis, which reaches a steady state within seconds in proportion to $\exp(-\mu/D\ \Phi)$. The complete description and theoretical analysis of this phenomenon allows us to analyse and manipulate molecules in water. We call this effect photochemical microscale electrophoresis (PME) and use it as a fast, purely optical tool for the simultaneous determination of electrophoretic mobilities, diffusion coefficients and charges of biomolecules ($Q \propto \mu/D$) such as DNA and proteins as well as the quantification of binding probabilities. We expect that the presented photochemically induced, electrokinetic reaction-diffusion-migration system will be a versatile playground for further research. It can be a valuable tool for the investigation of electrokinetic effects and for the development of optical methods such as zeta potential measurements or isoelectric focusing. Furthermore, it is likely that the optically controlled interaction of electrical fields with pH and ion gradients may lead to a novel testbed for intracellular processes.

BP 2.12 Mon 12:45 H 1058

Thermal gradients, a natural choice to support the origins of life — •Christof Mast[1], Lorenz Keil[1], Friederike Möller[1], Michael Kiess[1], Patrick Kudella[1], Mara Heinlein[1], Matthias Morasch[1], Hannes Mutschler[2], and Dieter Braun[1] — [1]LMU Munich, Amalienstrasse 54, 80799 München, Germany — [2]Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany

Life is a non-equilibrium system, which is nowadays maintained by a highly developed energy conversion machinery. Four billion years ago, other non-equilibrium mechanisms were needed to kick-start living processes. We propose ubiquitous heat fluxes as suitable driving force: Thermal gradients across water filled pores lead to a concurrent fluid convection and directed movement of dissolved charged molecules along the temperature difference. Combined, both effects accumulate the dissolved biomolecules in a length dependent manner. Oligonucleotides are pushed into a hydrogel phase, depending on their sequence and chirality: A mixture of strands with different sequence demixes into sequence-pure and homochiral hydrogels upon thermal accumulation, possibly selecting for interacting strands during the origin of life. The thermal non-equilibrium also creates and maintains a pH gradient over two units by the selective accumulation of charged buffer molecules, which shifts the local equilibrium in pH. In this system, early compartments of life may have cycled between different external pH conditions, implementing an important boundary condition for a primordial metabolism. [1] Keil et al. Nat Com, 2017, 10.1038/s41467-017-02065-3