

CPP 52: Biomaterials and Biopolymers (joint session with BP) II

Time: Thursday 15:00–18:45

Location: ZEU 222

CPP 52.1 Thu 15:00 ZEU 222

Observing the onset of amyloid fibril formation at interfaces with Reflection Anisotropy Spectroscopy — ●HEIKE ARNOLDS, SERGIO MAURI, CAROLINE SMITH, and PETER WEIGHTMAN — Surface Science Research Centre, University of Liverpool, Oxford Road, Liverpool L69 3BX, UK

The interaction of proteins with surfaces facilitates misfolding and leads to the formation of amyloid fibrils. This has a major impact on human health, because fibril formation during drug storage and injection decreases drug activity, for example in human insulin, and fibril formation at cell membranes is associated with diseases such as Alzheimer's. The key event is the formation of β -sheet structures which further self-assemble into amyloid fibrils, but there is little mechanistic understanding to date due to a dearth of experimental techniques which are sensitive and informative enough. Reflection anisotropy spectroscopy (RAS) provides structural information of adsorbates from the azimuthal angular variation of the optical spectrum about the direction of the incident light. It has been used for example to monitor the conformational change in cytochrome P450 in real time [1]. Here we apply the technique to the adsorption of human insulin on model methyl and amine terminated stepped Si(111) surfaces. By comparison to attenuated total reflection infrared spectra of the amide I band, we show that RAS can detect a helical β -sheet structure, which likely represents the onset of fibril formation.

[1]P. Weightman et al, Phys Rev E 88, 032715 (2013)

CPP 52.2 Thu 15:15 ZEU 222

UV treatment of stretchable polymer foils for bio-applications — ●RUXANDRA-A. BARB¹, BIRTE MAGNUS², THERESIA GREUNZ⁴, DAVID STIFTER⁴, RAINER MARKSTEINER², SIEGFRIED INNERBICHLER³, and JOHANNES HEITZ¹ — ¹Institute of Applied Physics, Johannes Kepler University Linz, Austria — ²Innovacell Biotechnologie AG, Innsbruck, Austria — ³Innerbichler GmbH, Breitenbach am Inn, Austria — ⁴CDL-MS-MACH, Johannes Kepler University Linz, Austria

Polymers are often used as substrates for cell cultivation. Stretchable polymer foils are required in a cell stretcher, which allows to investigate the behavior of cells during uni-axial mechanical strain or compression [1]. However, many stretchable polymers have weak cyto-compatibility. We demonstrate here that the cyto-compatibility of fluorinated ethylene propylene (FEP) or polyurethane (PU) can be significantly enhanced by UV photo-modification in a reactive atmosphere by means of a Xe2* excimer lamp emitting at 172 nm. Cells seeded on the treated polymer foils show enhanced cell adhesion and proliferation. Water contact angle and XPS measurements indicate that this is a result of improved wettability and a significant change in surface chemistry. However, tensile tests show that UV induced chain scissions can also lead to a degradation of the mechanical stability. But with suitable irradiation dose and foil thickness, repeatedly stretchable polymer foils with sufficient cell adhesion can be prepared.

[1] A. Gerstmaier, G. Fois, S. Innerbichler, P. Dietl, E. Felder, J. Appl. Physiol. 107, 613-620 (2009).

CPP 52.3 Thu 15:30 ZEU 222

Mechanics of engineered spider silk microparticles — ●MARTIN PETER NEUBAUER¹, CLAUDIA BLUEM², THOMAS SCHEIBEL², and ANDREAS FERY¹ — ¹Department of Physical Chemistry II, University of Bayreuth, Germany — ²Department of Biomaterials, University of Bayreuth, Germany

Spider silk fibers are well known for their high tensile strength and elasticity. Further, spider silk is biocompatible and -degradable. Thus, application perspectives can be envisaged for pharmaceuticals or cosmetics. Employing recombinant synthesis spider silk proteins are readily available and can be processed into different morphologies such as particles, capsules or films.[1]

We focus on mechanical properties of spider silk microparticles.[2] These could serve as fillers in composite materials or for drug delivery [3]. In this context, the understanding and controlling of mechanics is essential. From AFM force spectroscopy experiments we could show the drastic influence of hydration on the particles' elastic modulus which drops by orders of magnitude. Other investigated parameters include crosslinking and molecular weight. These mechanical studies

are accompanied by the examination of structure, swelling and thermal behavior.

[1] Humenik, M., Smith, A. M., Scheibel, S., Polymers 2011, 3: 640-661

[2] Neubauer, M. P., Bluem, C., Agostini, E., Engert, J., Scheibel, S., Fery, A., Biomater. Sci. 2013, 1: 1160-1165

[3] Bluem, C., Scheibel, T., BioNanoSci. 2012, 2: 67-74

CPP 52.4 Thu 15:45 ZEU 222

Multivalent Ligand Design — ●SUSANNE LIESE — FU Berlin, Berlin

The binding strength of multivalent ligands of different geometry and rigidity is studied, using an analytic statistical mechanics model. By varying the spacer length between the ligand units, the binding strength is optimized. It is found that for low association constants of the monovalent ligand, even an optimized multivalent structure, does not bind better than the monovalent correspondent. The critical association constant above which a multivalent ligand enhances binding, depends cubically on the distance between the receptor binding sites. In all systems we find that a multivalent ligand binds best, if the average spacer length is in the range of the receptor binding site distance and if the spacer is as stiff as possible.

CPP 52.5 Thu 16:00 ZEU 222

Structure/Property-Correlation of Alinate-Surfactant Mixtures at the Water Surface — ●PATRICK DEGEN¹, VICTORIA JAKOBI², MICHAEL PAULUS¹, and METIN TOLAN¹ — ¹Fakultät Physik/DELTA, TU Dortmund, Germany — ²Analytical Chemistry - Biointerfaces, Ruhr-Universität Bochum, Germany

Usually soft colloids, such as emulsion droplets or foam bubbles are stabilized by adsorbed layers of surfactants, polymers and mixtures of both. In recent years industrial researchers focus on polymers that are biocompatible such as gum acacia, chitosan or alginate. Such mixtures are found in pharmaceutical and food applications, in cosmetic products, detergents, and so forth. Nevertheless, the knowledge of basic properties of oil-water interfaces stabilized by surfactant-polymer mixtures is challenged by the complexities of the interactions involved. We present complementary investigations of surface tension and surface rheology properties on the alginate/surfactant system. In combination with dynamic light scattering and fluorescence spectroscopy this work provides new insights into the interactions between alginate and different surfactants in bulk and at the interface. Additionally, X-ray reflectivity measurements give information about the microscopic structure of such interfacial films. We demonstrate that some of the characteristic rheological features related to polymer - surfactant associations correlate with the X-ray reflectivity results, where the formation of large-scale complexes, depending on the surfactant concentration was observed.

CPP 52.6 Thu 16:15 ZEU 222

Determining the Specificity of Monoclonal Antibody HPT-101 to Tau-Peptides with Optical Tweezers — ●TIM STANGNER¹, CAROLIN WAGNER¹, DAVID SINGER², STEFANO ANGIOLETTI-UBERTI³, CHRISTOF GUTSCHE¹, JOACHIM DZUBIELLA³, RALF HOFFMANN², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Department of Experimental Physics I, D-04103 Leipzig, Germany — ²University of Leipzig, BBZ, D-04103 Leipzig, Germany — ³Humboldt University Berlin, Department of Physics, Berlin 12489, Germany

Optical tweezers-assisted dynamic force spectroscopy (DFS) is employed to investigate specific receptor/ligand bindings on the level of single binding events. Here, the binding of the phosphorylation-specific antibody HPT-101 to tau-peptides (pThr231/pSer235) with two potential phosphorylation sites is analyzed. According to ELISA-measurements, the antibody binds only specificity to the double-phosphorylated tau-peptide. It is shown by DFS that HPT-101 binds also to each sort of the mono-phosphorylated peptides. By analyzing the measured rupture-force distributions characteristic parameters are determined for all interactions. Using the extracted bond parameters, we build a simple theoretical model to predict features of the unbinding process for the double-phosphorylated peptide purely based on data on the monophosphorylated ones. Furthermore we introduce a method to estimate the relative affinity of the bonds. The values

obtained for this quantity are in accordance with ELISA, showing how DFS can offer important insights about the dynamic binding process that are not accessible with this common and widespread assay.

15 min. break

Invited Talk CPP 52.7 Thu 16:45 ZEU 222
Threading DNA through nanopores for biosensing applications — ●MARIA FYTA — Institute for Computational Physics, University of Stuttgart

The use of nanopores to read-out in an ultra-fast and cheap way the information inherent in DNA is being intensively investigated the last two decades. A biomolecule, like DNA, in a salt solution is electrophoretically threaded through a nanometer sized pore altering the ionic current that flows through the pore. Simultaneously, measuring the transverse tunneling currents across the nanopore can possibly lead to distinguishable electronic signatures for each DNA unit. Here, we will review some of our work related with the statistical and dynamical characteristics of the translocation process and the ionic current through the pore as obtained through multiscale simulations. Using more accurate simulations we will then report on our attempts to optimize the nanopore. Our efforts are focused on proper functionalization of the nanopore in order to enhance the transverse ionic current for reading-out the genetic information in DNA.

CPP 52.8 Thu 17:15 ZEU 222
DNA Interactions in Crowded Nanopores — NADANAI LAOHAKUNAKORN¹, SANDIP GHOSAL², OLIVER OTTO¹, KAROLIS MISUNAS¹, and ●ULRICH F. KEYSER¹ — ¹Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, CB3 0HE Cambridge, UK — ²Northwestern University, Evanston, IL 60208-3109, USA

The motion of DNA in crowded environments is a common theme in physics and biology. Examples include gel electrophoresis and the self-interaction of DNA within cells and viral capsids. Here we study the interaction of multiple DNA molecules within a nanopore by tethering the DNA to a bead held in a laser optical trap to produce a *molecular tug-of-war*. We measure this tether force as a function of the number of DNA molecules in the pore and show that the force per molecule decreases with the number of molecules [1]. A simple scaling argument based on a mean field theory of the hydrodynamic interactions between multiple DNA strands explains our observations. At high salt concentrations, when the Debye length approaches the size of the counterions, the force per molecule becomes essentially independent of the number of molecules. We attribute this to a sharp decrease in electroosmotic flow which makes the hydrodynamic interactions ineffective.

[1] N. Laohakunakorn, S. Ghosal, O. Otto, K. Misiunas, and U. F. Keyser. DNA Interactions in Crowded Nanopores. *Nano Letters*, 13(6):2798-2802, (2013).

CPP 52.9 Thu 17:30 ZEU 222
Diffusion regulation in the basal lamina — ●FABIENNA ARENDS^{1,2} and OLIVER LIELEG^{1,2} — ¹Zentralinstitut für Medizintechnik, Technische Universität München, Boltzmannstr.11, 85748 Garching — ²Fakultät für Maschinenwesen, Technische Universität München, Boltzmannstr.15, 85748 Garching

The permeability of the basal lamina, a biological hydrogel found at the basolateral side of the epithelium, is an important property for the design of both new drug delivery systems and biomimetic hydrogels. Moreover, it is highly desirable to understand the diffusion of colloidal particles and macromolecules such as drug delivery vehicles, nutrients, growth factors, and proteins across the basal lamina. The mobility of those objects in this highly complex gel is regulated by a broad range of factors including geometric constraints and different types of physical interactions between the particles/molecules and the hydrogel constituents.

Here, we quantify the diffusion of colloids and molecules within an extracellular matrix gel (ECM) purified from the Engelbreth-Holm-Swarm sarcoma, which is a model system for the basal lamina. For this quantification we use single particle tracking techniques and measure the formation of a concentration gradient of solutes across the ECM. From our data we aim at deciphering the underlying mechanisms responsible for the permeability properties of the hydrogel.

CPP 52.10 Thu 17:45 ZEU 222
Induction phase of entropic DNA segregation in bacteria — ●ELENA MININA and AXEL ARNOLD — Institute for Computational

Physics, University of Stuttgart, Allmandring 3, 70569, Stuttgart, Germany

Cell division is a complex mechanism which consists of two main processes – DNA replication and segregation. In primitive bacteria such as *Escherichia coli*, which has a rod-like shape and a single chromosome, the dsDNA molecule of the mother cell is split into two daughter strands which are complemented again. During the replication these daughter strands segregate, i.e. move towards opposite sides of the cell to create two new cells. It was previously shown that the segregation of confined linear polymers (DNA) is entropically driven and does not need to involve any active mechanisms [A. Arnold and S. Jun, *Phys. Rev. E* 76 (2007)]. However, the initial configuration of fully overlapping polymers is perfectly symmetrical. Initiation of segregation requires to break this symmetry. This period of time is called induction and has a rather broad distribution, which significantly reduces the efficiency of entropic segregation. In the present study we investigate the induction more closely and determine the mechanism that breaks the symmetry of the system. Combination of MD simulations with theory based on free energy calculation shows that the induction is not diffusive as it was predicted, but is a process related to the ordering of the polymer ends during breaking the system symmetry, when the tail of one strand tries to pass the tail of the other strand. Our findings might explain the segregation delay observed in experiments on *E.coli*.

CPP 52.11 Thu 18:00 ZEU 222
The influence of topology and thermal backbone fluctuations on sacrificial bonds — ●SORAN NABAVI¹, MATTHEW J. HARRINGTON², OSKAR PARIS¹, PETER FRATZL², and MARKUS A. HARTMANN¹ — ¹Institute of Physics, Montanuniversität Leoben, Leoben, Austria — ²Max-Planck-Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

One strategy to improve the mechanical performance of natural materials is sacrificial bonding that can be found in bone, wood, and in some softer biological materials like silk, mussel byssus threads. Sacrificial bonds (SBs) are reversible bonds which are weaker than the covalent bonds that hold the structure together. Thus, upon loading SBs break before the covalent bonds rupture. The rupture of SBs reveals hidden length providing a very efficient energy dissipation mechanism. Furthermore, SBs can reform after their rupture providing molecular repair and self-healing. We use Monte Carlo simulations to examine the influence of topology and SBs density on mechanical properties of single polymeric chains. The influence of SB density, topology and thermal backbone fluctuations on mechanical behavior are investigated by computationally mimicking tensile and cyclic loading test. Increasing the SBs density increases the work to fracture and also the energy dissipation in cyclic loading whereas the topology (determines the position and spacing of peak force) and thermal fluctuations (determine height of SB force) changes the mechanical properties. The results bear important implications for the understanding of natural systems and for the generation of strong and ductile biomimetic polymers.

CPP 52.12 Thu 18:15 ZEU 222
Dynamic glass transition in room temperature ionic liquids with calorimetric methods. — ●EVGENI SHOIFET^{1,2}, HEIKO HUTH¹, SERGEY VEREVKIN^{2,3}, and CHRISTOPH SCHICK^{1,2} — ¹Institute of Physics, Rostock University, Rostock, 18051, Germany — ²Interdisciplinary Faculty, Rostock University, Rostock, 18051, Germany — ³Institute of Chemistry, Rostock University, Rostock, 18051, Germany

Many ionic liquids are good glass formers. Nevertheless, only a few studies of the glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition (α -relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. We try to use calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs.

CPP 52.13 Thu 18:30 ZEU 222
Unusual behavior of vapor deposited glasses of 1-pentene and ethylcyclohexane investigated by fast-scanning and AC chip nanocalorimetry — ●YEONG ZEN CHUA¹, MATHIAS AHRENBERG¹, CHRISTOPH SCHICK¹, KATHERINE WHITAKER², MICHAEL TYLINSKI², and MARK EDIGER² — ¹Institute of Physics, University of Rostock,

Rostock 18051, Germany — ²Department of Chemistry, University of Wisconsin, Madison, Wisconsin 53706, United States

Glasses produced by physical vapor deposition exhibit different densities and relaxation behaviors, depending upon the deposition conditions. Glasses deposited at temperatures of about 0.85 of glass transition temperature T_g , called stable glass, have low enthalpy, low heat capacity, high kinetic stability and high density, while glasses deposited

at much lower temperatures than T_g have opposite properties. We have investigated the glasses of 1-pentene and ethylcyclohexane created from PVD in a wide range of deposition temperatures between 10 K and 120 K by fast-scanning and AC chip nanocalorimetry. Fast-scanning calorimetry provides information about the enthalpy of the deposited samples, while AC chip nanocalorimetry allows for a highly sensitive heat capacity measurement on the same samples.