BP 28: Posters: Biomaterials and Biopolymers

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

BP 28.1 Tue 14:00 Poster A

Raman spectroscopic analysis of drug-target interactions in malaria disease — •Torsten Frosch[1,2] and Juergen Popp[1,2] — [1]Leibniz Institute of Photonic Technology — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena

Raman spectroscopy provides extremely high chemical selectivity for the identification and quantification of antimalarial active agents [1,2]. A Raman spectroscopic elucidation of drug-target-interactions was be performed in physiological environment [3], while water did not cause a strong Raman signal. Raman spectra were acquired within intact cells. Highly spectrally resolved Raman difference spectra were acquired in order to elucidate small shifts of the molecular vibrations caused by the weak interactions. Defined stoichiometric ratios of heme (targets) and antimalarial drugs characterize the molecular interaction. With help of a thorough interpretation of these binding processes this work contributes towards the tailored design of new effective active agents against Malaria.

Acknowledgment: We thank Katja Becker for help with cell preparation.

References: [1] Frosch, T.; Yan, D.; Popp, J. Anal Chem 2013, 85, 6264-6271. [2] Frosch, T.; Schmitt, M.; Noll, T.; Bringmann, G.; Schenzel, K.; Popp, J. Anal. Chem. 2007, 79, 986-993. [3] Frosch, T.; Meyer, T.; Schmitt, M.; Popp, J. Anal. Chem. 2007, 79, 6159-6166.

BP 28.2 Tue 14:00 Poster A

The effect of urea on the swelling and collapse behavior of poly-N-isoproylacrylamide: a computational study — •Julian Michalowsky[1], Samantha Micciulla[2], Regine von Klitzing[2], and Jens Smiatek[1] — [1]Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin, 10623 Berlin, Germany

The effect of urea on the swelling and collapse properties of poly(N-isopropylacrylamide) (PNIPAM) molecules is presented. The results of all-atom Molecular Dynamics simulations imply that the macroscopic changes induced in the system by the increase of temperature and urea concentration can be related to microscopic details. The numerical simulations elucidate the main mechanism leading to the observed effects, which are the result of a subtle interplay between hydration properties and a concentration-dependent urea binding behavior. In particular, at low osmolyte concentration a small amount of direct bonded urea molecules to PNIPAM in addition to the hydrating water molecules leads to the stabilization of a more extended conformation. In contrast, at high osmolyte concentrations the binding between PNIPAM and urea becomes more favorable such that the number of hydrating water molecules is significantly decreased. Our numerical results therefore imply that a concentration-dependent binding behavior of urea governs the experimentally observed collapse and swelling properties of PNIPAM brushes in aqueous solution.

BP 28.3 Tue 14:00 Poster A

Swelling behaviour of individual corneocytes — •Hannes Heinel, Diana Voigt, and Robert Magerle — Chemische Physik, Fakultät für Naturwissenschaften, TU Chemnitz, 09107 Chemnitz, Germany

Corneocytes are dead, cornified cells that compose the outmost layer of the skin, known as stratum corneum. They contain a network of keratin intermediate filaments encased by a protein envelope, and display an extreme and reversible swelling upon hydration. M. E. Evans et al. have shown, that the expansion is due to the particular three-dimensional packing of keratin intermediate filaments [1,2]. With atomic force microscopy (AFM) we study the changes of morphology and nanomechanical properties of individual corneocytes upon hydration in humid air. Isolated corneocytes from a human donor are deposited on different substrates and imaged with AFM. The relative humidity of air is changed in-situ. [1] M. E. Evans, R. Roth, PRL **112**, 038102 (2014); [2] M. E. Evans, S. T. Hyde, J. R. Soc. Interface **8**, 1274 (2011)

BP 28.4 Tue 14:00 Poster A

Microrheological characterization of DNA nanotube networks — •Tina Händler[1], Carsten Schuldt[1,2], Martin Glaser[1], Jörg Schnauss[1], Josef A. Käs[1], and David M. Smith[2] — [1]University of Leipzig, Soft Matter Physics Division, Leipzig — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig

Studying the mechanics and dynamics of biopolymers has inspired many ideas and theories in polymer physics. One prominent example is actin, being the best-studied semiflexible polymer. Unfortunately, naturally occurring protein-based biopolymers are limited in their properties such as length, stiffness and interaction strengths. This highlights the advantage of having "programmable" model polymers at hand, which give the opportunity to experimentally test parameters otherwise unavailable in natural systems, and therefore expand theoretical approaches. Nanotubes formed from synthetic DNA strands are an ideal match to this need: they are semiflexible over their typical length scale and can be hybridized to have characteristics such as persistence length which are similar actin filaments or can be varied in a controllable way. We use this model system to measure the mechanical properties and dynamics of entangled networks with microrheological methods. The results can be employed to re-examine theories of semiflexible polymers and provide an insight into the internal structural dynamics of DNA helix tubes.

BP 28.5 Tue 14:00 Poster A

A unified theoretical approach to the inelastic mechanics of biopolymer gels, cells and cell aggregates — •Andrea Kramer[1], Matti Gralka[2], and Klaus Kroy[1] — [1]Institute for Theoretical Physics, Universität Leipzig, Germany — [2]Department of Physics, University of California, Berkeley, USA

Whereas classical viscoelastic models can often be applied to describe the mechanical response of biomaterials to small deformations, they cannot adequately be used to model the response to large deformations. Here, the transient breaking of bonds, e.g., crosslinks in biopolymer networks or cell-cell adhesions in cell aggregates, leads to a new class of response reminiscent of (pseudo-)plastic phenomenology. We present a schematic modeling framework for the construction of inelastic models for biological materials based on the inelastic Glassy Wormlike Chain (iGWLC) model [1]. Decomposing the total deformation into viscoelastic and inelastic components, we provide a unified description that is able to qualitatively explain recent experimental data for the nonlinear mechanics of fibrin and collagen gels, cells and cell aggregates [2,3].

[1] L. Wolff et al., New J. Phys. 12, 053024 (2010)
[2] S. Münster et al., PNAS 110, 12197 (2013)
[3] T.V. Stirbat et al., Eur. Phys. J. E 36, 84 (2013)

BP 28.6 Tue 14:00 Poster A

Higher ordered assembly of rigid biopolymers induced by depletion forces — •Martin Glaser[1], Teresa Tschirner[1,2], Maximilian Moebius-Winkler[2], Carsten Schuldt[1,2], Tina Händler[1], Tom Golde[1], Josef Käs[1], David Smith[2], and Jörg Schnauss[1] — [1]University of Leipzig, Faculty of Physics and Earth Sciences: Soft Matter Division, Leipzig, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany

The influence of depletion forces on processes like cellular organization has long been underestimated. An attractive potential induced within a system of rigid biopolymers can lead to the formation of higher ordered structures. The biopolymer actin can assemble, to loose networks, bundles and also clusters in a higher-level assembly like asters and nematic phases. In particular, the formation of asters was usually attributed to active processes driven by the molecular motor myosin. We present experimental evidence of bundle arrangements in star-like structures independent of other associated proteins. For the formation, we use established actin-bundling mechanisms such as counter-ion clouds and depletion forces. These structures can be formed solely by altering the concentration of actin and the according bundling agent in the system. Since no other proteins are involved, this effect demonstrates that higher ordered structure formations can be controlled only by self-assembly and accordingly energy minimization of the system. To demonstrate generality of this ordering effect beyond cellular biopolymers, we additionally present first experimental results on the formation of higher ordered structures by artificially designed DNA tubes.