CPP 7: Poster: Biopolymers and Biomaterials (jointly with BP)

Time: Monday 17:30–19:30 Location: Poster A

CPP 7.1 Mon 17:30 Poster A

Conformation Changes of F-actin under Shear — •Inka Lauter[1], Donald Guu[2], Minne Paul Lettinga[2], Rudolf Merkel[1], and Margret Giesen[1] — [1]Institute of Complex Systems: Biomechanics (ICS-7), — [2]Institute of Complex Systems: Soft Condensed Matter (ICS-3); Forschungszentrum Jülich

Polymers have versatile physical characteristics. Besides stiff and flexible polymers, the class of semiflexible polymers is of high interest in rheology as well as in biophysics. In our work we focus on the collective properties of in vitro polymerized solutions of filamentous actin (F-actin). We present recent data on fluorescently labeled single actin filaments in a solution of unlabeled actin filaments under external shear force. The studies were performed by means of a multipinhole-confocal microscope and a counter rotating shear cell. We show that under shear, filaments align perpendicular to the velocity gradient. Furthermore we studied filament curvatures as a function of actin concentration. The curvature distribution exhibits an exponential tail and the probability for high filament curvatures increases with actin concentration. The distribution of filament lengths, however, is unaffected even under high shear rates. This result is in contrast to classic rheometer data, which predict filament rupture at a certain strain level.

CPP 7.2 Mon 17:30 Poster A

Diffusion and Adsorption of Proteins in Nanoscaled Environments — •Sebastian Mörz[1], Dagmar Auerbach[2], Gregor Jung[2], and Patrick Huber[1,3] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Biophysical Chemistry, Saarland University, Saarbrücken, Germany — [3]Facultad de Física, Pontificia Universidad Católica de Chile, Santiago de Chile, Chile

During the recent years, some versatile developements in biochemistry have opened a wide field of applications. Examples are pore-suspending lipid bilayers or new means of drug delivery by encapsulation of biomolecules into mesoporous template materials. In nanometer scaled confinement, both the transport of biomolecules and their interaction with the porous environment are crucial to these applications, since the above mentioned systems employ artificial nanoporous matrices.

The aim of our research is to examine the diffusion and adsorption characteristics of proteins under such confinement in cylindrical nanochannels with special respect to the differences between the folded and the unfolded state of the proteins. Adsorption isotherms of folded and unfolded bovine heart cytochrome c in nanoporous silica have been measured at different pH-values, ranging from near-neutral pH to the isoelectric points of both the protein and the matrix. The diffusion of green fluorescent protein (GFP) in porous aluminum oxide was investigated using fluorescence correlation spectroscopy (FCS) for various pore diameters (25 to 75 nm) at pH 7 and at the isoelectric point of the membrane material (pH 9).

CPP 7.3 Mon 17:30 Poster A

Structural levels of organization in spider-silk - a combined mechanical and IR-spectroscopic study — •Markus Anton, Wilhelm Kossack, Roxana Ene, Christof Gutsche, and Friedrich Kremer — University of Leipzig, Institute of Experimental Physics I, Linnéstr. 5, 04103 Leipzig, Germany

Many efforts were undertaken to develop novel materials with promising mechanical qualities using spider silk as a pattern. Due to its unique mechanical properties, namely high tensile strength in combination with great elasticity, spider silk even surpass modern synthetic fibers like Kevlar [Kubik, *Angew. Chem. Int. Ed.* **41** (2002)].

Despite the successful synthesis of silk-like proteins, one is incapable to manufacture materials with similar properties on a large scale [Heim et al., *Angew. Chem. Int. Ed.* **48** (2009)], because of an incomplete understanding of spider silk's microscopic structure. Its mechanical properties are based on a refined architecture at the molecular and mesoscopic scale. Nanocrystals are interconnected by prestrained amorphous regions offering an internal pressure counterbalanced by the fiber's outer skin. By that structure, external stress is directly transferred to the nanocrystals resulting in a shift of the Alanin-specific absorption band [Papadopoulos et al., *Colloid. Pol. Sci.* **287** (2009), R. Ene et al, *Soft Matter* **5** (2009)].

To unravel this interplay between external and internal constrains a pressure- and temperature-dependent analysis of specific IR absorption bands by means of hydrostatic pressure provided by a diamond anvil cell was carried out.

CPP 7.4 Mon 17:30 Poster A

Frequency resolved depolarized light scattering studies of tRNA conformation in solution — •Christoph Angermann[1] and Thomas Hellweg[2] — [1]Universität Bayreuth, Physikalische Chemie 1 — [2]Universität Bielefeld, Physikalische und Biophysikalische Chemie

A custom built depolarized dynamic light scattering apparatus equipped with a confocal Fabry-Perot interferometer (FPI) with a free spectral range of 150 MHz was developed. The FPI is used to analyze the scattered light in the frequency domain. This is an important characteristic because the rotational motion of the particles modifies the depolarized component of the scattered light. Due to further development of this setup, it is easily possible to accumulate the noisy component efficiently leading to an enhancement of the signal to noise ratio. Combined with an iterative deconvolution method this apparatus can be used to analyze the rotational diffusion of tRNA from brewer's yeast in solution in a time range of 1 to 80 ns.

CPP 7.5 Mon 17:30 Poster A

(Visco-)Elasticity and thickness determination of polyelectrolyte multilayers by atomic force microscopy — •Johannes Hellwig, Cagri Üzüm, and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin

Thin films of polyelectrolyte multilayers can be easily prepared by using the Layer-by-Layer technique. These films show different growth behaviour, e.g. linearly or non-linearly, and also different mechanical properties. Mechanical properties can be influenced by the hard substrate below the film. Therefore the film thickness has to be taken into consideration. The growth behaviour and film thickness of PEMs can be determined by different methods using an Atomic Force Microscope (AFM). A common method called *scratch method* and a newly presented method called *full-indentation* was used to determine the thickness of soft films with a double layer number of 12 * 96. It was shown that both methods agree well within the experimental errors. In addition the elastic modulus of the films was determined by using an Colloidal Probe AFM where a colloidal probe attached to the end of a cantilever was indented into the PEM film. The mechanical properties of the PEMs was calculated from the deflection of the cantilever with a Herzian based elasticity model. Latest research focus on the non-elastic behaviour of PEMs.

CPP 7.6 Mon 17:30 Poster A

Excitation energy transfer dynamics in the light-harvesting complex LH2 determined by a mixed quantum-classical approach — •Jörg Liebers[1], Carsten Olbrich[1,2], Mortaza Aghtar[1], Michael Schreiber[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Germany — [2]Chemnitz University of Technology, Germany

In photosynthesis the harvesting of sun light is done by light-harvesting antenna complexes containing chlorophyll and carotenoid molecules. Starting from the available crystal structure of the light-harvesting systems 2 (LH2) of a purple bacterium all-atom classical molecular-dynamics (MD) simulations were applied to obtain the motion of the nuclei due to thermal fluctuations [1]. These fluctuations provide the input for quantum chemical calculations to calculate the excitation energies of the Q_y states of the single bacteriochlorophyll (BChl) molecules and also the Coulomb couplings between them. Using these time series of excitation energies and couplings, the spectral density and time-dependent Hamiltonians for this system were constructed which allows for a quantum dynamical investigation of the excitation energy transfer processes in the LH2 complex [2]. Here we use ensemble averaged wave packet dynamics with a quantum correction for temperature effects to calculate excitation dynamics and optical properties.

[1] C. Olbrich, U. Kleinekathöfer, J. Phys. Chem. B 114, 12427 (2010).

[2] C. Olbrich, J. Liebers, U. Kleinekathöfer, phys. stat. sol. (b) 248, 393 (2011).

CPP 7.7 Mon 17:30 Poster A

Environmental effects on the exciton dynamics in the FMO light-harvesting complex — •Mortaza Aghtar[1], Carsten Olbrich[1], Jörg Liebers[1], Johan Strümpfer[2], Klaus Schulten[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Germany — [2]University of Illinois at Urbana-Champaign, USA

Long-lived quantum coherent transfer has been observed experimentally in Fenna-Mathews-Olson (FMO) light-haversting complex at a temperature of 77 K. The cause for these long-lived coherence is still unclear. Thermal effects of the environment have been studied widely as a possible answer not only at low but also at physiological temperatures. To contribute to this debate, we apply all-atom classical molecular-dynamics (MD) simulations to obtain thermal fluctuations of the environment. The MD calculations provide the input for quantum chemical calculations to obtain the vertical excitation energies of the single bacteriochlorophyll (BChl) molecules [1]. The distribution of energies and couplings are analyzed together with possible spatial correlations. Using excitation energies and couplings, we have constructed the spectral density and Hamiltonian of the FMO complex which allows for the investigation of exciton dynamics and environmental effects [1,2].

[1] C. Olbrich, Th. la Cour Jansen, J. Liebers, M. Aghtar, J. Strümpfer, K. Schulten, J. Knoester, and U. Kleinekathöfer, J. Phys. Chem. B 115, 8609 (2011).
[2] C. Olbrich, J. Strümpfer, K. Schulten, and U. Kleinekathöfer, J. Phys. Chem. Lett. 2, 1771 (2011).

CPP 7.8 Mon 17:30 Poster A

Selective decalcification: A method to determine the phosphate distribution within the cuticle of isopod by confocal Raman spectroscopy — •Christian Reisecker[1], Bastian Seidel[2], Andreas Ziegler[2], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [2]Central Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The mineralized exoskeleton (cuticle) of isopods, is an excellent model to study biological composite materials. In spite of the diversity of crustacean species they share a similar structural principle for their cuticle: An organic matrix composed of chitin-protein fibers associated with various amounts of crystalline and amorphous CaCO3 and Ca3PO4. Scanning confocal Raman microscopy (SCRM) is a useful tool to study the chemical composition isopod cuticle and to allocate the distribution of organic and inorganic components. Carbonate minerals can easily detected but phosphates are more difficult to assign because of their lower content and of their lower Raman intensity. In this study selective decalification at pH=7 is applied to determine the phosphate distribution within the cuticle of three different isopods, which mainly differ in their phosphate content. While the calcite layer appears to be unchanged after the procedure no ACC can be detected in the endocuticle. Performing Cluster analysis phosphates can be allocated within endocuticle. The influence of the phosphate content in the mechanical properties of the cuticle SFM nanodindentation experiments are performed.

CPP 7.9 Mon 17:30 Poster A

Using confocal spectroscopy to determine the Mg content and the crystalline orientation of calcite within the exocuticle of isopods — •Katja Huemer[1], Christian Reisecker[1], Martin Laher[1], Bastian Seidel[2], Andreas Zielger[2], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [2]Central Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The exceptional properties of biological composites, such as the exoskeleton of crustaceans, are based on a complex hierarchical architecture of inorganic and organic components. The mineralized exoskeleton formed by the cuticle of crustaceans is an excellent model to study biological composite materials. The cuticle consists of an organic matrix composed of chitin-protein fibers associated with various amounts of crystalline and amorphous calcium carbonate. Using scanning confocal Raman microscopy (SCRM) for isopods is was possible to show that mineral phases have a layered arrangement where calcite is restricted to the outer area of the cuticle forming the outer protective layer. The aim of this study is to investigate the influence of the Mg content and crystalline morphology in the mechanical properties of the exocuticle the tergites of three isopod species. Using SCRM for the different species the Mg content can be determined and different types of oriented growth of nanocrystalline calcite can be discriminated. SFM nanodindentation experiments are performed to show the influence of these parameters in the local mechanical properties.

CPP 7.10 Mon 17:30 Poster A

Phase transitions in Chitosan/DPPC membrane multilayer as a function of hydration — Zoraya E. Lopez Cabana, Carmen M. Gonzalez Henriquez, •Ulrich G. Volkmann, Patrick Huber, Marcelo Cisternas, Rosario Ortega, and Mauricio Sarabia — Surface Lab, Facultad de Fisica, Pontificia Universidad Catolica de Chile, Chile

The main goal of this investigation is the formation of porous membranes of chitosan, a natural polymer. The porous character favors the incorporation of humidity that affects the thermal behavior of the multilayer. The membranes have been formed by spin coating on silicon wafers at 2000/6000 rpm. The thickness of the membrane was studied with Very High Resolution Null Ellipsometry and their topography by Atomic Force Microscopy (AFM). On top of the chitosan membrane a precise concentration of DPPC was evaporated by Physical Vapor Deposition (PVD) and homogeneous DPPC films ($\sim$ 80 Åthickness) were obtained. The characterization of the phase transition temperature of the multilayer Chitosan/DPPC was realized by imaging ellipsometry and *in situ* AFM and Raman spectroscopy. These transitions are consistent with those found by Meyer *et al.* [1].

[1] Meyer, H. W.; Semmler, K.; Rettig, W.; Pohle, W.; Ulrich, A. S.; Grage, S.; Selle, C.; Quinn, P. J. *Chem. Phys. Lipids* **2000**, 105, 149-166.

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