CPP 40: Biomaterials and Biopolymers I (joint session BP/CPP/MM, organized by CPP)

Time: Wednesday 15:00–18:15 Location: H40

CPP 40.1 Wed 15:00 H40

Self-assembled plasma protein nanofibers — •Christian Helbing[1], Tanja Deckert-Gaudig[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science, Department of Materials Science and Technology, Otto Schott Institute of Materials Research (OSIM), Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Jena, Germany — [2]Institute for Photonic Technology, Jena, Germany

Protein nanofibers (PNFs) are promising materials for numerous applications in the field of biomedical engineering. Especially, self-assembled PNFs based on plasma proteins have a high importance due their easy fabrication and high biocompatibility. However, knowledge about the self-assembly mechanism of such PNFs is limited. The aim of the current study is to deepen the understanding of the formation mechanism. We tested the hypotheses that morphology and inner structure of PNF depends on environmental conditions. In this work, we present results of self-assembled PNF structures formed in solution from a plasma protein combination. The observed morphology of the formed PNFs depended strongly on the formation conditions. The structural analysis suggest that a partial denaturation, i.e. a change in the secondary structure, of the plasma proteins is a necessary requirement for the formation of PNFs. The comparison of the secondary structure of the PNFs and the native proteins helps to improve the understanding of the self-assembly mechanism. The current results leads to a better control during the PNF formation.

CPP 40.2 Wed 15:15 H40

Automatically recognizing structural patterns in (bio)polymers — •Michele Ceriotti — École Polytechnique Fédérale de Lausanne

Atomistic simulations have been constantly increasing in accuracy and predictive power over the past decade, and materials and molecules of growing complexity are now amenable to modelling. There is however a dire need for algorithms to analyze the outcome of such simulations, to infer the elementary building blocks and the design principles that link atomic-scale structure and the emergence of meso-scale complex behavior. Here I will show how a probabilistic analysis of molecular motifs (PAMM) algorithm can be used to automatically recognize secondary structure patterns in proteins, and discuss how this approach could be used to identify new hydrogen-bond patterns in situations in which biopolymers are encountered in unusual conditions, such as in non-aqueous mediums or at inorganic interfaces.

Invited Talk CPP 40.3 Wed 15:30 H40

Competing oligonucleotide macromolecules: binding preferences instead of a ménage a trois — •Albrecht Ott — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

The description of macromolecular recognition is usually reduced to the consideration of molecular pairs. In the simplest descriptions the receptor pairs exhibit a lock and key interaction, which mainly depends on the shape of the molecular recognizers, and this is supposed to lead to a highly specific recognition process. Much more refined and quantitative physical descriptions have been proposed, however, they are again based on pairwise interaction, and we remain far from understanding molecular binding in competition as it occurs in a biological organism. Here we present experiments on DNA macromolecular binding in competition. We identify situations where the binding constant of one DNA strand is highly dependent on the presence of another, very similar competitor. We interpret our findings as the result of an interaction term that leads to a formal equivalent of a Landau phase transition. We present experimental results from in vitro transcription assays that highlight the existence of other non-trivial competitive situations that may act along similar lines.

CPP 40.4 Wed 16:00 H40

Poly(ethylene glycol) films and nanomembranes as flexible platform for humidity sensors and bioengineering — Musammir Khan and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We discuss possible applications of novel poly(ethylene glycol) (PEG) hydrogel films and membranes (PHFs and PHMs). They were fabricated by thermally activated crosslinking of amine- and epoxy-terminated, star-branched PEG oligomers and characterized by tunable thicknesses of 4 - 200 nm. As demonstrated, PHFs and PHMs can be used as highly sensitive elements in humidity sensors and moisture-responsive nanoelectronic devices, relying on resistive transduction technique. Their resistance change by ca. 5.5 orders of the magnitude upon relative humidity variation from 0 to 100%, which is unprecedented response for homogeneous materials. As another representative example, we show that PHFs and PHMs are able to host protein-specific receptors, providing, at the same time, protein-repelling and humidity-responsive matrix with a characteristic mesh size up to 8.4 nm. A noticeable grafting density of the test avidin protein, specifically attached to the biotin moieties coupled to the free amine groups in the PHMs, was achieved, whereas the analogous values for non-specifically adsorbed proteins were lower by a factor of 4-5. The engineering of PHMs with biomolecule-specific receptors and their loading with biomolecules are of potential interest for sensor fabrication and biomedical applications, including tissue engineering and regenerative therapy.

CPP 40.5 Wed 16:15 H40

Dynamic biointerfaces: new generation of cell instructive materials — •Chiara Fedele, Ravichandran H. Kollarigowda, Silvia Cavalli, and Paolo A. Netti — Center for Advanced Biomaterials for Healthcare, Istituto Italiano di Tecnologia, Neaples, Italy

Nowadays the growing interest in tissue engineering and biology for the in vitro control of cell fate has led to the design of dynamically actuable platforms through the implementation of stimuli-responsive materials in order to mimic the continuous remodeling of the extracellular matrix in living systems. Dynamic biointerfaces are conceived in order to be able to modify in a predictable spatiotemporal manner the cell-material crosstalk, overcoming the limitations of static conventional biomaterials. In our work, azobenzene-containing photosensitive polymers (e. g. polymer brushes, thin films, crosslinked free standing polymers) are designed as biomaterials to obtain patterned or reshaping substrates using photolithographic techniques or single laser beam instruments, in some cases even in presence of cells, allowing for a real-time modification of cell behavior.

15 min. break

CPP 40.6 Wed 16:45 H40

Tuning the Morphology of Langmuir Polymer Films through Controlled Relaxations of Non-Equilibrium States — •Renate Reiter, Sivasurender Chandran, and Günter Reiter — University of Freiburg, Experimental Polymer Physics, Freiburg, Germany

In general it is difficult to reproduce well defined morphologies of Langmuir polymer films (LPFs) because they have a high propensity to form non-equilibrium states. When these films are allowed to relax, a decay of the surface pressure with time might be observed indicating that the system is not equilibrated. Monitoring the temporal evolution of these relaxations and correlating them with snapshots of the corresponding morphologies sheds light on the associated structural reorganisation processes.

We present a systematic study based on different compression protocols designed to allow for relaxations of LPFs under well defined conditions. The homo peptide poly-γ-benzyl-L-glutamate (PBLG) was chosen for this study because it is a well investigated system that represents the relaxational behaviour of rod-like molecules which is expected to show less complexity than coiled polymer molecules. Our results demonstrate that experimentally manipulating the course of relaxations in LPFs has tremendous impact on the ordering of the molecules. Therefore various macroscopic properties of these biological relevant thin films are accessible.

CPP 40.7 Wed 17:00 H40

Impact of Silver Nanoparticles on the mechanical properties of Aquabacterium biofilms — •Yvonne Schmitt[1], Alexandra Grün[1], Dimitri Demeshko[2], Werner Manz[1], and Silke Rathgeber[1,2] — [1]Institute for Natural Sciences, University of Koblenz-Landau, Koblenz, Germany. — [2]Technology Institute for Functional Polymers and Surfaces (tifko) GmbH, Neuwied, Germany.

The antimicrobial properties of silver nanoparticles (AgNP) led to a

wide range of applications in consumer products. As a consequence, there is an increasing release of AgNP into aquatic environments. Biofilms, a conglomerate of extracellular DNA, polysaccharides and proteins, play an important role in sediment stabilization in riverine systems. AgNP are supposed to be a continuous source for silver ions (Ag^+) which can bind to functional groups of the biofilm constituents. This might lead to a decrease in the number of possible intermolecular interactions and, thus, reduced stability of the network. An impairment of the sediment stabilization due to enrichment of the AgNP in the biofilms might be detrimental to the whole ecosystem. In this work we studied the mechanical properties of an *A. citratiphilum* biofilm by means of rheology. The bacterium chosen is representative for a numerically dominant group of bacteria in different freshwater habitats. The biofilm was exposed to environmentally relevant concentrations of AgNP. In order to distinguish physical effects, resulting from the presence of the nanoparticles in the biofilms, from chemical effects, due to the activity of Ag^+, we studied biofilms exposed to Ag^+ as reference. We discuss our results in respect to their environmental implications.

CPP 40.8 Wed 17:15 H40

Characterization of the behaviour of amino acids at bioactive calcite interfaces — •Robert Stepić[1], Zlatko Brkljača[1,2], David M. Smith[2,3], and Ana-Sunčana Smith[1,2] — [1]Institute for Theoretical Physics and Excellence Cluster: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Nägelsbachstraße 49b, Erlangen, 91052, Germany — [2]Rudjer Bošković Institute, Bijenička 54, 10000, Zagreb, Croatia — [3]Center for Computational Chemistry, FAU Erlangen-Nürnberg, Nägelsbachstraße 25, Erlangen, 91052, Germany

The process of crystal growth controlled by biomolecules is known as biomineralization. This type of controlled growth results in crystals with a myriad of interesting properties, useful in a variety of applications. Therefore it is of great importance to gain deeper insights into the mechanistic details of interactions on the bioinorganic interface. For this purpose we present a systematic study of a set of amino acids, the elementary building blocks of peptides and proteins. Our methodology includes fully atomistic molecular dynamics simulations of the interface made of amino acids, water and slabs of calcite. Two different calcite slabs were taken into account, one with the stable (104) face and one with the unstable (001) face, which is associated with crystal growth. Free energies of binding to both surfaces for all the individual amino acids were determined using a series of sampling simulations with biasing potentials. These in turn reveal the importance of charged and polar groups in the interaction with calcite. This work provides reference data which can be helpful in further theoretical and experimental studies of calcite/peptide interfaces.

CPP 40.9 Wed 17:30 H40

Biomimetic Surface Templating of Silica Nanoparticles by Lysine-Leucine Peptide on Au Substrate — •Hao Lu[1], Yeneneh Yimer[2], Rüdiger Berger[1], Mischa Bonn[1], Jim Pfaendtner[2], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Chemical Engineering University of Washington, Seattle, USA

Fabrication of silica thin films and architectures has led to many applications in electronic and optical devices, cosmetics, and catalysis; recently, bioinspired silica fabrication approaches have attracted great attention because of low production cost and mild, sustainable fabrication methods. We are the first to demonstrate that the biomimetic molecules can also exert control over silica mineralization when bounded to inorganic surfaces. We use amphiphilic helical peptides based on leucine and lysine side chains (LKa14) carrying cysteine terminal groups as linkers, providing stable covalent bond to gold surfaces. Using XPS, VSFG, and AFM, complemented by molecular dynamic simulation, we have investigated the silica mineralization process at the molecular level directly at the surface: In analogy to solution mineralization, the LKa14 peptides on Au tend to assemble into ordered lateral structures, maintain their solution state helical folding and are oriented upright on the surface. The LKa14 peptides nucleate silica nanoparticles at the surface, which then grow into larger, globular structures. This surface mineralization process serves as a well defined model system for lateral protein assembly and biomineralization and is of potential interest for the design of silica-based biomimetic coatings.

CPP 40.10 Wed 17:45 H40

Reaction kinetics and diffusion in cell-free protein synthesis altered in polymer hydrogels — •Julian Thiele[1], Maike M. K. Hansen[2], David Foschepoth[2], Hans A. Heus[2], and Wilhelm T. S. Huck[2] — [1]Leibniz Institute of Polymer Research Dresden (IPF), Leibniz Research Cluster (LRC) and Department of Nanostructured Materials, Hohe Straße 6, 01069 Dresden, Germany — [2]Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, NL

Despite the viscous and highly crowded interior of a cell and its influence on diffusion and reaction kinetics, in vitro studies on protein synthesis often fail to take into account the density and spatial organization of the cytoplasm.

We mimic the complex cellular environment using a porous hydrogel matrix, and study the effects of macromolecular crowding on gene expression. While gene expression is strongly decreased by macromolecular crowding in conventional dilute bulk solutions, both gene transcription and translation are significantly enhanced 5x and 4x, respectively, when performed in a microscopic hydrogel environment.

These results highlight the need to consider the influence of the physical environment on complex biochemical reactions including macromolecular crowding as well as microscale confinement and spatial organization.

CPP 40.11 Wed 18:00 H40

Protein-protein interactions in crowded lysozyme solutions — •Karin Julius[1], Michael Paulus[1], Julian Schulze[1], Stefanie Roese[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund — [2]Fakultät Chemie, Technische Universität Dortmund, 44221 Dortmund, Germany

Inside cells, proteins are surrounded by different macromolecules, including proteins themselves, which cover approximately 30% of the available volume. It has been shown that this reduction of free space by macromolecules, the so called crowding effect, has a significant impact on the stability of proteins, rendering them more resistant to temperature or pressure denaturation. However, the influence of crowding on the protein-protein interaction potential that is mediated by the solvent is still unknown. The final goal of this project is the investigation of the pressure dependent interaction potential between proteins in aqueous protein solution as a function of the crowder concentration, mimicking intracellular solution conditions. For this purpose, small-angle x-ray scattering (SAXS) under high hydrostatic pressure will be applied. As we will focus on the effect of crowding, the well characterized model protein lysozyme is used at a concentration of 5 - 10 wt.-% in combination with the macromolecular crowder Ficoll PM 70 and its monomeric subunit sucrose.