CPP 48: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Wednesday 15:45–18:30 Location: H13

Invited Talk CPP 48.1 Wed 15:45 H13

Many Weak Interactions Make a Difference - from Fuzzy Biomolecular Self Assembly to Superselectivity — •Ralf Richter — School of Biomedical Sciences, Faculty of Biological Sciences, School of Physics and Astronomy, Faculty of Mathematics and Physical Sciences, and Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, LS2 9JT, United Kingdom

Multivalent interactions are key to molecular and cellular communication in biological systems, yet remain poorly understood. I shall present results of our efforts to better understand the role of multivalent interactions in two biological systems that involve biological polymers: (i) the nuclear pore permeability barrier, a meshwork of intrinsically disordered proteins that fills the nuclear pores and makes nucleo-cytoplasmic transport selective, and (ii) the interface between polysaccharide-rich extracellular matrix and the cell surface which is key to the communication of cells with their environment.

To study these systems on the supramolecular level, we take a multidisciplinary approach that combines surface science tools (to reconstitute well-defined model systems from the constituent molecules), biophysical characterization techniques (for quantitative analysis) and soft matter physics theory (to establish structure/property/function relationships).

The insights gained help us to uncover physical mechanisms underpinning functions, such as 'superselectivity' in the targeting of cell surfaces or the permeability of membranes, and help develop materials with new functions for applications in the life sciences.

CPP 48.2 Wed 16:15 H13

DNA crookedness regulates DNA mechanical properties at short length scales — •J.G. Vilhena[1], Alberto Marin-Gonzalez[2], Fernando Moreno-Herrero[2], and Ruben Perez[3] — [1]Department of Physics, University of Basel — [2]Centro Nacional de Biotecnologia, CSIC, Spain — [3]Universidad Autonoma de Madrid, Spain

Sequence-dependent DNA conformation and flexibility play a fundamental role in specificity of DNA-protein interactions. Here we quantify the DNA crookedness: a sequence-dependent deformation of DNA that consists on periodic bends of the base pair centers chain. Using extensive 100 μs-long all-atom molecular dynamics simulations, we found that DNA crookedness and its associated flexibility are bijective: unveiling a one-to-one relation between DNA structure and dynamics. This allowed us to build a predictive model to compute the stretch moduli of different DNA sequences from solely their structure. Sequences with very little crookedness show extremely high stretching stiffness and have been previously shown to form unstable nucleosomes and promote gene expression. Interestingly, the crookedness can be tailored by epigenetic modifications, known to affect gene expression. Our results rationalize the idea that the DNA sequence is not only a chemical code, but also a physical one that allows to finely regulate its mechanical properties and, possibly, its 3D arrangement inside the cell.

CPP 48.3 Wed 16:30 H13

Fast and on demand mussle-inspired adhesives by enzymatic polymerization of decapetides — •Maximilian Seuss[1], Justus Horsch[2], Patrick Wilke[2], Matthias Pretzler[3], Inga Melnyk[1], Dario Remmler[2], Annette Rompel[3], Hans G. Börner[2], and Andreas Fery[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]Humboldt-Universität Berlin — [3]Universität Wien

A novel strategy to generate adhesive protein analogues by enzyme-induced polymerization of peptides is presented. Inspired by the repetitive nature of certain peptide sequences in mussel-foot protein mfp-1 we designed a polymerization reaction using these sequences as macromonomers. Peptide polymerization relies on tyrosinase oxidation of tyrosine residues to Dopaquinone, which rapidly forms cysteinyldopa with free thiols from cysteine residues. This forms a covalent bond between macromonomers and generates adhesive polymers. The resulting artificial protein analogues show strong adsorption to different surfaces, even resisting hypersaline conditions. Adhesion energies up to 10.9 mJ/m^2 are found in single adhesion events and average values are superior to those reported for mussel foot proteins that constitute the gluing interfaces.

CPP 48.4 Wed 16:45 H13

Inequivalence of fixed-force and fixed-extension statistical ensembles for a flexible polymer tethered to a planar substrate — •Panayotis Benetatos[1] and Sandipan Dutta[2] — [1]Department of Physics, Kyungpook National University, Daegu, S. Korea — [2]Center for Soft and Living Matter, Institute for Basic Science, Ulsan, S. Korea

Recent advances in single macromolecule experiments have sparked interest in the ensemble dependence of force-extension relations (Gibbs versus Helmholtz). The thermodynamic limit may not be attainable for such small systems, that leads to inequivalence of the fixed-force and the fixed-extension ensemble. We consider an ideal Gaussian chain described by the Edwards Hamiltonian with one end tethered to a rigid planar substrate. We analytically calculate the force-extension relation in the two ensembles and we show their inequivalence which is caused by the confinement of the polymer to half space. The inequivalence is quite remarkable for strong compressional forces. We also perform Monte-Carlo simulations of a tethered wormlike chain with contour length 20 times its persistence length which corresponds to experiments measuring the conformations of DNA tethered to a wall. The simulations confirm the ensemble inequivalence and qualitatively agree with our analytical predictions for the Gaussian model. Our analysis shows that spatial confinement due to tethering causes ensemble inequivalence, irrespective of the polymer model.

15 min. break

CPP 48.5 Wed 17:15 H13

Transverse viscoelastic properties of cellulose fibers investigated by atomic force microscopy — •Caterina Czibula[1,3], Christian Ganser[1,3], Ulrich Hirn[2,3], and Christian Teichert[1,3] — [1]Institute of Physics, Montanuniversitaet Leoben, Austria — [2]Institute of Paper, Pulp and Fibre Technology, Graz University of Technology, Austria — [3]CD Laboratory for Fiber Swelling and Paper Performance, Graz University of Technology, Austria

Cellulosic fibers are used in the paper and textile industry. To gain more insight on how mechanical properties of cellulose fibers are related to properties of end-products like paper, our work focusses on the transverse viscoelastic behavior of single cellulose fibers. To reach this ambitious goal we implemented an atomic force microscopy (AFM) based method. Probing nanoscale mechanical properties of soft materials with AFM yields information on the performance of the material. With the Johnson-Kendall-Roberts model, the contact between AFM tip and sample surface can be well described. The evaluation of the experimental data combines contact mechanics and viscoelastic models which consist of springs and dashpots in series or parallel describing elastic and viscous behavior, respectively. Here, it will be demonstrated that the so-called Generalized Maxwell model yields reasonable results for single pulp as well as viscose fibers at five different relative humidity (RH) values and in water. The RH increase leads to a steady decrease of the viscoelastic properties. Especially in water, the viscoelastic behavior shows a pronounced decrease, proving that the interaction of the fibers in water is different than at varying RH levels.

CPP 48.6 Wed 17:30 H13

Elastic-Plastic Transition of Filament Networks — •Fanlong Meng[1] and Eugene Terentjev[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, U.K.

Filament networks are ubiquitous in biological systems, such as cytoskeleton, extracellular matrix and connective tissue. The elasticity of a permanently crosslinked filament network is relatively well understood [1, 2]. However, the filament networks are usually transient because the filaments can dynamically break from and re-bonded to crosslinks including various proteins and biological motors. Because of the complexity in the spatial and the temporal evolution of the network structure induced by crosslink dynamics, the rheological prop-

erties of a transiently crosslinked is poorly investigated. Recently, we proposed a model where the total energy of a transient filament network is a function of time due to the breakage and the re-formation of crosslinks [3]. With the model, we successfully explain experimental observations including stress relaxation, shape recovery, and necking formation. Moreover, we provide a phase diagram detailing the conditions for a transient filament network to behave elastically, plastically or in a mixed way. References: [1] F. Meng, E. Terentjev, Soft Matter 12, 6749 (2016) [2] F. Meng, E. Terentjev Polymers, 9, 52 (2017) [3] F. Meng, E. Terentjev, Macromolecules 51, 4660 (2018)

CPP 48.7 Wed 17:45 H13

Permanent Damage in Reversible Cross-linked Fiber Bundles — •Huzaifa Shabbir[1] and Markus Hartmann[2] — [1]Faculty of Physics, University of Vienna, Austria — [2]Ludwig Boltzmann Institute of Osteology at the Hanusch Hospital of WGKK and AUVA Trauma Centre Meidling, Vienna, Austria

Cross-linking is a common strategy to tailor the mechanical properties of polymeric systems. In natural systems, these cross-links are usually weaker than covalent bonds, which helps to maintain the structural integrity of the system preventing permanent damage [1].

Addition of cross-links to a polymeric system shows positive effects on many mechanical parameters, recent computational studies on cross-linked fiber bundles showed the surprising result that weak cross-links may deteriorate the strength of these systems [2]. This effect is strongly dependent on the coordination of cross-links [3], being most pronounced for the classical case of two-fold coordinated cross-links, i.e. one additional bond connecting two monomers. This presentation will discuss in detail the influence of cross-link coordination on this effect. In particular, Monte Carlo simulations have been used to detect the onset of permanent damage, the corresponding work and strength as a function of cross-link density and coordination. The results clearly indicate that systems with cross-links of higher coordination are more damage tolerant than classical two-fold coordinated cross-links.

[1] Fantner et al., Biophys. J. 90, 1411 (2006) [2] Nabavi & Hartmann, Soft Matter 12, 2047 (2016) [3] Shabbir & Hartmann, New Journal of Physics 19, (2017)

CPP 48.8 Wed 18:00 H13

Capabilities of photoresists based on polysaccharides for Direct LaserWriting — •Marie-Christin Heep[1], Agnes Koerfer[1], Maximilian Rothammer[2], Cordt Zollfrank[2], and Georg von Freymann[1,3] — [1]Physics Department and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Chair of Biogenic Polymers, TU Munich, Campus Straubing of Biotechnology and Sustainability, Germany — [3]Institute for Industrial Mathematics ITWM, Germany

Direct laser writing is a common method for fabrication of three dimensional micro- and nanostructures. The available materials have recently been expanded to polysaccharides [1]. These resists consist of a photo-curable polysaccharide, a photo initiator and a solvent. The exact mixture defines the properties of the final material. A detailed discussion on the crosslinking density and hence the stability of the written structures as well as on the resolution and the feature size of the resist will be provided. These properties are most crucial for applications. Furthermore, we examine the surface roughness of the resist as well as the ability to self-assemble. The self-assembling of the resist is investigated with respect to the concentration of initiator. Different solvents are taken into account, to observe their influence on the handling of the resist. The knowledge about the influence of the exact mixture on the properties of the material allows the development of new resist for specific requierenments. This also allows the use of self-assembling processes for micro- and nanostructures with a tailored disorder.

[1] M. Rothammer et al., Cellulose **25**, 6031 (2018).

CPP 48.9 Wed 18:15 H13

Towards an artificial human nail plate — •Kim Thomann[1], Andreas Späth[1], and Rainer H. Fink[1,2] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]CENEM, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

Human fingernails cannot be studied ex vivo with the same ease as for example hair since only clippings can be obtained which do not necessarily reflect the behavior of the whole nail. Thus, we aim to create an artificial nail plate model that resembles the adhesive characteristics of the human finger nail suited for ex vivo studies. In order to mimic the surface free energy (SFE) as well as the morphology of the nail, we first investigated the surface properties of the natural fingernail using a number of methods. In vivo contact angle (CA) measurements were performed to determine the SFE. Water CAs along resin replicas of fingernails were measured and scanning electron micrographs were taken to correlate SFE with topography. Our first approach for an artificial nail plate model is based on mixed alkane thiol self-assembled monolayers, terminated with either -OH or -COOH and -CH3. CA measurements revealed that either the total SFE or the relation between the polar and dispersive component could be replicated, but both requirements could not be met simultaneously. Thus, microcontact printing (micro-CP) is considered to produce patterned SAMs at various periods to match the nail's microstructure.