BP 13: Biopolymers

Time: Tuesday 17:15–18:45 Location: PC 203

BP 13.1 Tue 17:15 PC 203

Fibrin network dynamics in nanodroplets — •Heather M Evans[1], Enkhtuul Surenjav[1], Craig Priest[1], Ralf Seemann[1,2], Stephan Herminghaus[1], and Thomas Pfohl[1] — [1]Max Planck Institute for Dynamics and Self-organization, Göttingen, Germany — [2]Experimental Physics, Saarland University, Saarbrücken, Germany

This work explores complex dynamic phenomena of the blood clotting protein, fibrin. Protein "monomers" of fibrinogen assemble into fibers in the presence of the enzyme, thrombin, to ultimately form a three-dimensional fibrin network. Consequently, fibrin is a vital component of blood clots and provides an interesting yet relevant model system to study network properties. In order to study the development and manipulation of this robust network, we utilize new microfluidic designs that allow us to produce fibrin networks within nanodroplets. The droplets prohibit sticky surface interactions between the protein and the device walls. Furthermore, the incorporation of geometric structures on the microdevice enables the controlled deformation of individual droplets containing fibrin networks. The behavior of the networks is found to depend on parameters such as the network age and droplet velocity, as well as the relative protein concentrations. Using high resolution fluorescence microscopy, we analyze the elastic recovery of these networks through several cycles of mechanical deformation.

BP 13.2 Tue 17:30 PC 203

Morphological and Mechanical Characterization of Reconstituted Collagen Type I Networks — •Stefan Münster[1], Thorsten Koch[1], Philip Kollmannsberger[1], Louise Jawerth[2], David Vader[2], Gerd Schroeder-Turk[1], and Ben Fabry[1] — [1]Department of Physics, University of Erlangen-Nuremberg, Germany — [2]Department of Physics, Harvard University, Cambridge, USA

Collagen is the most abundant extracellular matrix (ECM) protein and serves as 3D culture environment for cell biology assays. Cell behavior in 3D sensitively depends on the mechanical properties of the ECM. Moreover, for computing cell tractions from the matrix deformations around invaded cells, knowledge of the matrix rheology is necessary.

Confocal images of collagen gels (2.4 mg/ml) show a narrowly distributed pore size of Ø1 μm. Macrorheology using a parallel-plate rheometer revealed predominantly elastic behavior that was approximately linear for strains <5%, with a shear modulus G' of 80 Pa, a loss modulus G" of 11 Pa, and a weak frequency dependency of both moduli according to a power-law with exponent 0.09. Microrheological behavior was measured by applying a 21 nN 'point' force to a ferrimagnetic Ø4.5 μm bead, and tracking the resulting 3D displacements of Ø1 μm fluorescent beads dispersed in the gel. Local strain fields were also determined by indenting the gel surface with a sphere and by shearing the bulk between two parallel glass plates. Under all conditions, the microscopic gel deformations for small strains closely followed that of an affine, predominantly elastic, isotropic and homogeneous continuum.

BP 13.3 Tue 17:45 PC 203

Microrheology of hyaluronan solutions: implications for the endothelial glycocalyx — •Nadja Nijenhuis[1], Daisuke Mizuno[2], Christoph F. Schmidt[3], Hans Vink[1], and Jos A.E. Spaan[1] — [1]University of Amsterdam, Amsterdam, The Netherlands — [2]Kyushu University, Fukuoka, Japan — [3]Georg-August-Universität, Göttingen, Germany

The endothelial glycocalyx (EG) forms an anti-adhesive surface at the luminal side of a blood vessel, acting both as a molecular sieve and as a mechanotransducer of fluid shear stress to the underlying endothelial cell layer. One of the components involved in these processes is the highly hydrated glycosaminoglycan (GAG) hyaluronan (HA). HA is the largest of the GAGs present in the EG. We used an optical tweezers setup and laser interferometry to measure the high bandwidth storage (G') and loss (G") modulus of HA solutions. The HA networks, consisting of approximately physiological molecular weight chains and concentrations had a frequency regime up to about 1000 Hz in which the mechanical response was more elastic than viscous. The addition of hyaluronidase to the entangled HA solution rapidly changed its rheological behavior: G' decreased, the entangled network character disappeared, and viscosity became dominant over elasticity.

BP 13.4 Tue 18:00 PC 203

Modelling of individual Hyaluronan-Aggrecan Complexes in the Extracellular Matrix — •Marcel Hellmann[1,2], Matthias Weiss[2], and Dieter W. Heermann[1] — [1]Institut für Theoretische Physik, Philosophenweg 19, Universität Heidelberg, D-69120 Heidelberg, Germany — [2]Cellular Biophysics Group, German Cancer Research Center, Bioquant Center, Im Neuenheimer Feld 267, D-69120 Heidelberg, Germany

The extracellular matrix (ECM) forms a protective layer of varying thickness around mammalian cells that acts as a rampart against potentially hostile invaders. To a large extent, the ECM consists of flexible hyaluronan (HA) filaments anchored in the cell's plasma membrane with rather rigid aggrecan complexes radially attached. In order to elucidate the influence of aggrecans on the ECM thickness, we have studied the behavior of an end-grafted, flexible polymer backbone with a single rigid side chain by means of Monte Carlo simulations.

We have found that already an individual flexible backbone with a single rigid side chain shows appreciable conformational changes compared to an undisturbed flexible chain: Depending on the side chain length (S) and the branching site (b), the backbone (length N) stretches from a mushroom-like to a more brush-like configuration. For $b = N$, i.e., when attaching the side chain to the free end of the backbone, the effect is strongest. Our data indicate that the thickness of the ECM may be tuned by simply altering the attachment of aggrecans to the HA backbone.

BP 13.5 Tue 18:15 PC 203

Why ion-terminated, finite polyalanine helices are stable in the gas phase — •Volker Blum[1], Joel Ireta[1,2], Alexandre Tkatchenko[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Universidad Autonoma Metropolitana-Iztapalapa, Mexico DF, Mexico

The formation of helical secondary structure in peptides is often associated with a "hydrophobic effect", but a series of landmark experiments indicate an *intrinsic* helical stability of isolated gas-phase polyalanine peptides, when terminated, e.g., by simple alkali ions [1]. We here quantify the mechanisms that stabilize Li^+ ion-terminated helices from first principles, including (i) the direct stabilization by saturating missing H-bonds near the C-terminus, (ii) indirect (de-)stabilization by the absence of H-bond cooperativity in short chains, (iii) the electrostatic presence of the positive ion, which more than offsets the missing H-bond cooperativity, and (iv) the stabilizing effect of non-local correlation (van der Waals) between side chains with increasing helix length. (i), (ii), and (iii) are covered by density-functional theory (DFT) in the PBE generalized gradient approximation; regarding (i), we show how details of the termination affect the stability hierarchy of different helix types (α, 3_{10}) For short helices Ala_n (n=1-10), we capture (iv) by quantum-chemical MP2 perturbation theory; this is used to corroborate a set of semi-empirical C6 corrections to DFT, which are then used to describe the limit of even larger helices. [1] Kohtani, Kinnear, Jarrold, JACS **122**, 12377 (2000).

BP 13.6 Tue 18:30 PC 203

How Large are Cooperative Effects in Hydrogen Bonded Molecular Chains? — •Martin Fuchs[1], Joel Ireta[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Univ. Autonoma Metropolitana Iztapalpa, Mexico

Intermolecular hydrogen bonds play an eminent role in a wide range of materials. In particular, they are critical for the secondary structure stabilization of biopolymers like proteins and nucleic acids. Arrays of hydrogen bonds (hbs), such as in chains or helices, often display a cooperative strengthening of the individual hbs. This cooperativity is crucial for understanding the stability and properties of hydrogen bonded materials. Here we investigate the hb cooperativity in model chains of HCl, HF, HCN, formamide, and 4-pyridone, i.e. molecules forming weak to strong hbs. We calculate the hb strength of infinitely long chains using density-functional theory (DFT) with the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA). We show that for large intermolecular separations, the hbs in the infinite chain strengthen by 20% over the respective molecular dimers, consistent with dipolar electrostatics [1]. At the equilibrium separation, the hbs strengthen significantly further (up to 260% for HF), with ad-

ditional stabilization from induced dipolar interactions. Comparing with results from higher-level calculations (MP2 and quantum Monte Carlo) we find that DFT faithfully describes the cooperativity in these systems in which the hbs are close to linear. [1] P.B. Allen, J. Chem. Phys. **120**, 2951 (2004).