BP 23: Biomaterials and biopolymers I (joint session BP/CPP)

Time: Thursday 9:30–12:45 Location: H10

BP 23.1 Thu 9:30 H10

A unifying perspective on rigidity in under-constrained materials — •Matthias Merkel[1,3], Karsten Baumgarten[2], Brian Tighe[2], and Lisa Manning[1] — [1]Department of Physics, Syracuse University, Syracuse, NY, USA — [2]Delft University of Technology, Delft, The Netherlands — [3]Centre de Physique Théorique, Université Aix-Marseille, France

We present a novel approach to understand rigidity in under-constrained materials, including sub-isostatic spring networks as well as 2D and 3D vertex models for dense biological tissues. We show that the onset of rigidity is determined by a purely geometric criterion. This allows us to analytically predict the elastic material properties close to the transition, which depend only on few geometric coefficients. We obtain exact expressions for the magnitudes of bulk modulus and shear modulus discontinuities at the rigidity transition, several scaling relations of the shear modulus, and the magnitude of the anomalous Poynting effect. Moreover, we show that the ratio of the excess shear modulus to the shear stress is inversely proportional to the critical shear strain with a prefactor of three, which we expect to be a general hallmark of rigidity in under-constrained materials induced by geometric incompatibility. This could be used in experiments to distinguish whether strain-stiffening as observed for instance in biopolymer networks arises from nonlinear characteristics of the microscopic material components or from effects of geometric incompatibility.

BP 23.2 Thu 9:45 H10

Heat and light - non-equilibrium tools to break early symmetry — Matthias Morasch[1], Corinna Kufner[2], Stefan Krebs[3], Hannes Mutschler[4], Wolfgang Zinth[5], Dieter Braun[1] und •Christof Mast[1] — [1]Systems Biophysics, LMU Munich, Amalienstr. 54, 80799 Munich, Germany — [2]Harvard-Smithsonian Center for Astrophysics, Harvard University, 60 Garden Street, Cambridge, MA 02138 — [3]Gene Center, LMU Munich, Feodor-Lynen-Straße 25, 81377 Munich, Germany — [4]MPI Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany — [5]BMO, LMU Munich, Öttigenstrasse 67, 80538 Munich, Germany

Modern lifeforms perpetuate their highly evolved molecular structures by using them to convert external energy-fluxes for self-replication and evolution. It is an open question how this closed cycle could start around four billion years ago. At that time, no sophisticated enzymes were available to initiate that process from the initially random and racemic pool of early prebio-polymers. We investigate how physical non-equilibria could help this issue by breaking early symmetry and locally enrich oligomer pools with a reduced sequence space and with a homochiral backbone. We are especially interested in the effect of thermal gradients across small water-filled pores and of incident UV-light. Thermal convection chambers could have selected for interacting, hence homochiral, sequences by their thermophoretic and lengthdependent concentration while UV-light is known to damage oligomers in a sequence dependent manner.

BP 23.3 Thu 10:00 H10

Kinetic Control of Peptide Self Assembly Pathways — •Joshua T. Berryman and Ali Asghar Hakami Zanjani — University of Luxembourg, Luxembourg

Naturally occurring peptides may aggregate to form 3D amyloid-like crystals, or may take on quasi one-dimensional amyloid fibril structures. Mltiple distinct polymorphic structures often exist as subbranches within both the crystallising and fibril-forming pathways, differing either in overall symmetry or in only local conformational degrees of freedom.

We examine and discuss a system of aggregating peptides in which the available polymorphs are observed to differ in the macroscopic chirality of their assembly, with right-twisted fibrils, left-twisted fibrils, and non-twisted crystals forming sometimes even in the same sample. Using atomistic and also coarse-grained calculations we develop a structural and kinetic model for assembly of the amyloid-forming peptides and validate against light scattering and microscopy results [1,2]. We are able to provide a simple analytical expression to predict if a given set of experimental conditions (parameterised by temperature, concentration and pH) will lead to left-handed fibrils, right-handed fibrils or mesoscopic twist-free microcrystals [1].

[1] Reynolds et al., Nat. Comms. 8:1338 (2017)
[2] Lara et al., J. Am. Chem. Soc. 136(12):4732 (2014)

BP 23.4 Thu 10:15 H10

Early Stage Self Assembly of Flexible Peptides — •Ali Asghar Hakami Zanjani and Joshua T. Berryman — University of Luxembourg, Luxembourg

We use accelerated simulation methods to investigate the early stage nucleation processes of a homologous series of hexapeptides: ILQINS (from hen's egg-white lysozyme), IFQINS (from human lysozyme) and TFQINS (a disease-related mutation in humans). We observe that the majority of initially formed one-dimensional single beta sheets in these systems have antiparallel alignment of peptide strands, in contrast to experimentally observed mature multi-sheet aggregates which have parallel strand alignment in all structures found to date [1-3].

We confirm the stability of the antiparallel aggregates by molecular dynamics simulations showing greater configurational stability for the antiparallel rather than parallel single beta sheets [4]. As mature antiparallel aggregates have not been observed for these systems we assume that such structures represent a kinetic trap, with limited potential to mature into amyloid fibrils or the related microcrystals. The existence of this kinetic trap offers the possibility to control amyloid formation by chemically directing small structures either towards or away from the antiparallel structures, depending if formation of macroscopic aggregates is considered beneficial or harmful.

[1] Reynolds et al., Nat. Comms. 8:1338 (2017)
[2] Lara et al., J. Am. Chem. Soc. 136(12):4732 (2014)
[3] Sievers, PhD Dissertations, (ProQuest, UMI: 3322087, 2008)
[4] Cooper, Beta-Sheet Geometry, (Birkbeck College, 1995)

BP 23.5 Thu 10:30 H10

The force spectroscopy of a biomimetic polymer in molecular simulations via perturbation theory — •Aviel Chaimovich[1], Christian Leitold[2], Kurt Kremer[3], and Christoph Dellago[4] — [1]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam — [2]University of California, Santa Barbara 93106 — [3]Max Planck Institute for Polymer Research, Mainz 55128 — [4]University of Vienna, 1090 Vienna

It has become a common practice of probing various aspects of biological polymers via force spectroscopy. Considering that many proteins exhibit similar phenomena, we are interested in their corresponding universal signatures. For this purpose, we invoke molecular simulations of a biomimetic polymer: Although this homopolymer is solely based on a bead-spring model with a square-well potential, it is capable of universally capturing the protein-like unfolding of any heteropolymer [1]. Foremost, via the Wang-Landau procedure, we calculate at zero force the free energy as a function of the potential energy of the polymer [2]. We continue via perturbation theory, determining the free energy at nonzero force, applying it on different sets of monomeric sites. We in turn find scaling relations for the activation and transition of the biomimetic unfolding, relating these to various polymeric characteristics (e.g. the radius of gyration). Our findings consequently have important ramifications for protein unfolding.

[1] M. P. Taylor, W. Paul, and K. Binder (PRE, 2009). [2] C. Leitold and C. Dellago (JCP, 2014).

BP 23.6 Thu 10:45 H10

Heated microbubbles condense and encapsulate prebiotic molecules and enhance ribozymatic activity — •Matthias Morasch[1], Alan Ianeselli[1], Alexandra Kühnlein[1], Saidul Islam[2], Kristian Le Vay[3], Hannes Mutschler[3], Matthew W. Powner[2], Christof B. Mast[1], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich, Amalienstrasse 54, 80799 München — [2]Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, UK — [3]Max-Planck Institute for Biochemistry, Am Klopferspitz 18, 82152, Martinsried, Germany

Interfaces in an otherwise homogeneous system can drastically change local reaction dynamics. Here, we studied microscale water cycles by the application of a temperature gradients to microbubbles in water and found that it triggered a wide range of processes crucial for the origin of life. We could show that biomolecules increase in concentration more than 1000-fold by the capillary flow at the air-water interface.

RNA precursors are found to crystallize around the bubble, allowing for a possible enantiomeric selection, while monomers undergo an enhanced phosphorylation. In the presence of vesicles, nucleic acids are concentrated and encapsulated in vesicle clusters, which are frequently ejected into the bulk solution. In addition, self-complementary RNA is demonstrated to form sequence-pure hydrogels, while the catalysis of the hammerhead ribozyme drastically increased at the interface compared to the bulk. The studied setting is hypothesized to be ubiquitous on early Earth.

15 minutes break.

BP 23.7 Thu 11:15 H10

Mechanical properties of UV-irradiated collagen fibrils studied with atomic force microscopy — •Marcus Schulze, Melanie Rogge, and Robert Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Straße 16, 64287 Darmstadt

Collagen is a widely used component for the synthesis of substrates in the field of Tissue Engineering (TE). Cell adhesion and proliferation on theses substrates is strongly dependent on their mechanical properties which makes a controlled adjustment of these properties a key requirement for a more elaborated substrate design. Among several approaches, the irradiation of the collagen-based substrates with UV light proved itself a valuable technique to modify the mechanics without introducing cytotoxicity. For the evaluation of the influence of UV light on the mechanical properties of collagen fibrils in a liquid environment the atomic force microscope was used. Varying combinations of UV light sources (UV-A, UV-B, and UV-C) and fluids (deionized water and phosphate buffered saline (PBS)) were applied to two kinds of samples. The indentation modulus was measured on surface supported fibrils and a tensile modulus was derived from bending experiments on freely suspended collagen fibrils. Results suggested an increase in modulus within 30 minutes of treatment with UV-B or UV-C light in PBS.

BP 23.8 Thu 11:30 H10

The effect of surface functionalization and pH on protein-gold nanoparticle interactions — •Brahmaiah Meesaragandla[1,2], Isabel Garcia[3], Luis.M Liz-Marzán[3,4], and Mihaela Delcea[1,2] — [1]Institute of Biochemistry, University of Greifswald, Greifswald, Germany — [2]ZIK HIKE, University of Greifswald, Greifswald, Germany — [3]CIC biomaGUNE and CIBER de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), San Sebastián, Spain — [4]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

In this work, we have investigated the interactions between differently functionalized gold nanoparticles (citrate, PEG-OMe, PEG-COOH, PEG-NH2, and glycan coated AuNPs) and human serum albumin (HSA) with pH using UV-Vis absorption, dynamic light scattering (DLS), and circular dichroism (CD) spectroscopy techniques. HSA exhibit different isomeric forms and undergoes conformational changes at different pH conditions (e.g. pH 3.8, 7.4, and 9.3). Both UV-Vis and DLS measurements have indicated the formation of protein corona. CD spectroscopy studies suggested that HSA conjugated to AuNPs undergoes a change in the secondary structure (decrease in alpha-helix) at various pH for all functionalized AuNPs. This change in protein secondary structure might be due to the type of dominant interaction between NPs and HSA (i.e electrostatic, hydrogen bonding). Our results indicated that both, surface charge and pH of the medium, influences the changes in HSA structure.

BP 23.9 Thu 11:45 H10

Temperature dependence of the elastic modulus of vapor deposited phospholipid bilayers on solid substrates — Maria J. Retamal[1], •Rodrigo Catalan[2], Marcelo Cisternas[2], Nicolas Moraga[2], Diego Diaz[2], Tomas P. Corrales[3], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[1], and Ulrich G. Volkmann[2] — [1]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [3]Department of Physics, UTFSM, Valparaiso, Chile — [4]TUHH, Hamburg, Germany

Phospholipid membranes (PMs) play a key role in most physiological processes. Besides the function of membrane proteins, changes in the fluidity of the phospholipid membrane are crucial in the permeability of certain molecules, such as oxygen or glucose. We analyze with Atomic Force Microscopy (AFM) and Surface Force Spectroscopy (SFS) the temperature dependence of Young's modulus (YM) of non-functional PMs (DPPC, DMPC and DSPC). Phospholipids were vapor-deposited in high vacuum onto silicon substrates. AFM measurements in liquid confirm the self-assembly of the phospholipid bilayer and YM measurements with SFS indicate the main transitions of the phospholipid bilayers. We show that PMs made by PVD in high vacuum preserve their structure and mechanical properties after proper hydration. This study opens new pathways to assemble phospholipid mixtures by means of solvent-free membrane formation. Acknowledgements: FONDECYT Nos. 3160803 (MJR), 1180939 (UGV), 1171047 (MSA) and 11160664 (TPC), CONICYT Fellowship (MC) and CONICYT-PIA ACT 1409.

BP 23.10 Thu 12:00 H10

Sequence effects on size, shape, and structural heterogeneity in Intrinsically Disordered Proteins — •Upayan Baul[1], Debayan Chakraborty[2], Mauro L. Mugnai[2], John E. Straub[3], Devarajan Thirumalai[2], and Joachim Dzubiella[1] — [1]Institute of Physics, Albert-Ludwigs-University of Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]Department of Chemistry, The University of Texas at Austin, Austin, Texas 78712 — [3]Department of Chemistry, Boston University, Boston, Massachusetts 02215

Intrinsically disordered proteins (IDPs) lack well-defined three-dimensional structures, thus challenging the archetypal notion of structure-function relationships in proteins. We present the development of a coarse grained simulation model that quantitatively characterizes the structural features of IDPs as a function of sequence and length (N_T). For diverse IDP sequences, with N_T ranging from 24 to 441, our simulations not only reproduce the radii of gyration (R_g) obtained from experiments, but also predict the scattering intensity profiles in near quantitative agreement with Small Angle X-ray Scattering experiments. While R_g values are well-described by the standard Flory scaling law, $R_g = R_0 N_T^{\nu}$, with $\nu = 0.588$, analyses reveal that the extent of conformational heterogeneity for IDPs is highly sequence-dependent, even though ensemble-averaged properties suggest synthetic polymer-like behavior in a good solvent. In conclusion, we comment on the effects of external stimuli such as salt concentration and temperature on the conformational properties of polypeptide sequences.

BP 23.11 Thu 12:15 H10

Co-survival and competition relationship between bacteria analyzed in millifluidic droplet sequence — •Xinne Zhao[1], Larysa Baraban[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute of Materials Science and Max Bergmann Center of Biomaterials Dresden, TU Dresden, Dresden, Germany — [2]Center for advancing electronics Dresden, cfaed, Dresden

Analysis of living systems, e.g. bacterial or cells populations plays significant role in fundamental research of population diversity, and evolution.1 Here, we present an optical detection system, combining the encapsulation of bacteria into numerous emulsion droplets to monitor their long term behavior and their relationship in co-culture environment. The bacteria we choose here are BFP E.coli and YFP E.coli which can express blue fluorescence and yellow fluorescence separately under different light illuminations. By detecting the emission wavelength from different E.coli, we can obtain the information of growth state of each bacteria strain. Compared to the classical cell culture methods, the strategy we use here can avoid the influence of getting sample during bacteria growing, as well achieve real-time and automatic monitoring. In order to find out the co-survival and mutual competition relationship between the two bacteria strains, we plan to get the reference growth curve of individually culturing both strains, co-culture them with different initial cell concentration ratios, add antibiotics, as well as compare their maximum cell concentration and generation time.

[1] R. Illing et al, Biomicrofluidics, 2016, 10, 024115.

BP 23.12 Thu 12:30 H10

Collagen gels determine the viscoelastic properties of tissue without hindering the diffusion of the aqueous solvent — Frank Sauer[1], Linda Oswald[1], Angela Ariza de Schellenberger[3], Heiko Tzschätzsch[3], •Felix Schrank[3], Tony Fischer[2], Jürgen Braun[4], Claudia T. Mierke[2], Rustem Valiullin[5], Ingolf Sack[3], and Josef A. Käs[1] — [1]Soft Matter Physics Division,Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — [2]Biological Physics Division,Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — [3]Department of Radiology, Charité-Universitätsmedizin, Berlin, Germany — [4]Institute of Medical Informatics,Charité-Universitätsmedizin, Berlin, Germany —

[5]Applied Magnetic Resonance, Felix Bloch Institute for Solid State Physics, Leipzig, Germany

Collagen accounts for the major extracellular matrix component in many tissues providing mechanical support for cells. Little is known whether water diffusion interacts with viscoelastic properties of tissues. We are combining highfield MR based diffusion measurements, novel compact tabletop MRE and confocal microscopy in collagen networks of different cross-linking states (untreated versus additional treatment with glutaraldehyde). The MRE-measured shear modulus is sensitive to interactions on the intrafiber level (e.g. fiber stiffness) and is able to depict the pronounced transition from viscous-soft to elastic-rigid gel properties. 3D pore size analysis indicate an unaltered overall network structure and MR based diffusion measurements further allude that there is free extracellular diffusive water transport in connective tissue.