

CPP 38: Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)

Time: Wednesday 15:00–16:45

Location: ZEU/0255

Invited Talk

CPP 38.1 Wed 15:00 ZEU/0255

Engineering, processing and application of recombinant spider silk proteins — ●THOMAS SCHEIBEL — Universität Bayreuth, Lehrstuhl Biomaterialien, Prof.-Rüdiger-Bormann-Str. 1, 95440 Bayreuth

Proteins reflect one fascinating class of natural polymers with huge potential for technical as well as biomedical applications. One well-known example is spider silk, a protein fiber with excellent mechanical properties such as strength and toughness. We have developed biotechnological methods using bacteria as production hosts which produce structural proteins mimicking the natural ones. We employ silk proteins in application forms such as fibers, hydrogels, particles or films with tailored properties, which can be employed especially for biomaterials applications. In case of implants or catheters cell adhesion plays a crucial role for the overall function of the to-be-used material. To change the properties of in-use polymers and to adopt their biocompatibility, we established coatings based on engineered spider silk proteins. Spider silk hydrogels can be employed as new bioinks for biofabrication. Their elastic behavior dominates over the viscous behavior over the whole angular frequency range with a low viscosity flow behavior and good form stability. Cell-loaded spider silk constructs can be easily printed without the need of additional cross-linkers or thickeners for mechanical stabilization. Our bio-inspired approach serves as a basis for new materials in a variety of medical, biological, or technical applications.

CPP 38.2 Wed 15:30 ZEU/0255

Inferring Structure-Property Relationships with Artificial Intelligence: A Lignin Case Study — ●MATTHIAS STOSIEK and PATRICK RINKE — Department of Physics, Atomistic Modelling Center, Munich Data Science Institute, Technical University of Munich

The potential of lignin as an abundant, underutilized biopolymer is increasingly being realized. A key challenge for the targeted production of lignins remains the poorly understood relation between lignin properties and its complex structure. Artificial intelligence (AI) methods could reveal such structure-function relationships but remain elusive in biomaterials research.

95 structurally diverse lignins are extracted from birch wood combining the Aqua Solv Omni (AqSO) biorefinery process and AI-guided data acquisition [1, 2]. Each lignin sample is characterized with 2D NMR spectroscopy and complemented with measurements of key lignin properties such as antioxidant activity.

To establish structure-function relationships, we correlate regions of the NMR spectra with corresponding property measurements. With a feature importance analysis, we identify structural relevant features for each property and provide a chemical interpretation. For instance, we find that more β -O-4 bonds lead to lower surface tension in water indicating a more linear lignin structure. Our structure-inference approach is designed to be general and applicable to a wide range of materials and characterization data.

[1] D. Diment et al., *ChemSusChem*, e202401711 (2024). [2] M. Alopaus, M. Stosiek et al., *Sci Data* 12, 996 (2025).

CPP 38.3 Wed 15:45 ZEU/0255

A minimalist view on biopolymer phase separation and aging — ●JASPER MICHELS — Max Planck Institute for Polymer Research, Mainz, Germany

Phase separation of proteins is a ubiquitous process by which cells regulate biological processes. In aberrant cases, such as encountered in neurodegeneration, initially liquid condensates age to become more solid-like. Understanding the interplay between phase separation and aging seems essential in the development of new therapeutic strategies. We apply minimal models that aim to capture the essence of biological transitions in terms of driving forces and thermodynamics. Models discriminating between mono- and multivalent directed association on the one hand and non-specific interactions on the other appear surprisingly versatile in reproducing and predicting biopolymer phase behavior, while at the same time providing essential mechanistic insight. We

will review our efforts, combining theory with experiments and demonstrating how relatively simple descriptions can (re)produce complex multi-component phase behavior. We will also present a dynamic version of the model, which provides for a thermodynamically fully consistent and intuitive description of the experimentally observed changes in viscoelasticity during aging. Our calculations explain how the stickiness of the proteins changes with time and concentration and how the coupling between association and solvation determines condensate viscoelasticity.

CPP 38.4 Wed 16:00 ZEU/0255

Cellulose-colloid hybrid materials for refractive index tuning — ●STEPHAN V. ROTH — Deutsches Elektronen-Synchrotron DESY, Hamburg, Sweden — KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose nanofibrils (CNF) with tailored (negative) surface charge are ideal for stable, nanoporous, structure-guiding network for thin film composite materials. Colloid materials offer the possibility for tunable structural colors, templates for metamaterials, and refractive index tuning. Here, core-shell-colloids with a hydrophobic core and positively charged, hydrophilic shell are used as additive in CNF thin films to tune their refractive index. The imbibition and self-assembly of the colloids as a function of colloid diameter in the CNF network was quantified, with colloids smaller than the pores in the CNF network penetrating into the thin film. Subsequent heat treatment allows for nanoscale composite formation on the level of the ~ 10 nm sized CNF bundles, while humidity treatment homogenizes the colloid distribution. Furthermore, the influence of the colloid size on the CNF structure inside the thin film was investigated and related to the mechanical properties of the colloid-CNF composite.

CPP 38.5 Wed 16:15 ZEU/0255

A universal material basis for biocompatible printed electrolytes in Organic Electrochemical Transistors (OECTs) — ●MORITZ FLEMMING, PAUL ZECHEL, RAKESH NAIR, LAURA TEUERLE, HANS KLEEMANN, and KARL LEO — Institute of Applied Physics, Technische Universität Dresden

Organic Electrochemical Transistors (OECTs) stand out for their interplay between ionic and electronic conduction, making them ideal analogues to biological synapses for neuromorphic computing or biosensors. Furthermore, they can be printed into integrated circuits on flexible substrates, allowing for low-cost and high throughput fabrication of full electronic systems. However, most OECT electrolytes for integrated circuits still lack biocompatibility and suffer from rheology-related printing challenges. This talk presents a novel material basis that can be combined with an ionic liquid to fabricate a biocompatible electrolyte for OECTs. It allows rheological adjustments to enable the use of electrolyte in both inkjet and screen printing. Furthermore, the electrolyte is UV-curable, enabling it to transition into solid-state structures after printing. Extended ink and device lifetimes for screen-printed structures enable the fabrication of state-of-the-art OECTs that can operate in ambient air more than 30 days after fabrication. Ultimately, a fully biocompatible and screen-printed OECT on a leaf substrate is demonstrated.

CPP 38.6 Wed 16:30 ZEU/0255

Nonequilibrium dynamics of the helix-coil transition in polyaniline — ●MAXIMILIAN CONRAD¹, FABIO MÜLLER¹, SUMAN MAJUMDER², and WOLFHARD JANKE¹ — ¹Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — ²Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India

As a continuation of our previous work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyaniline are investigated in an explicit solvent. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. We compare the phenomenology of the transition between the two studies and investigate the dynamics.