

CPP 41: Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Wednesday 17:00–18:45

Location: ZEU/0255

CPP 41.1 Wed 17:00 ZEU/0255

Coarse-grained simulations of network-forming DNA nanostructures — ●TAKAHIRO YOKOYAMA^{1,2} and ARASH NIKOUBASHMAN^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — ²Technische Universität Dresden, Dresden, Germany

DNA nanotechnology offers exceptional nanoscale designability through precise control of DNA sequences. These individual DNA strands can form predetermined building blocks, which then hierarchically assemble into super-structures such as nanotubes, nanocapsules, or nanostars. The latter can assemble further into (percolated) networks, where sequence-level design enables systematic control of the rheological and mechanical network properties. This multi-scale self-assembly can lead to cascading effects, where even a single unpaired nucleotide on the building block level can act as a highly flexible hinge that dramatically alters the network mechanics. To understand how such variations on the nucleotide-scale affect the network properties, we designed a series of DNA networks by systematically altering the arm number and junction flexibility of the star-shaped building blocks using coarse-grained molecular simulations of the oxDNA model. Our study revealed that the bulk modulus of the network decreased with increasing number of DNA arms; this counter-intuitive behavior stems from the addition of flexible junctions on the single-star level, which preferentially absorb deformation and soften the overall network. This result highlights the importance of precise nanoscopic design on the order of one nucleotide to obtain optimal network properties.

CPP 41.2 Wed 17:15 ZEU/0255

Characterizing interactions between glycoproteins and RNA at the lipid membrane interface — ●HORACIO V. GUZMAN¹ and VIVIANA MONJE² — ¹Biophysics & Intelligent Matter Lab, Material Science Institute of Barcelona, CSIC, Spain — ²Department of Chemical and Biological Engineering, State University of New York at Buffalo, 308 Furnas Hall, Buffalo, USA

Biological membrane interfaces interacting with proteins, nucleic acids, and glycans are integral to many cellular processes. The interplay between membrane lipids and biopolymers is highly sensitive to their flexibility grade, secondary structure, and electrostatics. Consequently, the cell membrane interface experiences changes in local lipid distribution and fluctuation in local properties. Projecting biophysical and structural membrane and biopolymer properties onto a two-dimensional plane simplifies the quantification of molecular signatures by reducing the dimensional space and identifying relevant entropic and short-range interactions at the interface of interest, as well as, characterizing interaction patterns and spatial correlations of complex lipid bilayers as they interact with biopolymers. We compare lipid-lipid interaction patterns in membrane-only systems to the corresponding systems containing small proteins and RNA fragments, respectively. These analyses quantify the effect of peripheral biopolymers on local lipid composition, structure, packing, deformation ratio of the biopolymer, and surface topology of the membrane upon adsorption. Such characterization is crucial for starting with the next-generation rational design of lipid vesicles and lipid-coated RNA drug delivery systems.

CPP 41.3 Wed 17:30 ZEU/0255

Nanoscale characterization of piezoelectric nanofibers blended with Salmon Gelatin — ●MARTÍN CHAVARRÍA-VIDAL¹, DRAGICA BEZJAK², MARÍA SAAVEDRA-FREDES¹, BENJAMÍN SCHLEYER-THIERS¹, ILKA HERMES³, and TOMÁS P. CORRALES¹ — ¹Universidad Técnica Federico Santa María, Valparaíso, Chile — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — ³Leibniz Institute of Polymer Research, Dresden, Germany

We electrospin salmon gelatin (SG) mixed in a polyvinyl alcohol (PVA) matrix containing chitosan (Ch). Furthermore, we used a coaxial electrospinning approach to blend these nanofibers together with polyvinylidene fluoride (PVDF). Such biomaterials could lead to the potential development of biocompatible and piezoelectric heart patches. After electrospinning our polymers, we observe by SEM two size distributions. Mechanical characterization of the large nanofibers obtained by AFM reveals two Youngs moduli peaks, centered at 1.77

GPa and 209 MPa. Small nanofibers also show a two component mechanical moduli distribution with peaks at 565 MPa and 1.33 GPa (10.1016/j.bbadv.2025.100168). EDS shows that both distributions contain Fluor. However, complimentary PFM measurements indicate that large nanofibers have a piezoelectric response comparable to pure electrospun PVDF, while the small ones do not exhibit such response. These measurements lead us to believe that the large nanofibers are mainly β -phase PVDF, while the smaller ones are composed of PVA/SG/Ch with α -phase PVDF (10.1177/15589250221125437).

CPP 41.4 Wed 17:45 ZEU/0255

Structural investigations using in situ SAXS on flexible bio-based vitrimeric carbon nanocomposites — ●SARATHLAL KOYILOTH VAYALIL^{1,2}, VAISHNAV B², VIRANCHIKA BIJALWAN², SRAVENDRA RANA², and AJAY GUPTA² — ¹Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — ²Applied Science Cluster, UPES, Dehradun, India

In this work, in situ small- and ultra-small-angle X-ray scattering has been employed to investigate the real-time structural evolution of 3D-printed vitrimeric thiol-acrylate photopolymers and their carbon-based nanocomposites designed for healable strain-sensing and soft-robotic applications. Flexible bio-acrylate based vitrimers reinforced with graphene/CNT fillers at varying concentrations are examined to elucidate temperature-dependent phase segregation and enable direct visualization of nano- and microscale filler morphologies, their spatial distribution, and their evolution across key thermal transitions (T_g and T_v of the polymer matrix). The effects of the stress/strain and cyclic-thermal cycles on the filler aggregates affecting the composites conductivity in carbon-filled samples are also evaluated. These insights into nano- and microscale morphology, reinforcement, and conductive behavior help us understand the dynamic structure-property relationships governing vitrimer-based conductive networks

CPP 41.5 Wed 18:00 ZEU/0255

Nanomechanical testing of suspended single nanofibers and humidity-induced glass transition — ●BENJAMIN SCHLEYER-THIERS¹, DIEGO BENAVENTE², YUSSER OLGUIN^{2,3}, and TOMÁS P. CORRALES^{1,3} — ¹Physics department of Universidad Tecnica Federico Santa María, Valparaíso, Chile — ²Technological and Scientific Center (CCTVal), Valparaíso, Chile — ³Biotechnology Center Daniel Alkalay Lowitt

In this work we will study the interaction of water molecules with polymeric nanofibers made from hygroscopic biopolymers and contrast them in environments with variable relative humidity. For this, we will suspend single nanofibers over micropatterns etched on silicon. In this suspended configuration, we shall perform three-point bending tests utilizing the environmental Atomic Force Microscope (AFM) and detect bending forces of the nanofiber, at different relative humidities. As bending tests are performed over the suspended nanofiber, the position-dependent stiffness can be plotted to find its mechanical modulus through bending models. The stiffness of single nanofibers drops with the increase in relative humidity, hinting a glass transition induced by this environmental condition. To test this behavior, we attempt to perform fracture experiments on a micro structured grid made by photolithography.

CPP 41.6 Wed 18:15 ZEU/0255

Probing light-induced drug release to lipid monolayers — ●IPSITA PANI, MICHAEL HARDT, and BJÖRN BRAUNSCHWEIG — Institute of Physical Chemistry, University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Light-induced drug release using photoresponsive nanocarriers is increasingly explored for targeted therapeutic applications. While most studies characterize release in bulk aqueous environments, drug release across aqueous-organic interfaces is equally important, as these interfaces represent the entry point into cells. We recently demonstrated light-induced drug release to air-water interface.[1] In cancer therapeutics, passive diffusion of anticancer drugs across lipid membranes is a key transport mechanism, yet direct quantitative data on drug-lipid interactions and their effect on release remain limited. Here, using arylazopyrazole photosurfactant nanocarriers and doxorubicin as a represen-

tative anticancer drug, we investigate how interfacial lipid composition governs light-induced drug release. By combining Langmuir monolayers with interface-specific vibrational sum frequency generation (SFG) spectroscopy, we quantitatively estimate drug release at lipid-adsorbed interfaces as a model membrane. To systematically probe headgroup effects, we employ four dimyristoyl lipids- DMPC, DMPG, DMPS, and DMPE which share identical acyl chains but differ in charge and polarity. These results elucidate how lipid-drug interactions modulate release efficiencies at membrane-like interfaces, providing insights key to the design of photoresponsive nanocarriers for targeted drug delivery. [1] Pani et al. Chem. Sci., 2024, 15, 18865-18871.

CPP 41.7 Wed 18:30 ZEU/0255

Hetero-aggregation of microplastic particles — THOMAS WITZMANN¹, ANJA F. R. M. RAMSPERGER², HAO LIU², YIFAN LU³, HOLGER SCHMALZ², LUCAS KURZWEG⁴, TOM C. D. BÖRNER⁴, KATHRIN HARRE⁴, ANDREAS GREINER², CHRISTIAN LAFORSCH², HOLGER KRESS², CHRISTINA BOGNER³, STEPHAN GECKLE², ANDREAS FERY¹, and •GÜNTER K. AUERNHAMMER¹ — ¹Leibniz-Institut

für Polymerforschung Dresden, Germany — ²Universität Bayreuth, Germany — ³Universität zu Köln, Germany — ⁴Hochschule für Technik und Wirtschaft Dresden, Dresden

Microplastic particles (MPP) in the environment are surrounded by a layer known as an 'eco-corona'. This is made up of natural organic matter (NOM), such as biomolecules, humic substances, and other natural molecules. NOM substantially alters the surface properties of MP particles, thereby influencing their interaction with other surfaces in an aqueous environment and their aggregation behaviour. We studied the interactions of eco-corona-covered MP particles on the nanoscale using colloidal probe-AFM. Measurements were performed at different ionic concentrations to mimic changing environmental conditions. We found that the eco-corona can pull on the silica colloidal probe via polymer bridging. This mechanism leads to aggregation and, consequently, sedimentation in the environment. By comparing our AFM results with experiments and simulations at different length scales, we consistently found that this type of heteroaggregation is conducive to stable aggregate formation and retains MPPs in sediments.