# CPP 49: Gels, Polymer Networks and Elastomers I

Time: Thursday 11:30–12:45 Location: ZEU/0255

CPP 49.1 Thu 11:30 ZEU/0255

**Nanoparticle–Polymer Coupling in Magnetic Gels Studied by Means of Computer Simulations and Experiments** — •Rebecca Stephan[1], Surojit Ranoo[2,4], Patrick Kreissl[1], Chinmay Pabshettiwar[1], Jessica Kubis[2], Christian Holm[1], Annette M. Schmidt[2], Regine von Klitzing[3], and Rudolf Weeber[1] — [1]Institute for Computational Physics (ICP), Universität Stuttgart — [2]Institute of Physical Chemistry, Department of Chemistry, University of Cologne — [3]Institute for Condensed Matter Physics, Technical University of Darmstadt — [4]Laboratoire Colloïdes et Matériaux Divisés, ESPCI Paris

Magnetic gels - soft hydrogels with embedded magnetic nanoparticles (MNPs) - combine the viscoelastic properties of a gel with the magnetic behavior of the MNPs. Their response to an external magnetic field enables tunable mechanical and dynamic properties such as shape, stiffness, and swelling. The microscopic coupling mechanisms between the MNPs and the surrounding polymer matrix are crucial for the material's stimuli-responsive properties. However, these mechanisms are not yet fully understood.

In this work, we juxtapose results for PAAm hydrogels with embedded cobalt ferrite nanoparticles with coarse-grained molecular dynamics simulations coupled to lattice-Boltzmann hydrodynamics. In both cases, we probe the coupling using magnetic AC susceptibility spectra. Our findings demonstrate that the local polymer environment and the surface heterogeneity of the magnetic particles - chemical or topographical - play an important role in MNP-polymer coupling.

CPP 49.2 Thu 11:45 ZEU/0255

**Strain-stiffening critical exponents of fibre networks under uni-axial deformation** — •Atharva Pandit[1] and Abhinav Sharma[1,2] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Deutschland — [2]Bereich Theorie der Polymere, Leibniz-Institut für Polymerforschung, 01069 Dresden, Deutschland

Disordered fibre networks exhibit a floppy to rigid mechanical phase transition as a function of connectivity. Sub-isostatically connected networks can undergo this transition via straining. Critical exponents governing this transition have been estimated theoretically and by numerical simulations of various types of networks. We present improved results, achieved through a combination of refined numerical simulations, larger system sizes and incorporation of theoretical predictions for better post-simulation analysis. A linear evolution of the critical strain and critical exponents is observed as the network is sheared while being subjected to non-volume-preserving uni-axial deformations.

CPP 49.3 Thu 12:00 ZEU/0255

**Probing Mechanical Properties of Magnetic Gels Using Computer Simulations** — •Yashas Tejaskumar Gandhi, Christian Holm, and Rudolf Weeber — Institute For Computational Physics, University of Stuttgart, Germany

Magnetic gels are liquid swollen polymer networks embedded with magnetic nanoparticles (MNPs). Their motion, shape and mechanical properties can be governed by an external magnetic field. The mechanical properties of a magnetic gel depend on both the polymer network and the embedded MNPs. They can also be heated by applying an AC magnetic field due to viscous and hysteresis losses.

There are two ways to probe the mechanical properties of magnetic gels: at the nanoscopic level using AC susceptometry, and at the macroscopic level by measuring stress under deformation. While macroscopic measurements are relatively straightforward, they are computationally demanding. The Gemant-DiMarzio-Bishop theory provides a framework for connecting magnetic AC susceptibility data to nanoscale mechanical properties. Our objective is to test this theory in computer simulations by comparing nanoscale measurements with macroscale measurements.

The polymer network is modelled as a coarse-grained bead-spring system. We also incorporate a solvent model for hydrodynamic interactions in the system. Shear deformation is applied using periodic Lees-Edwards boundary conditions. Our simulations use the 'Extensible Simulation Package for Research on Soft Matter Systems (ESPResSo)' simulation package.

CPP 49.4 Thu 12:15 ZEU/0255

**Dynamic control of rigidity via geometric frustration** — •Santiago Gomez Melo[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]ITP, Philosophenweg 19, Heidelberg — [2]BioQuant, Im Neuenheimer Feld 267, Heidelberg

Recent advances in materials design and 4D-printing now allow one to realize programmable metamaterials that upon receiving a suitable stimulus dynamically change their unconventional macroscopic properties. For mechanical metamaterial, these tunable features have so far been restricted to geometric quantities, such as the Poisson ratio and the strain-to-twist ratio, but the effective elastic moduli have not been addressed yet. Here we combine central force network theory and responsive hyperelasticity to show that it is also possible to dynamically control the elastic moduli, and more specifically the shear modulus, by programming geometric frustration into a stimuli-responsive structure. This phenomenon, known as geometric incompatibility, produces a rigidity phase transition in which the elastic modulus changes by several orders of magnitude. It results from inducing a state of self-stress that eliminates the floppy modes of the system by producing second-order rigidity. The underlying physical principle seems to be also at work in biological systems, most prominently in epithelial monolayers, but here it is predicted for entirely synthetic materials, like temperature-sensitive hydrogels and nematic elastomers, opening up the perspective of designing a new class of dynamic metamaterials.

CPP 49.5 Thu 12:30 ZEU/0255

**Aqueous Foams stabilized by PNIPAM Microgels: Effect of Cross-linker and Concentration** — •Joanne Zimmer, Kevin Gräff, Luca Mirau, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

Aqueous foams are abundant in everyday life, important for industrial applications and interesting from a fundamental point of view. In this work, aqueous foams are generated by sparging gas (nitrogen) through an aqueous dispersion of PNIPAM microgels, which are used as foam stabilizers. The microgel cross-linker content as well as the microgel concentration are varied and prove to significantly influence the foam formation properties (foamability) and the foam stability. A lower cross-linker content as well as a higher microgel concentration elevate the foamability, generate foams with higher liquid content and smaller bubbles and increase the foam stability. These observations are correlated with the microgel behaviour at the single air-water interface, i.e. pendant drop measurements and Langmuir trough. Our findings highlight good agreement across both length scales: an increase in foamability correlates with a faster decrease in surface tension, and a higher foam stability with a higher surface elastic modulus of a microgel-covered single air-water interface. The ability of the microgels to form a collective polymer network seems to dominate these processes.