

CPP 22: Gels, Polymer Networks and Elastomers I

Time: Wednesday 9:30–11:15

Location: H 0106

Invited Talk

CPP 22.1 Wed 9:30 H 0106

Production of various hybrid bio-based gel ink made of polymer grafted nanocellulose, suitable for 3D printing application — ●JULIEN R.G. NAVARRO, XUEHE JIANG, FERAS DALLLOUL, ENGUERRAND BARBA, and BENEDIKT MIETNER — Institute of Wood Science, University Hamburg, Germany

The use of biodegradable and renewable material resources, which can replace petroleum-based products, to produce performant functional materials are one of the greatest challenges for a future sustainable society. Within this philosophy, bio-based polymers such as nanocellulose have attracted considerable attention. However, nanocellulose needs further chemical surface modification to be considered as suitable ink material in specific applications or for being processed through 3D gel-printing. This talk will focus on the opportunity and the advantages of modifying the CNF surface chemically through the selective grafting and cross-linking of numerous polymers on its surface, with and without the presence of inorganic nanoparticles. The grafting of those specific entities onto the CNF surface not only affect the behavior of the CNF in suspension, but allows also to introduce numerous new properties before being processed through 3D-printing. In this talk, several gel-ink examples with various properties (luminescent, self-healing, anti-microbial) will be presented and their ability to be 3D printed will be shown.

CPP 22.2 Wed 10:00 H 0106

Predicting birefringence patterns and actuation of 3D-printed structures of liquid crystalline elastomers — ●SANTIAGO GOMEZ MELO, LI-YUN HSU, CLARA VAZQUEZ-MATEL, RASMUS SCHRÖDER, EVA BLASCO, FALKO ZIEBERT, and ULRICH SCHWARZ — Heidelberg University, Heidelberg, Germany

Liquid crystalline elastomers (LCEs) are a promising class of material to achieve autonomous deformation in response to external stimuli. Their actuation stems from the nematic-isotropic transition of a programmed molecular orientation, in which the LCE locally strains differently along the parallel and perpendicular directions. Recently, interest in this system has increased due to the possibility to 3D-print such materials as structures with arbitrary shapes. Here we show that the orientation in the sample can be controlled by positioning PDMS-scaffolds at the boundaries. Because they introduce strong anchoring boundary conditions, they determine the minimal energy solution of the Landau-de Gennes free energy of the LCE. We show both theoretically and experimentally that the use of suitable scaffold geometries allows for the engineering of diverse textures of the director field, which are then imprinted into the LCE by direct laser writing. To demonstrate successful design, we show that the calculated and measured birefringence patterns agree very well with each other. A similar test can be performed for mechanical actuation by temperature changes, which is predicted by modelling the LCE-microdevice as neo-Hookean material with an active deformation contribution.

CPP 22.3 Wed 10:15 H 0106

Insights into Modelling Cellulose Aerogels: A Computational Approach — JANNIK JARMS¹, ●NINA BORZECKA¹, and AMEYA REGE^{1,2} — ¹Institute of Materials Research, German Aerospace Center, Köln, Germany — ²School of Computer Science and Mathematics, Keele University, Staffordshire, England

There is an increasing demand for advanced sustainable materials that can be tailored for very specific applications. In this respect, aerogels have attracted considerable attention due to their extraordinarily high porosity, due to which they provide solutions for various applications such as insulation, sorbents, support for catalysts, etc.

The cellulose aerogel structure is formed due to polycondensation of D-glucose molecules. The structure formation is computationally designed with coarse-grained molecular dynamics. The system of beads represents the monomers, that during synthesis form polymer chains, and subsequently, the final gel structure. The system exhibits the Langevin dynamics which mimics the Brownian motion. The interaction of monomers and polymer chains was implemented as an ensemble of structural and polymer interaction model represented with Hooke's law and Lennard-Jones potential respectively.

The developed approach indicates good agreement with the experiments. Obtained computationally microstructures were characterized

in terms of pore structure. Combining experimental and numerical research creates an opportunity for deeper understanding the fundamentals of synthesis of these novel, promising materials.

CPP 22.4 Wed 10:30 H 0106

Systematic Organophilization of Montmorillonite: The Impact Thereof on The Characteristics of NBR and SBR Based Nanocomposites and Their Blends — ●HISHAM ESSAWY and SALWA EL-SABBAGH — National Research Centre, Cairo - Egypt

Different montmorillonites either, completely hydrophilic (Mont-0), amphiphilic (Mont-25, Mont-50, and Mont-75) or completely hydrophobic (Mont-100) were used as reinforcing fillers for styrene butadiene rubber (SBR) and acrylonitrile butadiene rubber (NBR) individually to predict the influence of the different forms on the properties of the rubbers (rheometric characteristics and mechanical properties). The shifts in the glass transition temperatures (T_g) after the clay insertion were determined from dynamic mechanical thermal analysis (DMTA) to investigate the preference and action of each form. In addition, the storage moduli were used as indications to the corresponding mechanical properties of the samples. The influences could be verified after comparing the impacts of aging conditions on the properties of rubber compositions. The obtained data may provide a platform to suggest the mechanism by which these forms can in some cases act as compatibilizers in addition to their reinforcing/plasticizing effect when employed with the physically incompatible NBR/SBR (50/50) blend, which helps to optimize the properties of nanocomposites based on these blends. The proposed mechanism of action showed good correlation with the results of the mechanical properties and x-ray diffraction (XRD) investigations as well.

CPP 22.5 Wed 10:45 H 0106

Surfactants as a tool for tuning the volume phase transition temperature VPTT of microgels — ●YULIA GORDIEVSKAYA¹, JOACHIM JELKEN¹, SE-HYEONG JUNG², NINO LOMADZE¹, ANDRIJ PICH^{2,3}, ELENA YU. KRAMARENKO⁴, and SVETLANA SANTER¹ — ¹University of Potsdam, Potsdam, Germany — ²RWTH Aachen University, Aachen, Germany — ³Aachen Maastricht Institute for Biobased Materials (AMIBM), Maastricht University, Geleen, The Netherlands — ⁴Moscow, Russia

Microgels are well-known to be highly responsive systems able to undergo volume phase transitions under changes in various environmental conditions. Due to this feature, they are used as nanocontainers, sensors, micropumps, and actuators in microfluidic systems. We showed the light-driven remote control of the volume phase transition temperature VPTT of p(NIPAM-AAc) microgels between 32°C and up to 95°C in the solution of azobenzene containing surfactants[1,2]. To discuss the mechanism of light-triggered VPTT shift we provided the theoretical calculations covering a wide range of surfactant concentrations and solvent quality. The factors determining the VPTT are electrostatic and hydrophobic interactions in the system and the translational entropy of counterions.

[1] Jelken, J., Jung, S. H., Lomadze, N., Gordievskaya, Y. D., Kramarenko, E. Y., Pich, A., & Santer, S. Adv. Funct. Mater., 2022, 32(2), 2107946. [2]. Schimka S., Gordievskaya Y.D., Lomadze N., Lehmann M., von Klitzing R., Romyantsev A.M., Kramarenko E.Y., Santer, S. J. Chem. Phys., 2017, 147(3), 031101

CPP 22.6 Wed 11:00 H 0106

Magnetic Controllability in Magnetic Nanogels — ●IVAN NOVIKAU¹ and SOFIA KANTOROVICH^{1,2} — ¹University of Vienna, Vienna, Austria — ²Ekaterinburg, Russia

Magnetic Nanogels (MNGs) have emerged as versatile soft materials, especially promising for biomedicine due to the bio-compatibility of external magnetic fields. Recent research has focused on incorporating magnetic nanoparticles (MNPs) into nanogels for targeted drug delivery, enhanced uptake by tumor cells, and advancements in medical imaging and therapy.

This study utilizes molecular dynamics (MD) simulations and the Lattice-Boltzmann (LB) scheme to investigate the magnetic controllability of MNGs. Specifically, we explore the effective transfer of MNP torque to the polymer matrix, providing insights into guiding MNGs through the circulatory system.

For the suspensions of MNGs we calculate the magnetic susceptibility, and analyse the influence of an external magnetic field on vis- | coelastic properties, with a specific focus on the dynamic moduli.