

## CPP 67: Polymer and Molecular Dynamics, Friction and Rheology

Time: Friday 9:45–12:15

Location: H13

CPP 67.1 Fri 9:45 H13

**Nanomechanische Charakterisierung von funktionalen Celluloseeinzelfasern** — ●JULIA AUERNHAMMER<sup>1</sup> und ROBERT STARK<sup>2</sup> — <sup>1</sup>Technische Universität Darmstadt, Institut Materialwissenschaften, Physics of Surfaces, Alarich-Weiß-Straße 16, 64287 Darmstadt — <sup>2</sup>Technische Universität Darmstadt, Institut Materialwissenschaften, Physics of Surfaces, Alarich-Weiß-Straße 16, 64287 Darmstadt

Der heutige Alltag ist ohne Applikation von Papier, wie in Printmedien, Verpackungsprodukte oder gar in technischen Spezialpapieren, kaum vorstellbar. All diese Anwendungen machen sich die einzigartigen Eigenschaften von Papier zu nutze. Papier ist porös und kann ohne externe Pumpen kapillargetriebenen Flüssigkeiten transportieren. Im Vergleich zu porösen Kunststoffen ist es chemisch und thermisch stabiler, reißfest und kann nach Gebrauch recycelt oder energetisch verwertet werden. Zum Design von Papieren mit funktionalen Eigenschaften werden die Papiere oft mit hydrophoben Polymeren modifiziert um die Nassreißfestigkeit zu verbessern. Mit Hilfe der Rasterkraftmikroskopie und der Korrelation zur Konfokalmikroskopie und Fluoreszenzmikroskopie wird hier ein detailreiches Bild der Verteilung des Polymerfilms auf einzelnen Cellulosefasern aufgezeigt. Zudem wird die räumliche Ausdehnung der Einzelfaser bei steigender Luftfeuchtigkeit sowie die damit verbundenen Veränderungen der lokalen mechanischen Eigenschaften an der Oberfläche der Einzelfaser herausgearbeitet. Weiterhin zeigt der Mikrozugversuch am Rasterkraftmikroskop das Verhalten von Einzelfasern bei mechanischer Beanspruchung unter verschiedenen Luftfeuchtigkeiten.

CPP 67.2 Fri 10:00 H13

**Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers** — ELIAS M. ZIRDEHI and ●FATHOLLAH VARNIK — ICAMS, Ruhr-Universität Bochum, Germany

The addition of small molecules is found to enhance the dynamics of structural relaxation in polymers and glasses [1]. This effect turns out to be a non-monotonic function of the particle size [2]. Through a detailed analysis of the non-Gaussian parameter for the particles and monomers, it is shown that the time scales of cooperative motion for the two constituents exhibit a separation when decreasing the size of particles. This decoupling of dynamics is also apparent in the ratio of diffusion coefficient and relaxation times of two species. Loss of the coupling effect makes the monomers become weakly influenced by the fast dynamics of the smaller particles. On the other hand, the larger particles are strongly coupled to polymers while being less mobile, which leads to a rather weak enhancement effect on the polymers dynamics. The strongest effect on polymers dynamics is observed in the intermediate particle sizes where the particles have high mobility as well as sufficiently strong coupling to the polymer matrix. A potential application of this effect can be the tuning of the triggering temperature in shape memory polymers. This issue is also briefly discussed.

1. Elias Mahmoudinezhad, Axel Marquardt, Gunther Eggeler and Fathollah Varnik, *Procedia Computer Science* 108, 265-271 (2017).

2. Elias M. Zirdehi, Fathollah Varnik, Non-monotonic particle size effect on the glass transition in polymer-particle blends (under rev.).

CPP 67.3 Fri 10:15 H13

**Rheology of Nonequilibrium Polymer Melts** — ●MANJESH K. SINGH, HSIAO-PING HSU, and KURT KREMER — Max Planck Institute for Polymer Research, Mainz, Germany

Polymers have become very popular in everyday use because of ease in processing of polymeric materials. Polymers are processed to different complex shapes from the molten state. Polymer melts display rich viscoelastic behavior in the typical length and time scales. The processing of polymer melts become difficult with increase in molecular weight (Mw) because of increase in viscosity. The long polymer chains in a melt have to move in a specific way due to the topological constraints "entanglements" imposed by neighboring chains. This happens because of the fact that the in a polymeric systems each monomers are connected to their neighboring monomers and can not crossover each other. Increase in number of entanglements with increase in Mw leads to increase in viscosity.

We have used complementary experimental and simulation ap-

proaches to study the development of entanglements in a fully disentangled melt of collapsed polymer chains and changes in viscosity, moduli and glass-transition temperature during the process.

CPP 67.4 Fri 10:30 H13

**Cyclization and relaxation dynamics of finite-length collapsed self-avoiding polymers** — ●JULIAN KAPPLER<sup>1,2</sup>, FRANK NOÉ<sup>1</sup>, and ROLAND R. NETZ<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, 14195 Berlin, Germany — <sup>2</sup>Cambridge University, Cambridge CB3 0WA, United Kingdom

The loop formation kinetics of polymers governs the dynamics of protein folding and gene expression regulation. The quantity of main interest is the cyclization time  $\tau_{cyc}$ , i.e. the mean time it takes the two polymer ends to find each other. We study the cyclization and relaxation dynamics of ideal as well as interacting polymers as a function of chain length  $N$ . For the cyclization time of ideal chains we recover the known scaling  $\tau_{cyc} \sim N^2$ , for a self-avoiding slightly collapsed chain we obtain from Langevin simulations and scaling theory a modified scaling  $\tau_{cyc} \sim N^{5/3}$ . The cyclization and relaxation dynamics of a finite-length collapsed chain scale differently; this unexpected dynamic multi-scale behavior is rationalized by the crossover between swollen and collapsed chain behavior.

CPP 67.5 Fri 10:45 H13

**Network dynamics in hydrogen-bonding telechelic polymers: associate lifetime, structural relaxation and phase separation** — ●MARTIN TRESS<sup>1</sup>, KUNYUE XING<sup>1</sup>, PENGFEI CAO<sup>2</sup>, SHIWANG CHENG<sup>3</sup>, TOMONORI SAITO<sup>2</sup>, VLADIMIR NOVIKOV<sup>1</sup>, and ALEXEI SOKOLOV<sup>1,2</sup> — <sup>1</sup>University of Tennessee Knoxville, Department of Chemistry, Knoxville, Tennessee, USA — <sup>2</sup>Oak Ridge National Lab, Chemical Sciences Division, Oak Ridge, Tennessee, USA — <sup>3</sup>Michigan State University, Department of Chemical Engineering and Material Science, East Lansing, Michigan, United States

Supra-molecular networks formed by reversible bonds between polymer chains exhibit extraordinary properties, e.g. extreme toughness & elongation at break or self-healing. We study short telechelic polymers with different H-bonding ends and backbones [Xing, Tress et al., *Macromolecules* 10.1021/acs.macromol.8b01210]. The H-bonds increase the glass transition temperature (Tg), though in flexible polydimethyl siloxanes it does not vary with H-bond strength whereas in much stiffer polypropylene glycol Tg varies significantly. In contrast, viscosity strongly depends on H-bond strength in the former while it is unchanged in the latter. Complementary measurements of mechanical and dielectric relaxation indicate that this due to competing lifetimes of supra-molecular associations and chain relaxation. Furthermore, viscoelastic properties are enhanced tremendously by phase separating ends, controlled by Tg of these aggregates. The concept of bond lifetime renormalization [Stukalin et al., *Macromolecules* 46 (2013) 7525] describes the results qualitatively but appears to fail quantitatively.

15 min. break

CPP 67.6 Fri 11:15 H13

**Filtering polymeric topologies in spatially-modulated nano channels** — ●LISA B. WEISS<sup>1</sup>, MATTIA MARENDA<sup>2</sup>, CRISTIAN MICHELETTI<sup>2</sup>, and CHRISTOS N. LIKOS<sup>1</sup> — <sup>1</sup>Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — <sup>2</sup>SISSA, International School of Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy

Polymers of various topologies are of importance in biology, rheology and material science. Macromolecules of distinct topology consist of the same type and number of monomers, making it challenging to separate them using chemical approaches. Nevertheless, topology influences strongly their response to flow fields in concentrated and dilute solutions. Previously, successful separation strategies for linear and circular polymers have been developed, which unfortunately fail in the case of knotted ring polymers. Thus, we present a novel separation strategy employing spatially-modulated channels, building up on topology-dependent diffusivities in such channels. We take hydrodynamic interactions via the multi-particle collision algorithm into account. In equilibrium, we find an astonishing inversion of diffusivities in modulated channels compared to bulk, which can be rationalized

by a Fick-Jacobs approach. Applying a flow enables a reliable separation of circular polymers from their knotted counter parts in weak flows. Looking in detail at the relevance of the size of the narrowing, we identify a regime of strong restrictions on polymer translocations in the case of pore sizes smaller than the average knot size. Here, the essential crossings act as a parachute preventing translocation.

CPP 67.7 Fri 11:30 H13

**Accelerating molecular dynamics simulations with population annealing** — •HENRIK CHRISTIANSEN<sup>1</sup>, MARTIN WEIGEL<sup>2</sup>, and WOLFHARD JANKE<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — <sup>2</sup>Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, England

We adapt Population Annealing to Molecular Dynamics simulations and demonstrate its ability to accurately simulate systems with rugged-free energy landscapes. For this we simulate the folding of met-enkephalin, a short peptide commonly used to test the performance of algorithms. A comparison with Parallel Tempering, the de facto standard for the simulation of complex systems with a rugged free-energy landscape using Molecular Dynamics, is presented. Further, we show that it is possible to use adaptive temperature steps in Population Annealing, i.e., the temperature set has not to be known beforehand, like in Parallel Tempering, but can be determined on-the-fly.

CPP 67.8 Fri 11:45 H13

**Dynamic Properties of Multiblock Copolymers** — •FABIAN BERRESSEM, FRIEDERIKE SCHMID, and ARASH NIKOUBASHMAN — Institute of Physics, Johannes Gutenberg-University Mainz

The ability of copolymers to self-assemble into well-defined nanostructures is of enormous importance in academic studies as well as in industry. This remarkable property makes it possible to create large volumes of materials with specific nanostructures and tailored properties. Previous research has focused mainly on the self-assembly of diblock copolymers, as the synthesis of these macromolecules is well-established. Recent advances in chemical synthesis have made it pos-

sible to create more complex polymers such as multiblock copolymers. Self-assembled structures of multiblock copolymers contain many loops and bridges, which can significantly alter their rheological properties due to entanglement effects. Thus, it is important to consider the chain conformations on a microscopic level to fully understand the macroscopic flow properties of the melts. The arrangement of the individual polymers, and hence the distribution of loops and bridges, strongly depends on the specific polymer properties as well as the employed manufacturing processes, e.g., solvent casting or spray coating. As a first step, we studied through self-consistent field theory (SCFT) the domain spacing and the loop and bridge distribution of lamella-forming multiblock copolymers in equilibrium, and found semiquantitative agreement with experiments. We then combined SCFT with molecular dynamics simulations of Lennard-Jones chains to determine the anisotropic shear viscosity of block copolymer melts.

CPP 67.9 Fri 12:00 H13

**Influence of interface hydration on sliding of graphene and molybdenum disulfide single-layers** — •HU LIN, ABDUL RAUF, NIKOLAI SEVERIN, IGOR M. SOKOLOV, and JÜRGEN P. RABE — Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Humidity influences friction in layered materials in peculiar ways. For example, while water improves the lubricating properties of graphite, it deteriorates those of molybdenum disulfide (MoS<sub>2</sub>). The reasons remain debated, not the least due to the difficulty to experimentally compare dry and hydrated interface frictions. For this, we strain the mica substrate and detect strain in graphene and MoS<sub>2</sub> by changes in Raman and photoluminescence spectra, respectively. The spectra show that the hydration of interfaces between a mica substrate and single-layers of graphene and MoS<sub>2</sub> with a molecularly thin water layer affects strain transfer from the substrate to the 2D materials. Strain relaxation in graphene changes from stick-slip in dry contact, to viscous when hydrated. In contrast, there is no viscous relaxation in MoS<sub>2</sub> regardless of hydration. Our work provides a novel approach for better understanding the impact of hydration on friction in layered materials.