CPP 56: Molecular and Polymer Dynamics, Friction and Rheology I

Time: Friday 10:45–12:00 Location: HÜL/S386

Invited Talk CPP 56.1 Fri 10:45 HÜL/S386

Liquid Dynamics at Interfaces — •Michael Vogel — Institut für Physik kondensierter Materie, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Liquids at interfaces are of great importance in nature and technology, for instance, in biological cells, clay minerals, and energy materials. Typically, the dynamics of liquids at interfaces significantly differ from those in the bulk. We combine nuclear magnetic resonance and broadband dielectric spectroscopy with molecular dynamics simulutations to determine the magnitude and range of these interface effects in broad frequency and temperature ranges. It is shown that the free energy landscape imposed by an interface on an adjoining liquid enables a basic understanding of the altered dynamical behavior [1]. It will be discussed that a knowledge of interface effects allows one not only to obtain valuable insights into the properties of confined water and, when avoiding crystallization, the anomalies and vitrification of bulk water [2-4], but also to steer ion transport in electrolyte-host systems for improved lithium-ion battery and proton-exchange membrane materials [5-7].

[1] S. Hefner et al., Phys. Rev. Lett. 133, 106201 (2024)
[2] V. Schiller and M. Vogel, Phys. Rev. Lett. 132, 016201 (2024)
[3] J. H. Melillo et al., PNAS 121, e2407030121 (2024)
[4] E. Steinrücken et al., J. Phys. Chem. Lett. 14, 4104 (2023)
[5] M. Stevenson et al., Adv. Funct. Mater. e15706 (2025)
[6] S. F. Winterstein et al., J. Am. Chem. Soc. 145, 27563 (2023)
[7] A. F. Privalov et al., J. Phys. Chem. Lett. 14, 9335 (2023)

CPP 56.2 Fri 11:15 HÜL/S386

The analytical and numerical investigation of star-shaped copolymers with three arms in confined geometries — •Zoriana Danel[1], Joanna Halun[2], and Paweł Karbowniczek[1] — [1]Cracow University of Technology, Poland — [2]Institute of Nuclear Physics, Poland

The influence of star copolymer topology on the depletion interaction potentials, the depletion forces, the radius of gyration and the monomer density profiles is investigated analytically and numerically. The method of analytical calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star-shaped copolymers with three legs in combination f=2-1 in a Θ-solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the case of one repulsive and the other inert surface is proposed. Besides, molecular dynamic simulations of a dilute solution of star-shaped copolymers in a good solvent with three number of legs with N=801 monomers (300+300+200+1) for combination f=2-1 and N=701 monomers (300+200+200+1) for combination f=1-2 confined in a slit with different boundary conditions are performed and the results of the monomer density profiles for the above mentioned cases are obtained for the narrow and wide slit region. Furthermore, the numerical calculations of the radius of gyration for star-shaper copolymers in combination f=2-1 and f=1-2 are performed. The obtained results are interesting from scientific and practical point of view, because of their potential application in materials engineering, nano-technology, biotechnology and medicine.

CPP 56.3 Fri 11:30 HÜL/S386

Polymer melt dynamics in the light of viscoelastic hydrodynamic interaction — •Hendrik Meyer — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 67034 Strasbourg, France

Our group has shown that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D [1] and 2D [2] and excellent agreement between theory and molecular dynamics simulation is found. The theory was developed for momentum conserving dynamics as well as Langevin dynamics. The physical mechanism considers that hydrodynamic interactions are time dependent because of increasing viscosity before the terminal relaxation time. We show that this mechanism is generally active and relevant in melts including entangled systems, rings or stars.

[1] PRL 107, 178301 (2011); PRE 85, 051807 (2012). [2] PRL 109, 248304 (2012); Soft Matter 9, 4249 (2013).

CPP 56.4 Fri 11:45 HÜL/S386

Knots in Polymers under Shear Flow — •Maurice P. Schmitt[1], Andrey Milchev[2], and Peter Virnau[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

Knots in polymers and biological macromolecules, such as DNA and proteins, are crucial to their structure and function. However, the effect of external forces on knots in polymers is still insufficiently understood. Here, we investigate the impact of shear and Poiseuille flow on knotted flexible polymers using Molecular Dynamics (MD) and Multi-Particle Collision Dynamics (MPCD) simulations. We find that under simple shear (Couette flow), initially loose knots in polymer coils tighten beyond a critical shear rate. Further increase of the shear rate leads to tumbling motions of the chains in flow and fluctuating knot sizes. In contrast, knotted polymer globules subjected to shear unfold into pearl-necklace-like conformations, whereby knots spread across multiple sub-globules and undergo dynamic topological transitions. In Poiseuille flow, knots also tighten under increasing flow strength, with fluctuations in knot size emerging at high shear rates. Unexpectedly, the slit thickness significantly influences the tightening process even at constant mean shear rate. These findings reveal that both Couette and Poiseuille flow induce major structural and topological transformations in knotted polymers, offering insight into the behavior of knots under hydrodynamic forces in confined and driven environments.