CPP 23: Polymer and Molecular Dynamics, Friction and Rheology

Time: Wednesday 9:30–11:15 Location: H34

Invited Talk CPP 23.1 Wed 9:30 H34

Advanced combined rheometer setups to in-situ correlate molecular dynamics and molecular structure formation with mechanical properties — •Manfred Wilhelm — Karlsruhe Institut für Technologie, Karlsruhe, Germany

Molecular understanding of mechanical properties over a broad length and time scale is crucial to develop advanced materials. Our research aims to design and built unique combined rheometer setups that can monitor in-situ molecular observables, such as molecular dynamics or chemical functional groups that are directly correlated to the macroscopic mechanical responses. These combined experimental setups overcome the experimental challenges associated with offline measurements and facilitate the understanding of structure-property relationships.

CPP 23.2 Wed 10:00 H34

Nonequilibrium Dynamics of the Helix-Coil Transition in Polyalanine — •Maximilian Conradi[1], Henrik Christiansen[1,2], Suman Majumder[3], Fabio Müller[1], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]NEC Laboratories Europe GmbH, Kurfürsten-Anlage 36, 69115 Heidelberg, Germany — [3]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India

In this work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyalanine are investigated. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. At the start of the transition short 310-helices form, leading to the molecule becoming more rod-like midway through the collapse. Afterwards, α-helix formation becomes the prevalent ordering mechanism leading to multi-leg hairpin structures, representative for the equilibrium behavior of longer chains. The dynamics of this transition is explored in terms of the power-law scaling of various associated relaxation times as a function of the chain length.

CPP 23.3 Wed 10:15 H34

Porous Particles Formation in the Drying of Polymer Solution Droplets — •Mengmeng Wu, Hsiao-Ping Hsu, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Due to the unique properties such as large specific surface area, high permeability and low density, porous polymer nano- or micro-spheres are promising for various applications including biomedical, pharmaceutical, tissue engineering and degradable electronic applications. We develop a coarse-grained polymer solution droplet model to study the particle structure formation of drying polymer solution droplets. By maintaining below the glass transition temperature, highly porous particles are generated followed by a fast evaporation and cavitation of solvents. For a drying droplet in an environment with low thermal conductivity, the temperature experiences a decrease owing to solvent vaporization. Such temperature reduction results in a decrease in evaporation rate during evaporation, consequently impacting the drying dynamics of polymer droplets. Our investigation explores how the cooling of droplets during solvent evaporation influences the final morphology of polymer particles.

CPP 23.4 Wed 10:30 H34

Polymer chains under oscillatory force in solvents of variable quality — •Bogumiła Szostak[1,2], Ron Dockhorn[2], Jens-Uwe Sommer[2], and Jarosław Paturej[1,2] — [1]University of Silesia in Katowice, Bankowa 12, 40-007 Katowice, Poland — [2]Leibniz Institute of Polymer Research Dresden, Hohe Straße 6 D-01069 Dresden, Germany

Polymers are key materials in soft condensed matter with diverse applications. Recently, significant attention has been given to understanding the micromechanical behavior of single macromolecules under applied forces. Using molecular dynamics, we examined how constant and periodic forces affect polymer chain conformations in dilute solutions, modeled for good and poor solvents. We systematically calculated the projection of the end-to-end vector in the force direction as a function of the applied force. This analysis led to the construction of force-extension diagrams, which revealed conformational transitions of polymers from a globular state to an extended chain. Analysis of hysteresis loops for periodic forces showed that longer force periods allowed more time for the system to respond, resulting conformational reorganization. These results were compared with analytical solutions of the Rouse model under periodic perturbation and scaling laws, providing a valuable benchmark and deeper insight into the observed dynamics. We also characterized the relationship between dissipated energy and the frequency of the applied sinusoidal stretching force. These findings provide new insights into the mechanical behavior of polymer chains under oscillatory forces, enhancing our understanding of their dynamic properties and potential applications.

CPP 23.5 Wed 10:45 H34

Role of Trapped Water Molecules at Sliding Contacts in Lattice-Resolved Friction Investigated with Molecular Dynamics — •Miljan Dašić and Igor Stanković — Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Understanding nanoscale friction within an environment which contains water, is crucial for engineering friction-based mechanisms and characterizing surfaces. From the point of view of Friction Force Microscopy (FFM) experiments, it has been understood that the lattice resolution in water environments originates from a dry contact state, in case of which all water molecules get expelled from the gap between the microscope's tip and the studied substrate.

We have developed an All-Atom Molecular Dynamics simulation setup, for revisiting this understanding by performing a detailed analysis of the impact of water molecules present in the system on the dynamic behavior of the nanotribological contact between an amorphous SiO2 probe and a monolayer MoS2 substrate.

Our analysis of stick-slip patterns shows the entrapment of water molecules at the contact interface. These trapped water molecules act as an integral part of the probe and participate in its interaction with the substrate, hence affecting the probe's dynamics and preventing long slips. Surrounding water molecules from the capillary or layer of water exhibit a replenishing effect, acting as a water reservoir during the sliding process. Such a phenomenon enables the preservation of lattice-scale resolution across a range of normal loads.

CPP 23.6 Wed 11:00 H34

The analytical investigation of star polymers in confined geometries — •Zoriana Danel[1], Joanna Halun[2], and Maciej Dudek[3] — [1]Cracow University of Technology — [2]Institute of Nuclear Physics — [3]Academy WSB

The analysis of the influence of star polymer topology on the depletion interaction potentials, the depletion forces and Pincus force was carried out analytically. The method of calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star polymers with f=3, 4, 5 legs 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 was proposed. Besides, we performed the investigation of the elastic properties of star polymers with different number of legs in a semi-infinite space confined by single wall with different boundary conditions and calculated Pincus force in the above mentioned cases. Calculations were carried out for star polymers with f=3,4,5 legs attached to the substrate by one or two arms. The acquired results showed that the Pincus force is affected by the number of arms attached to the surface. The obtained results are interesting from scientific and industrial point of view, because of their potential use in the production of paints, varnishes and new functional materials. Star polymers, due to their topology and shape can find practical application in nano - technology, as well as in biotechnology and medicine for drug and gene transmission.