DY 20: Soft Particles in Flows III (Focus session, joint DY/CPP)

Organized by S. Gekle, G. Gompper, C. Wagner

Time: Tuesday 14:00–15:45 Location: ZEU 160

Invited Talk DY 20.1 Tue 14:00 ZEU 160

Particle based simulations of viscoelastic Soft Matter — •Wim Briels — University of Twente, Enschede, The Netherlands

In order to describe flow of soft matter in complex geometries detailed information is needed about how stresses depend on velocity gradients and concentration. Besides this, often compressible flow equations must be solved concomitantly with diffusion equations.

Since it is difficult to collect the appropriate information and to accurately represent it with a constitutive model, it is natural to develop particle based methods that can be applied to large portions of matter. In order to achieve this goal, large mesoscale objects must be represented by single particles, which move such that both the thermodynamic and the viscoelastic properties of the system are recovered.

The rheological response of Soft Matter usually results from a strong interplay between processes at all time and length scales, including the ones that have been removed by coarse graining. I will discuss a model in which the internal dynamics of the particles is reinstated through the introduction of a few structural parameters. I will apply our approach to describe the rheology of pressure sensitive adhesives and telechelic polymers. If time permits I will address some issues concerning the application of Brownian dynamics simulations of flowing soft matter in complex geometries.

DY 20.2 Tue 14:30 ZEU 160

Telechelic star polymers under shear. — •Diego Jaramillo-Cano[1], Manuel Camargo[2], and Christos N. Likos[1] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria. — [2]CICBA, Universidad Antonio Nariño Campus Farallones, Km 18 via Cali-Jamundí, 760030 Santiago de Cali, Colombia.

Telechelic star polymers(TPSs) are macromolecules formed by a number of diblock copolymers(arms) anchored to a common central core, being the internal monomers solvophilic and the end monomers solvophobic. Recent studies have demonstrated that TPSs constitute self-assembling building blocks with specific softness, functionalisation, shape and flexibility: depending on different physical and chemical parameters, e.g. number of arms f, solvophobic-to-solvophilic ratio α and solvent quality λ, the conformation of TSPs features a well defined number of attractive spots on the surface(patches). In this work, we exhaustively study the conformation of isolated TSPs under shear by means of a combination of MPCD for the solvent and standard MD for the monomers. By employing the Lees-Edwards boundary condition, we systematically evaluate star shape descriptors, patches distinctive features and star rotation frequency as a function of the Weissenberg number Wi for low functionality of the TPSs. We cover a wide range of parameters for representative systems given by f=18, α=0.3,0.5,0.7, λ=1.0,1.1 and Wi=1-1400. Since the conformation of single stars is expected to be preserved in low-density bulk phases, the presented results are a first step in understanding and predicting the rheological properties of semi-dilute suspensions of this kind of polymers.

DY 20.3 Tue 14:45 ZEU 160

Soft colloid suspensions in external flow fields — •Roland G. Winkler and Gerhard Gompper — ICS and IAS, Forschungszentrum Jülich, 52428 Jülich, Germany

Soft colloids, like linear polymers as well as more complex polymeric structures such as star polymers or polymer networks exhibit large conformational changes and an intriguing dynamics when exposed to, e.g., a shear flow [1]. The flow field leads to polymer stretching, associated with a shape change of the soft colloids, and alignment, which depend on the specific structure of the particle. The particular structure even more determines the nonequilibrium dynamics. We will present simulation results of the nonequilibrium properties of such polymeric structures obtained by combining the multiparticle collision dynamics method, a mesoscale simulation approach for fluids [2], with molecular dynamics simulations for embedded polymeric objects. Moreover, the rheological characteristics of semidilute suspensions of linear [3] and star polymers [4] as well as end-functionalized semiflexible polymers [5] will be discussed.

[1] R.G. Winkler *et al.*, Curr. Opin. Colloid Interface Sci. **19**, 594 (2014)
[2] G. Gompper *et al.*, Adv. Polym. Sci. **221**, 1 (2009)
[3] C.-C. Huang *et al.*, Macromolecules **43**, 10107 (2010)
[4] S. P. Singh *et al.*, J. Chem. Phys. **141**, 084901 (2014)
[5] J. S. Myung *et al.*, J. Chem. Phys. **143**, 243117 (2015)

DY 20.4 Tue 15:00 ZEU 160

Soft particles at a fluid interface — •Jens Harting[1,2,3], Hadi Mehrabian[2,3], and Jacco Snoeijer[3,2] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Str. 248, 90429 Nürnberg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands — [3]Physics of Fluids Group, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands.

Particles added to a fluid interface can be used as a surface stabilizer in the food, oil and cosmetic industries. As an alternative to rigid particles, it is promising to consider highly deformable particles that can adapt their conformation at the interface. In this study we compute the shapes of soft elastic particles using molecular dynamics simulations of a cross-linked polymer gel, complemented by continuum calculations based on linear elasticity. It is shown that the particle shape is not only affected by the Young's modulus of the particle, but also strongly depends on whether the gel is partially or completely wetting the fluid interface. We find that the molecular simulations for the partially wetting case are very accurately described by the continuum theory. By contrast, when the gel is completely wetting the fluid interface the linear theory breaks down and we reveal that molecular details have a strong influence on the equilibrium shape. See: Soft Matter 12, 1062-1073 (2016)

DY 20.5 Tue 15:15 ZEU 160

Migration-transition of sedimenting soft particles in vertical flows — •Andre Förtsch, Matthias Laumann, Diego Kienle, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth

The dynamics of soft, heavy (light) particles is investigated in plane Poiseuille flows between two vertical walls and in the limit of a vanishing Reynolds number. We observe, that heavy (light) soft particles migrate to (away from) the center of a parabolic Poiseuille flow profile with the flow direction parallel to the gravitational force, similar as for buoyant particles. If the flow direction is reversed and antiparallel to gravitation, we find a surprising reversal of the migration direction and heavier (lighter) particles migrate away from (to) the center of a parabolic flow profile. This transition of the migration direction is determined numerically by the Stokesian particle dynamics and the Lattice-Boltzmann-Method as well as analytically in case of small deformations of a ring polymer. The migration away from the center is slowed down due to hydrodynamic particle-wall interactions. The parameter dependence of the final off center particle position may be used for separating different particles.

DY 20.6 Tue 15:30 ZEU 160

Synthesis and characterization of asymmetric, viscoelastic micro-swimmers with a propulsion mechanism based on chemical reactions — •Monika Pella and Heinz Rehage — Physikalische Chemie II, Technische Universität Dortmund, D-44227 Dortmund, Deutschland

Analyzing the movement and self-organization of living cells, it is generally difficult to distinguish between physical interactions and biological processes. More detailed insights into the basic mechanisms of the swimming motions of living cells can by enabled by the investigation of artificial model swimmers. Hydrogel capsules are especially suitable for this purpose because they have similar mechanical properties as biological cells. Active chemical compounds can be stored as fuel in the core of these capsules, serving as an energy source for the propulsion of these particles. Accordingly, each swimmer has its own impellent and can move independently from each other. We investigated in different types of capsule swimmers using oxygen formation as backstroke that pushed the particles forward. Particularly the trajectories, the velocities, the attachments at solid walls, the physical-chemical properties

and the typical swarming behavior of these artificial capsule swimmers are interesting. In addition to these experiments, we also analyzed the capsule swimming motion in the regime of small and large Reynold numbers.