RODLIKE COLLOIDS IN SHEAR FLOW: A MULTI-PARTICLE-COLLISION DYNAMICS STUDY

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Recently, there has been an increased interest in shear-induced phase transitions, and especially in inhomogeneous steady states which may exist between two coexisting phases. To gain insight into the underlaying microscopic mechanisms, we perform mesoscale simulations of solutions of rodlike colloids.

Studying the dynamical properties of colloids and polymers, respectively, in solution requires the adequate inclusion of hydrodynamic interactions. For an efficient treatment of such systems by computer simulations, the large length and time scale differences call for a coarse grained and simplified description of solvent dynamics. A particle based mesoscale simulation method – which we denote as Multi-Particle-Collision dynamics (MPCD) method – has attracted considerable attention, because it can naturally be coupled to a solute and combined with, e.g., molecular dynamics simulations.

Performing a series of simulations exploiting the MPCD method combined with molecular dynamics simulations, we demonstrate that the proper dynamics of flexible molecules in solution (Zimm dynamics) is obtained. In particular, the scaling of the Rouse mode amplitudes follows the predictions of the Zimm model. Similar studies of rodlike colloids display the influence of the hydrodynamic interactions on the diffusion and rotational dynamics. Applying a shear flow, we study the structural and dynamical properties of the colloids at various densities.

The method and results of the various simulations will be presented in the lecture.