

Theoriekolloquium

Am **9. Juli 2015** um **14.15 Uhr** in **W2 1-143** hält

Frau Prof. Dr. Friederike Schmid

einen Vortrag mit dem Titel

Studying mesoscale flow phenomena with dissipative particle dynamics

Dissipative Particle Dynamics (DPD) is a relatively new method for studying soft materials and complex fluids at a coarse-grained level. In the talk, I will introduce the DPD method, discuss recent ideas on DPD-based methods to simulate flow on mesoscales, and present selected applications.

Specifically, I will discuss flow in confined and structured environments. Structuring is an efficient tool to modulate the hydrodynamic boundaries at surfaces. We have performed Dissipative Particle Dynamics simulations of flow past superhydrophobic striped surfaces in microchannels, which demonstrate how anisotropic surface patterning may result in an anisotropic slip tensor. The simulation results are in excellent agreement with theoretical predictions. As an application, microchannels with variable surface slip can be used to separate enantiomeric particles by chirality.

Another topic of current interest is the simulation of electrohydrodynamic phenomena. Mesoscale simulations of electrokinetic phenomena are challenging due to the long range nature of both hydrodynamic and electrostatic interactions. In solutions of high ionic strength, the electrostatic interactions are partly screened, but the ions in solution still influence the hydrodynamic flows. We have developed a new hybrid DPD-Brownian Dynamics method which was specifically designed to enable efficient DPD-based simulations of electrolytes at high salt concentrations. The method is applied to the simulation of electroosmotic flow on superhydrophobic surfaces, and the results are compared to recent theoretical predictions by A. Belyaev and O. Vinogradova.

Interessierte sind herzlich eingeladen.

gez. Prof. Dr. Alexander Hartmann