

41st SFB 716 Colloquium

May 16, 2013 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites colleagues and interested person to the upcoming colloquium. In this lecture series renowned researchers and members of our subprojects talk about their research findings regarding dynamic simulation of systems with large particle numbers.

TALK 1

**Prof. Dr.
Wolfgang Paul**

Martin Luther
Universität Halle,
Department of
Physics

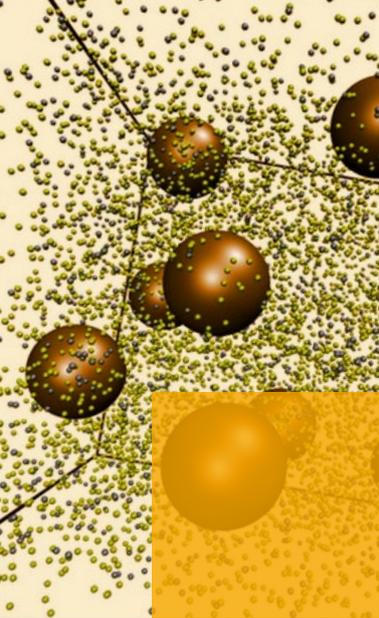
Structure and dynamics of a confined polymer melt: MD simulations of 1,4-polybutadiene between graphite walls

Composite materials made of polymers into which hard nano-objects are dispersed are abundant in technological applications. A very old application is car tires, i.e., styrene-butadiene rubber filled with carbon black nano-particles; a very modern one are carbon-nanotube reinforced polymers. In all these cases one hopes that the composite material will show properties which are improved compared to what each of the components would offer, very often, as in the two above examples, it is the mechanical behavior which ones tries to improve.

The special properties of the composites originate in the interface region between the filler and the matrix, and dispersing nano-objects is aimed at creating a large interface. For a polymer in contact with a hard filler, it is the change in behavior of the soft material next to the interface

which is relevant. And thinking about mechanical behavior, one has to consider the influence such a hard filler interface might have on the glass transition in the polymer matrix.

We will present chemically realistic Molecular Dynamics simulations of 1,4-polybutadiene (one of the components in the car tire) confined by graphite walls. The structural changes induced by the presence of hard walls give rise to changes in the relaxation properties of the matrix near the wall, and we will discuss how different experimentally accessible relaxation functions are altered. We will focus especially on dielectric experiments and their relation to the question of glass transition shifts in confinement.



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TALK 2

Dominic Röh

University of Stuttgart,
Institute for Computational
Physics

Subproject D.6

Hydrodynamic Correlations slow do Crystallization of Soft Colloids

Crystallization is commonly assumed to be a quasi-static process that is unaffected by details of particle transport other than the bulk diffusion coefficient. Therefore colloidal suspensions are often seen as a model system for experimentally more difficult systems such as metal melts, despite the need for a solvent.

We report molecular dynamics simulations of the crystallization in a suspension of Yukawa-type colloids. In order to investigate the role of hydrodynamic interactions mediated by the solvent, we modeled the solvent both, implicitly and explicitly using Langevin dynamics and the fluctuating Lattice Boltzmann method, respectively.

Our simulations show a dramatic reduction of the crystal growth velocity even at moderate hydrodynamic coupling, compared to the simulations without hydrodynamic interactions. A detailed analysis shows that this slowdown is due to the wall-like properties of the crystal surface, which reduces the colloidal diffusion towards the crystal surface by hydrodynamic screening. Crystallization in colloidal systems therefore differs strongly from pure melts, thereby making them less useful as a model system than previously thought.