

32th SFB 716 Colloquium

19 April 2012 | 4 pm

**New
location!**

University of Stuttgart
Campus Vaihingen
Pfaffenwaldring 27
Hörsaal V 27.01

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.
Roland Netz**

Free University
Berlin, Department
of Physics

Simulation approaches to friction and hydration in biomatter

The dynamics of biomatter is considerably slowed down by internal friction effects, effective forces between macromolecular assemblies involve slowly equilibrating hydration layers. Insight can be gained from all-atomistic simulations with explicit water that use novel concepts for efficient simulations. Three connected lines of work will be discussed:

- 1) The friction of surface-adsorbed peptides is very low on hydrophobic substrates but large on polar, hydrophilic substrates[1]. A modified Amonton's law is introduced, which generally describes the dynamics of hydrogen-bonded matter on the nano-scale[2].
- 2) The contribution of internal friction to the folding of peptides is traditionally probed by changing the solvent viscosity and extrapolating down to vanishing solvent viscosity. We apply the same procedure to simulations of short disordered and alpha-helix forming peptides, the

results can be favorably compared with results borrowed from polymer theory[3].

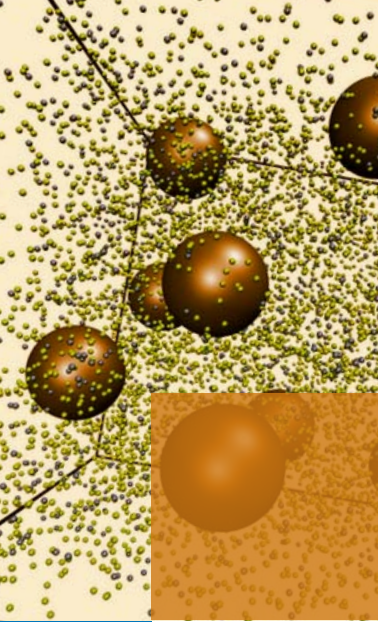
- 3) The so-called hydration repulsion between polar surfaces in water is studied using a novel simulation technique that allows to efficiently determine the interaction pressure at constant water chemical potential[4]. The hydration repulsion is shown to be caused by a mixture of water polarization effects and the desorption of interfacial water.

[1] Polypeptide friction and adhesion on hydrophobic and hydrophilic surfaces: A molecular dynamics case study. A. Serr, D. Horinek and R.R. Netz, JACS 130, 12408 (2008).

[2] Viscous Friction of Hydrogen-Bonded Matter. A. Erbas, D. Horinek, R.R. Netz, JACS 134, 623–630 (2012).

[3] Peptide Chain Dynamics in Light and Heavy Water: Zooming in on Internal Friction. J. Schulz, L. Schmidt, J. Dzubiella, R.R. Netz, JACS dx.doi.org/10.1021/ja211494h (2012).

[4] From simple surface models to lipid membranes: Universal aspects of the hydration interaction from solvent-explicit simulations. E. Schneck, R.R. Netz, Current Opinion in Colloid & Interface Science 16, 07–611 (2011).



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INFORMATION

15 minutes

Status information

TALK 2

Dominic Röhms

University of Stuttgart,
Institute for Computational
Physics (ICP)

Subproject D.6

Effects of hydrodynamic interactions in heterogeneous nucleation of colloids

Nucleation, the early stage of crystal growth, is still a rather poorly understood process. We investigate the heterogeneous nucleation in a colloidal model system near a wall using Molecular Dynamics computer simulations. In our coarse-grained simulations, the particles interact via a screened Coulomb (Yukawa-) potential representing charged colloids in water. Our focus lies on the influence of the hydrodynamic interaction, which is often neglected, since nucleation is considered as a quasi-static process. However, recent experiments have shown, that the kind of thermalization of the sample has a drastic influence on the nucleation rate.

In our simulations, we incorporated hydrodynamic interactions by coupling the particles to a lattice fluid. Since the com-

putation of the hydrodynamic interaction is still orders of magnitude more expensive than classical interactions, we have recently enabled our MD simulation software ESPResSo to employ GPUs for the calculation of the lattice fluid. By this, we can investigate systems, that previously required a small computer cluster, using a single GPU. Using a cluster equipped with GPUs, allows us to systematically investigate the influence of hydrodynamics on the heterogeneous nucleation, and explain why laminar flow conditions, as found e.g. in typical experimental settings between microscope sliders, can lead to enhanced nucleation by pre-ordering.