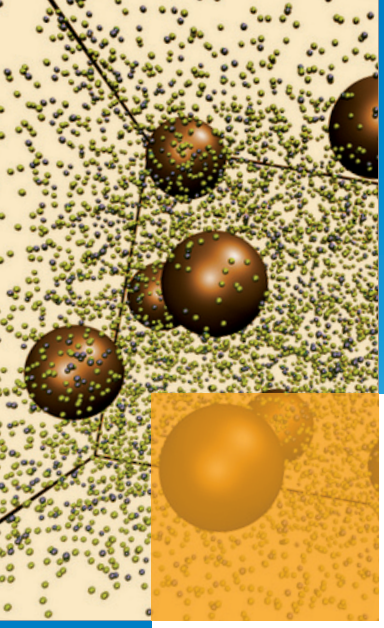


University of Stuttgart
SFB 716

Colloquium of the SFB 716

June 14th, 2018 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites to the upcoming colloquium. In this lecture series guest speakers and members of our subprojects inform about their results regarding the dynamic simulation of systems with large particle numbers.

TALK

Prof. Dr.
Ralf Drautz

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

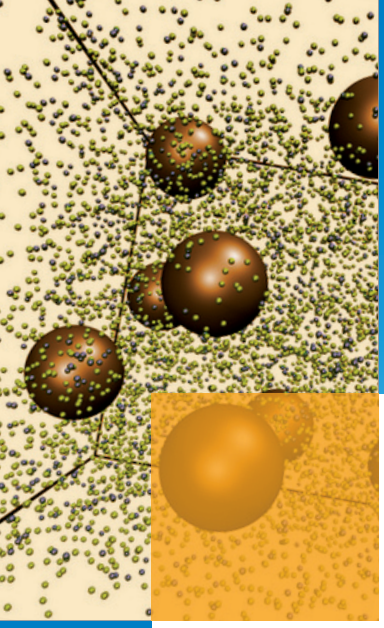
Ruhr-Universität Bochum

From electrons to interatomic interactions and to properties of materials

Density functional theory (DFT) provides a solid basis for the simulation of materials properties. The computational expense of DFT often makes the calculation of materials properties difficult. We coarse grain the interatomic interaction from DFT to allow for faster and larger simulations. The resulting analytic Bond-Order Potentials (BOPs) contain the important contributions to bond formation, including magnetism and charge transfer, naturally within their remit. The BOPs are orders of magnitude faster than DFT and allow for the direct sampling of thermodynamic observables.

I will discuss the application of the BOPs to simulating finite temperature properties in iron. I will further discuss the simulation of nucleation and solid-solid transformations with relevance to high-temperature materials. A short summary of recent activities for a more systematic validation of interatomic potentials will also be given.

www.sfb716.uni-stuttgart.de



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TALK

Kai Szuttor,
Florian Weik

Prof. Dr.
Christian Holm
Subproject C.5
Institute for Computational Physics (ICP)
University of Stuttgart

A multiphysics model for the simulation of DNA nanopore translocation

We present our progress in developing a multi-physics model for the simulation of DNA nanopore translocation. We show how salient physical properties of the coarse-grained DNA model we presented earlier can be included in an all-continuum description of the system. Further, we will show newer developments of the electrokinetics model we use. Namely, work towards a consistent inclusion of thermal fluctuations and a octree based solution for adaptivity in the diffusion part of the implementation.