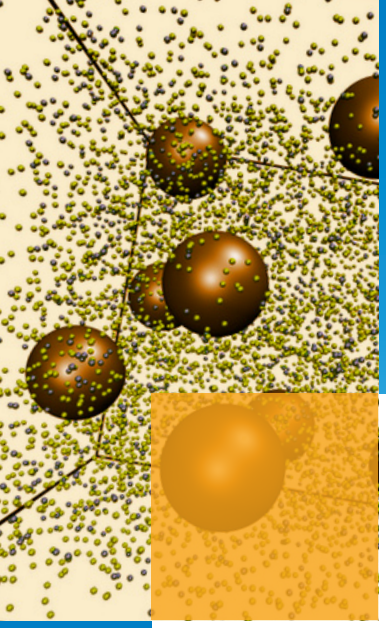

University of Stuttgart
SFB 716

Colloquium of the SFB 716

May 11th, 2017 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites colleagues and interested persons 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.

www.sfb716.uni-stuttgart.de

TALK

Prof. Dr. Christian Elsässer

Fraunhofer Institute for Mechanics of Materials IWM, Freiburg

Search for substitutes of hard-magnetic materials containing less critical elements by computational high-throughput screening

The discovery and design of new hard-magnetic intermetallic phases for high-performance permanent magnets are addressed by means of efficient and predictive computational high-throughput-screening approaches. The challenge is to identify substitutes for established hard-magnetic materials like Nd2Fe14B, which have outstanding functionalities but also constraining criticalities. To find promising candidates for new hard-magnetic phases, quantum-mechanical screening calculations based on density functional theory (DFT) are carried out to search for crystal structures and chemical compositions of intermetallic phases composed of transition-metal, rare-earth, and further substitutional or interstitial alloying elements, which have comparably good intrinsic ferromagnetic properties but contain less amounts of critical rare-earth elements than, e.g., the most prominent compound Nd2Fe14B.

References: N. Drebov, A. Martinez-Limia, L. Kunz, A. Gola, T. Shigematsu, T. Eckl, P. Gumbsch, and C. Elsässer, *New J. Phys.* 15, 125023 (2013); W. Körner, G. Krugel, and C. Elsässer, *Sci. Rep.* 6, 24686 (2016).

TALK

Ewa Anna Oprzeska-Zingrebe

Institute for Computational Physics (ICP), Subproject C.8 (Milestone-Presentation)

Interactions between a short DNA oligonucleotide and urea in the light of Kirkwood-Buff theory: a Molecular Dynamics simulation study

In nature, a wide range of biological processes, such as transcription termination or intermolecular binding, is dependent on the formation of specific DNA secondary and tertiary structures. These structures can be both stabilized or destabilized by the osmolytes, coexisting with the nucleic acids in the cellular environment. In our study, we investigate a simple 7-nucleotide DNA hairpin with the sequence d(GCGAAGC) in the presence of varying concentrations of urea.

The interaction between DNA and urea in unbiased molecular dynamics simulations has been analysed according to Kirkwood-Buff theory. We implemented the local/bulk partitioning model, complemented by the analysis of preferential hydration and preferential interaction coefficients, to get insight into the distribution of the cosolute in the vicinity of the DNA oligonucleotide. The free energy landscape of unfolding has been approached via Metadynamics upon the addition of a bias potential. This study allows us to get a more comprehensive understanding of the stability of the DNA structures in the presence of urea.