



# Colloquium of the SFB 716

July 12<sup>th</sup>, 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

Jörg Baz  
M.Sc.

### Predicting the Influence of Complex Solvent Environments on Thermophysical Properties

Jun.-Prof.

Niels Hansen  
Subproject A.9

Institute of  
Thermodynamics  
and Thermal  
Process  
Engineering (ITT)

University of  
Stuttgart

Part I:

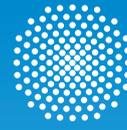
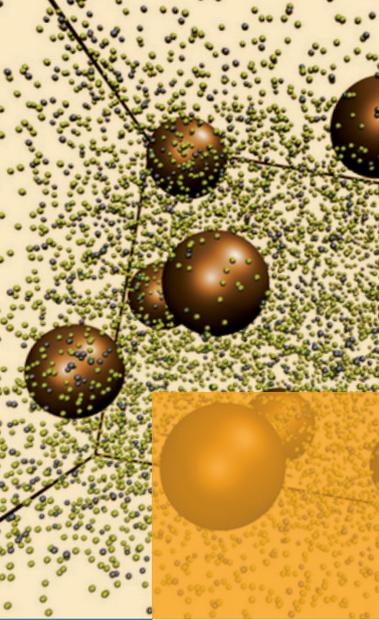
Functional organic materials composed of dye-based molecules that stack into various structures by non-covalent intermolecular forces have fascinating optical and mechanical properties. These novel materials are of increasing importance for many high-technology applications. Here is a need for a rational design of such materials based on the engineering of dye-dye interactions and the prediction of how these interactions impact the properties of nano- or bulk state materials. Perylene di-imide derivatives (PDIs) emerged as a prototype class of molecules for the elucidation of the transition from monomeric to bulk materials via the supra-molecular state.

We discuss the influence of the molecular architecture and the solvent composition on the thermodynamic fingerprint of the aggregation and investigate the ability of classical molecular dynamics simulations to be used in rational materials design.

Part II:

Deep eutectic solvents (DES) are used for biocatalysis reactions more and more. Low saturation vapor pressure, hard flammability as well as little toxicity are only a few advantages compared to previously used substances. Choosing the right solvent composition can lead to low viscosities with simultaneously low water activity which are required conditions for reactions and process design.

In this project static and dynamic mixture properties for a DES based on choline chloride and glycerol mixed with water are investigated due to their concentration and temperature dependence using means of molecular dynamics simulations.



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## TALK

Prof. Dr.  
Barbora

Kozlikova

Department of  
Computer Graphics  
and Design

Masaryk University,  
Brno (CZE)

## Visualization of Large Ensembles of Molecular Dynamics Simulations

In this talk, I will present one of the most currently intriguing problems in studying the behavior of molecular structures, the exploration of large ensembles of molecular dynamics simulations. I will outline several possible solutions we have developed in the last years in tight collaboration with the domain experts and will present our latest results and challenges for the future research.