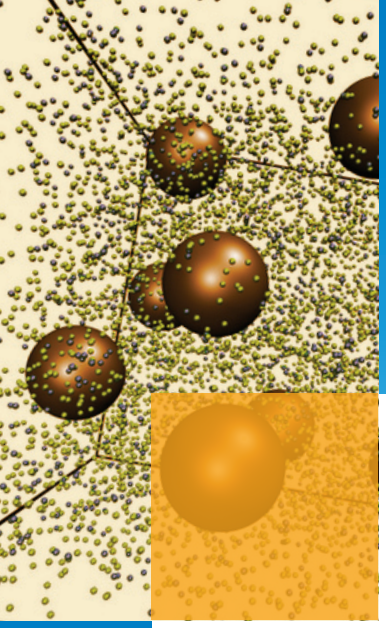


University of Stuttgart
SFB 716

www.sfb716.uni-stuttgart.de

Colloquium of the SFB 716

July 13th, 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.

TALK

Sebastián Miranda

Universidad Andrés Bello, Santiago, Chile

Theoretical Insights into the enzymatic reaction mechanisms of dehydratases and dehalogenases

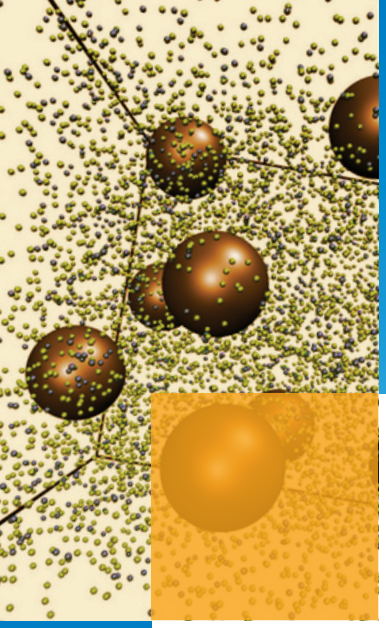
Enzymes are macromolecular systems capable of performing fascinating chemical transformations that otherwise would be difficult or even impossible. These molecular machines are the main responsible of life, and their continuous understanding has leaded towards the design of new promising devises in fields such as remediation, chemical catalysis, energy conversion, biosensors among others.

We propose to uncover the main factors that govern the mechanisms by which two very different enzymes are able to perform difficult chemical transformations.

The first case corresponds to fluoroacetate dehalogenase (FAcD), an enzyme capable of removing a fluorine atom from fluoroacetate (FAc). This represents a challenging process as the carbon fluorine (C-F) bond is the strongest carbon-halogen bond found in nature. To achieve this task, it proceeds by an initial concerted nucleophilic substitution (S_N2) reaction that eliminates the fluorine atom as fluoride, followed by a hydrolysis reaction to release the product.

The understanding of the first elementary step of this reaction provides useful insights for the design of new methods for the remediation of sewage water by eliminating the fluorinated compounds. The reaction mechanism was analyzed in terms of structural and electronic processes aiming to define the role of the catalytic site. Together with this, we shed light into the nature of the selectivity mechanism towards fluoroacetate over chloroacetate.

The second case of study corresponds to (R)-2-Hydroxyisocaproyl-CoA dehydratase, a radical enzyme that uses an iron-sulfur cluster as a cofactor. This enzyme catalyzes an atypical dehydration that could be useful to obtain very difficult molecular targets associated to the pharmaceutical industry,



Colloquium of the SFB 716

that otherwise would need several steps in their synthesis, increasing the costs of the process. This particular enzyme catalyzes the transformation of hydroxyisocaproyl-CoA to isocaprenoyl-CoA. The first step of the reaction involves an electron transfer towards the substrate, which initiates the transformation through radical intermediates.

We aim to present a complete mechanistic proposal for this complex chemical transformation, exploring the role that these radical intermediates have in the catalysis, which at this date is not fully understood.

TALK

Steffen Hirschmann

Institute for Parallel and Distributed Systems (IPVS), Subproject D.9

Dynamic Rebalancing for Short-Range MD Simulations with ESPResSo

The parallel simulation of dynamic, heterogeneous scenarios with large particle numbers on distributed HPC systems poses severe challenges in short-range molecular dynamics: We need to employ load-balancing techniques to account for load imbalances arising from the heterogeneous particle distributions to minimize the time to solution. Moreover, we need to employ load-balancing dynamically during runtime to account for the change in the heterogeneity of the particle distributions.

In this talk we will present approaches to tackle these problems. First, we need to determine optimal algorithms for load-balancing. Second, we have to extend the simulation software under consideration to arbitrarily shaped domains. And third, we need efficient methods and implementations for load balancing and communication across domain partitions and compute nodes.

Our first application which we currently extend to support dynamic load-balancing is ESPResSo. We will report on the current state of our work on the way to large scale simulations.