Title: Simulation Methods for Structure Formation and Function of biomolecular nanoscale Systems

Lecturer: Wolfgang Wenzel

Topics:

- Molecular Models for biomolecules and nanosystems
- Simulation techniques:
  - Monte Carlo Sampling for Thermodynamics
  - Molecular Dynamics for Kinetics
  - High Performance Computing
- Applications:
  - Protein Structure Formation and Function
  - Drug Design
  - Bio-Nano Interactions (Nanoparticles meet Proteins)

Abstract:

The concurrent growth of computationalpower, advances in simulation methodology and shrinking size of experimentally accessible objects have generated an increasing area of overlap where “virtual” experiments can complement, and sometimes even guide, laboratory experiments. In this lecture I will give a brief overview of a subset of presently interesting questions at the interface of the life- and the nanosciences and the corresponding methods that are available to address them.