

Elective module “Computational Engineering Science”

Lecturer	Prof. Dr. habil. Martin O. Steinhauser
Module Components	4 SWS lecture, accompanied by homework assignments
Preliminary Examination	none
Module Examination	Submitted written homework assignments (submission period: 8 weeks)
Further Information	This lecture introduces many tricks of the trade in Computational Science, in particular for the Molecular Dynamics and Monte Carlo Simulation Methods. Examples of previous successful research projects conducted by master students can be found on the Department Website of the Lecturer.

Keep in mind to register for every preliminary and module examination on the HIS-platform within the published time frame.

Short Outline of elective module contents

Students acquire interdisciplinary knowledge of theoretical concepts and computational methods in particular in Molecular Dynamics, Discrete Element and Monte Carlo simulations which will be applied to specific research problems of Materials Science, Chemistry, and (Bio-)Physics. All basics will be developed within the course – no previous knowledge is necessary; learning by doing applies! The lecture will be accompanied by homework assignments which include classical analytic problems, but also simple programming tasks which can be mastered with the research codes that will be provided in the lecture.

Successful completion of this course will prepare the student to engage subsequently in a Master Thesis in the scientific area of Computational Science with Applications in Chemistry, Biology, or Materials Science.

On successful completion of this module the students are able to:

- understand, describe and apply the theoretical basics of major simulation methods;
- understand and apply specifically the methods of Molecular Dynamics, Monte Carlo and Discrete Element simulations to scientific problems;
- implement and optimize their own research code from scratch to perform basic simulation tasks;
- start working towards a Master Thesis at the forefront of research in a selected area of Computational Science.