Data:	ADVTCMS. MA. Nr. 3587 / Examination number: 44511	Version: 12.08.2024	Start Year: WiSe 2018
Module Name:	**Atomistic Simulation Methods**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with the current state-of-the-art simulation methods for atomistic problems and most recent developments in computational methods for the nanoscale. They will be introduced to the fundamentals of statistical mechanics and interatomic potentials. Participants will also be introduced to the usage of machine learning methods in atomistic simulations, particularly for interatomic potentials. They will also be taught novel methods for visualization and analysis of their simulation results. Students will use widely-available open-source simulation software in hands-on exercises. They will learn the theoretical underpinnings of these advanced methods and will be able to apply those to new problems.		
Contents:	Key topics include: Statistical mechanics; Molecular dynamics; Monte Carlo methods; Kinetic Monte Carlo; Interatomic potentials; Machine learning potentials; Visualization and analysis methods including machine learning motivated methods.		
Literature:	D. Frenkel, B. Smit. Understanding Molecular Simulation: From algorithms to applications, Wiley VCH R. Lesar. Introduction to Computational Materials Science, Cambridge University Press E. Tadmor, R. Miller. Modeling Materials: Continuum, atomistic and multiscale techniques, Cambridge University Press J.M. Haille. Molecular Dynamics: Elementary Methods, Wiley VCH		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Software Tools for Computational Materials Scientists, 2024-07-16 Theory, Modelling and Simulation of Microstructures, 2024-07-01 basic experience with a Linux environment (bash/shell); knowledge of crystallography		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 8 students or more) [MP minimum 15 min / KA 90 min]		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 8 und mehr Teilnehmern) [MP mindestens 15 min / KA 90 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		