

Data:	ADVTCMS. MA. Nr. 3587 / Examination number: 44511	Version: 16.02.2022	Start Year: WiSe 2018
Module Name:	<b>Atomistic Simulation Methods</b>		
(English):			
Responsible:	<a href="#">Eidel, Bernhard / Prof. Dr.-Ing. habil.</a>		
Lecturer(s):	<a href="#">Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.</a>		
Institute(s):	<a href="#">Institute of Mechanics and Fluid Dynamics</a>		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with the most recent developments in computational materials science and current state-of-the-art simulation methods for atomistic problems. They will learn the theoretical background of advanced methods on the nanoscale and will be able to apply those to new problems.		
Contents:	This course will cover atomistics subjects such as atomic interactions, validation of potential functions, structure generation, surface energies as well as simulation and critical assessment of three-dimensional nanoscale specimens. Students will get an overview over current developments and will also be able to study such phenomena by hands-on simulations using open source software. Theoretical background and application of advanced methods for data analysis and visualization of atomic defect structures complement this course. The main emphasis of the exercises is on applying the methods from the lecture to problems with materials scientific relevance.		
Literature:			
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:	<b>Recommendations:</b> 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]		
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.		