SYLLABUS

Materials Modeling 7.5 credits T7002T

Materialmodeller

Course syllabus admitted: Autumn 2023 Sp 1 - Present

DECISION DATE
2021-02-17

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LULEÅ TEKNISKA UNIVERSITET

Materials Modeling 7.5 credits T7002T

Materialmodeller

Second cycle, T7002T

Education level	Grade scale	Subject	Subject group (SCB)
Second cycle	G U 3 4 5	Materialteknik	Materials Technology

Main field of study

Materials Science and Engineering

Entry requirements

Solid state physics (F7006T or equivalent), Applied mathematics (M0026M or M7018, or equivalent)

Selection

The selection is based on 30-285 credits

Course Aim

After completion of the course students suppose to: - understand the multi-scale nature of materials and the need to use a hierarchical approach to model them; - be familiar with a number of models which are formulated for different scales present in any material; - have knowledge of concept of modelling of the material properties based on a unit cell consisting of atoms; - be able to choose and apply models derived from an atomistic structure to predict basic material properties; - have good understanding of the link between nano-, micro- and macro- material scales and be able to demonstrated it by defining input and output parameters required by different models.

Contents

- Multi-scale nature of materials (nano-, micro-, macro-) - Link between different size scales - Hierarchical approach in material modelling - Atomistic method in materials modelling, aspects of different approaches will be presented, such as: total energy calculations, molecular dynamics simulations ab intio methods - General overview of numerical techniques in materials modelling Application of the numerical techniques to solve material modelling problems will be addressed during the course and some of the commercial software packages will be discussed.

Realization

Each course occasion´s language and form is stated and appear on the course page on Luleå University of Technology's website.
Lectures, seminars and laboratory work.

Examination

If there is a decision on special educational support, in accordance with the Guideline Student's rights and obligations at Luleå University of Technology, an adapted or alternative form of examination can be provided.
Approved written exam and mini-projects.

Unauthorized aids during exams and assessments

If a student, by using unauthorized aids, tries to mislead during an exam or when a study performance is to be assessed, disciplinary measures may be taken. The term “unauthorized aids” refers to aids that the teacher has not previously specified as permissible aids and that may assist in solving the examination task. This means that all aids not specified as permissible are prohibited. The Swedish version has interpretative precedence in the event of a conflict.

Overlap

The course T7002T is equal to MPC003

Course offered by

Department of Engineering Sciences and Mathematics

Modules

Code	Description	Grade scale	Cr	Status	From period	Title
0002	Laboratory work	U G#	3	Mandatory	A07	
0003	Written exam	G U 3 4 5	4.5	Mandatory	A21	

Study guidance

Study guidance for the course is to be found in our learning platform Canvas before the course starts. Students applying for single subject courses get more information in the Welcome letter. You will find the learning platform via My LTU.

Last revised

by Head Faculty Programme Director Niklas Lehto 2021-02-17

Syllabus established

The syllabus was established by the Department of Applied Physics and Mechanical Engineering 2007-02-28, and remains valid from autumn 2007.