

MSE-641

Methods of Modelling and Simulation of Materials Science

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Cursus	Sem.	Type
Materials Science and Engineering		Obl.

Language of teaching	English
Credits	1
Session	
Exam	During the semester
Workload	30h
Hours	14
Courses	6
Exercises	6
TP	2
Number of positions	

Frequency

Every year

Remark

Next time: 2018, March 1 to 2 and 5 to 7

Summary

Intermediate programming in Mathematica Computation and visualization of structures and structural relations, of mechanical properties of materials, of quantum mechanical properties and band structures. Computation of instabilities and phase transitions.

Content

Intermediate programming in Mathematica
 Computation and visualization of structures and structural relations.
 Computation and visualization of mechanical properties of materials.
 Computation and visualization of quantum mechanical properties and band structures.
 Computation of instabilities and phase transitions.

Keywords

materials science, problem solving, applied programming

Learning Prerequisites**Recommended courses**

Some programming experience in any language.

Beginner level knowledge of crystal structure, thermodynamics, kinetics, quantum mechanics, mechanical properties.

Assessment methods

in class evaluation