EPFL

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	Oral presentation
Workload	30h
Hours	**14**
Courses	6
Exercises	6
TP	2
Number of positions	

Frequency

Every year

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

Students will complete a small independent project ans either make a 5 minutes presentation or a 5 minute video illustrating their results