Methods of Modelling and Simulation of Materials Science

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Cursus
Science et génie des matériaux

Sem. Obl.

Type

Language English
Credits 1
Session Oral presentation
Exam
Workload 30h
Hours 14
Lecture 6
Exercises 6
Practical work 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

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

Learning Prerequisites
Recommended courses
Some programming experience in any language.
Beginner level knowledge of crystal structure, thermodynamics, kinetics, quantum mechanics, mechanical properties.