MH2046 Quantum Metallurgy 6.0 credits

Kvantmetallurgi

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment

On 2023-06-09, the Dean of the ITM school has decided to establish this official course syllabus to apply from autumn term 2023 (registration number M-2023-1203)

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Materials Science,Materials Science and Engineering

Specific prerequisites

Basic knowledge about quantum mechanics and the Schrödinger equation as well as ab initio calculations and density-functional theories (DFT) equivalent to MH1026 Materials Physics, 6 higher education credits.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After passing the course, the participant should be able to:

- Apply the basic principles of quantum metallurgical strategies and its limitations with regard to the size of the evaluated systems and the time scale
- Identify which type of materials science problem (threshold displacement energy, mechanical, kinetic etc) that is possible to solve or can be solved by means of ab initio tools, and reach the expected precision and the reliability for ab initio modelling for different properties and materials
- Justify and use one of the available ab initio programs, install the structure for the corresponding ab initio modelling and select the main parameters for first principle calculations

Course contents

Basic statistical physics, molecular dynamics,
Monte Carlo methods, overview of quantum mechanics, band structure, Fermi level, the nature of the chemical binding, density functional theory, calculation of structural stability in metals and alloys and energy for different defects.
Calculation of mechanical and electric properties, simulation of phase transitions.
Accuracy and limitations of the technology.
Overview of softwares.

Examination

- PRO1 - Project Assignment, 6.0 credits, grading scale: A, B, C, D, E, FX, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.