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

Course syllabus for MH2046 valid from Spring 2011

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

SK1110 Physics or corresponding knowledge on electrostatics and electrodynamics,

Material Physics or corresponding knowledge on solid state physics.

Basic engineering mathematics including differential equations.

Language of instruction

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

Intended learning outcomes

After the course, the student should be abel to:

- Identify materials science problems where the quantum metallurgy approach will be useful.
- Formulate materials science problems in a way so they are accessible for the quantum metallurgy approach.
- Interact with experts to perform calculations by means of the quantum metallurgy approach.
- Calculate energies of various defects.
- Interact with experts to calculate mechanical and electric properties.
- Predict the behavior of small systems using the quantum metallurgy approach.
- Interact with experts to calculate some kinetic properties.
- Estimate accuracy and limitations of the technique.

Course contents

Overview, Basis of statistical physics, Molecular dynamics, Monte Carlo methods, Overview of quantum mechanics, band structure, Fermi level, nature of chemical bond, Density-functional theory, Calculation of structural stability of metals and alloys and energy of various defects. Calculation of mechanical and electrical properties, simulation of phase transitions. Accuracy and limitations of the technique. Overview over softwares.

Course literature

Utdelat material

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.