FMH3700 Introduction to the EMTO Program Package 1 9.0 credits

Introduction to the EMTO Program Package 1

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

Establishment

Course syllabus for FMH3700 valid from Spring 2019

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

Basic knowledge of solid state physics; quantum mechanics; density functional; electronic structural methods. Good knowledge of Unix, Linux and Windows OS

Language of instruction

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

Intended learning outcomes

The aim of the course is to acquire basic knowledge in the first-principles quantum-mechanical modeling of random alloys using the EMTO computer program. Today there are a limited number of theoretical tools, which are suitable for the ab initio description of alloys. The particular strength of the EMTO method, which places the EMTO program into the focus of modern computational materials design, is that this approach properly accounts for the anisotropic lattice distortions in random alloys, and therefore it can be used to study the atomic level phenomena behind the thermo-physical, chemical, structural, mechanical, etc. properties of chemically and magnetically alloys. After this introductory course, the students will get basic experience of using the EMTO program; they will be able to apply the EMTO method to simple systems and calculate fundamental bulk properties (equation of state and elastic properties) of monoatomic as well as chemically disordered multi-component alloys.

Course contents

The EMTO package, components and usage;
Installation;
Preparing the calculation: structural information, real space cluster; chemically ordered and disordered systems;
Brillouin zone sampling;
Green's function;
Executing the program parts;
Reading and understanding the output;
Extracting data from the output:
Equation of state; DOS;
Fermi surface;
Examples;

Examination

- RAP1 - Report, 9.0 credits, grading scale: P, 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.

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

Other requirements for final grade

Written report

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.