



FMH3304 Computational Thermodynamics- Assessment of Thermodynamic Properties 6.0 credits

Termodynamisk modellering- utvärdering av termodynamiska egenskaper

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 FMH3304 valid from Spring 2014

Grading scale

Education cycle

Third cycle

Specific prerequisites

The thermodynamics of alloys, the software Thermo-Calc classical version/consol version.

Language of instruction

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

Intended learning outcomes

The course intends to give the students basic understanding of how thermodynamic properties of different phases can be evaluated and used to create consistent thermodynamic descriptions of alloy system. The course turns to doctoral students who want to get into basic thermodynamic modelling and calculations. The course covers, how different phases are modelled and which type of experimental information that can be used to fit the model parameters i.e. phase diagrams and thermochemical information such as activity, enthalpy of formation, heat capacity etc, but also ab initio calculated information.

On completion of the course, the student should be able to:

- connect crystallography to thermodynamic models
- read relevant scientific literature and from this be able to extract experimental information for use in thermodynamic evaluations correctly and to compare with calculated results.
- use ab initio calculated information in thermodynamic evaluations.
- write a scientific article about evaluation of a specific alloy system.

Course contents

Thermodynamic modelling by means of the Calphad method i.e. including different experimental techniques and how the information is used, use of ab initio-information, assessment technique.

Course literature

Lukas, Fries, Sundman, Computational Thermodynamics - The Calphad Method, Cambridge University Press, ISBN 978-0-521-86811-2

Utdelade vetenskapliga artiklar

Examination

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.

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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.