



MH1028 Computational Thermodynamics for Materials Design 6.0 credits

Termodynamisk modellering för materialdesign

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

Establishment

The official course syllabus is valid from the autumn semester 2026 as decided by the Faculty Board: PA-2026-011. Decision date: 2026-08-26

Grading scale

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

Education cycle

First cycle

Main field of study

Technology

Specific prerequisites

MH2027 Thermodynamics of Materials, or similar

Intended learning outcomes

After the course the students should have basic knowledge of:

- Thermodynamics of unary, binary and higher-order systems
- Thermodynamic models for phases with sublattice (called Compound Energy Formalism) and be able to
- Perform simple thermodynamic calculations using computer programs
- Calculate and use phase diagrams
- Use both Swedish and English terminology
- Basic concepts in the Calphad methodology

Course contents

- Basic thermodynamics for unary, binary and higher-order systems
- Thermodynamic models based on example Gibbs energy
- Gibbs energy and driving force
- Phase equilibria and phase diagrams
- Thermodynamic computations
- The Calphad methodology

Examination

- TEN1 - Written examination, 3.0 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Computer Exercise, 3.0 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.

Transitional regulations

Contact the course coordinator

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.