

Electronic Structure Theory, 7.5 credits

Elektronstrukturteori, 7.5 hp

Third-cycle education course

6FIFM33

Department of Physics, Chemistry and Biology

Valid from: First half-year 2025

Approved by

Approved

Registration number

Entry requirements

Entry requirement for studies on third-cycle education courses

- second-cycle degree,
- 240 credits in required courses, including at least 60 second-cycle credits,
or
- acquisition of equivalent knowledge in some other manner

This course does not assume any previous knowledge in first-principles simulations. However, an elementary knowledge in quantum and solid-state physics is required for understanding the course material.

Specific information

This course is aimed at giving a theoretical background behind state-of-the-art methods for quantum simulations of materials properties. A series of 10 lectures will be devoted to the basics of the solution of the electronic structure problem in solids using plane wave basis sets and all-electron techniques.

Learning outcomes

By the end of the course the students will be able to get:

Knowledge and understanding

- of theoretical methods for quantum simulations of materials properties;
- of the basics of the solution of the electronic structure problem

Competence and skills with

- project using VASP package
- numerical methods in solid state physics

Contents

The lectures introducing the methods will be complemented with computer exercises. During these practical classes, the students will run a mini-project, which include several simulations using VASP package, to apply the techniques discussed in the lectures and be acquainted with this package. Examination will be in the form of an oral project presentation.

Educational methods

Lectures and* *computer exercises

Examination

Examination will be in the form of an oral project presentation.

Grading

Two-grade scale

Course literature

- R. M. Martin "Electronic Structure. Basic Theory and Practical Methods"
(Cambridge University Press, Cambridge, 2004).

General information

The course is planned and carried out according to what is stated in this syllabus. Course evaluation, analysis and suggestions for improvement should be fed back to the Research and PhD studies Committee (FUN) by the course coordinator.