

# **Electronic structure theory, 7.5 credits**

Elektronisk strukturteori, 7.5 hp

Third-cycle education course

6FIFMB2

Department of Physics, Chemistry and Biology

Valid from: Second 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:

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

