

**Density Functional Theory, 6.0 credits**

Täthetsfunktionalteori, 6.0 hp

Third-cycle education course

6FIFMA8

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
- Basic knowledge in quantum mechanics. Acquired either through an undergraduate course in quantum mechanics or a chemistry course with a sufficient quantum mechanics component.

## Learning outcomes

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

### *Knowledge and understanding*

- get knowledge about the main concept and the historical development of density functional theory (DFT)
- apply the concepts to periodic crystalline systems
- apply the concepts to molecular systems

### *Judgement and approach*

- summarize, represent and discuss special topics related to density functional theory.
- be able to discuss current research and publications related to or utilizing density functional theory at a basic level

## Contents

The course gives an introduction to density functional theory (DFT) and show the foundations for applications in solid state physics, chemistry and biology. It will consist of three parts: Introduction to DFT (Florian Trybel), DFT for periodic solids (Ferenc Tasnádi), and DFT for molecular systems (Bo Durbeej).

### **Introduction to DFT**

This part of the course will explain the theoretical foundations of density functional theory and present a walk-through the historical developments in quantum mechanics leading to the development of DFT and its applications. It gives an introduction to Hartree-Fock and Thomas-Fermi Theory, introduces the Hohenberg-Kohn theorems and the Kohn-Sham equations. Basic approximations for the exchange-correlation functional will be introduced.

### **DFT for periodic solids**

This part of the course will discuss:

- (1) the application of DFT for periodic, crystalline systems.
- (2) the concept of periodic boundary conditions, lattice and Bloch functions as well as Wannier functions on an introductory level.
- (3) the basics of electronic structure theory, the calculation of forces and electronic topology.
- (4) the calculation of phonons, basics of molecular dynamics simulations and a short introduction to machine-learning interatomic potentials based on DFT calculations.
- (5) beyond standard methods: DFT+U, short introduction to dynamical mean-field theory (DMFT) for correlated systems.

This part of the course also provides a basis for the Electronic Structure Theory (6FIFM33, 7.5 credits) course, which gives more details on the applications of density functional theory for solids.

### **DFT for molecular systems**

This part of the course will discuss:

- (1) the fundamentals of applying DFT to finite molecular systems.
- (2) wave function-based methods beyond Hartree-Fock theory.
- (3) hybrid functionals and meta-GGAs.
- (4) time-dependent density functional theory (TDDFT) on an introductory level.

## Educational methods

Whiteboard as well as presentation-style lectures

## Examination

Oral examination

## Grading

Two-grade scale

## **Course literature**

Literature will be discussed during the course.