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 though 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-Kohm 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.