Linnæus University

Jnr: 2016/5155-3.1.2.2

Course syllabus

Faculty of Technology
Department of Physics and Electrical Engineering

4FY530 Täthetsfunktionalteori med tillämpningar inom atom- och kondenserade materiens fysik, 7,5 högskolepoäng

Density Functional Theory with applications in atomic and condensed matter physics, 7.5 credits

Main field of study
Physics

Subject Group
Physics

Level of classification
Second Level

Progression
A1F

Date of Ratification
Approved by Faculty of Technology 2016-09-26
The course syllabus is valid from autumn semester 2017

Prerequisites
Physics 90 credits (including a course in quantum mechanics 7.5 credit and an introductory course in solid state physics 7.5 credit), mathematics 45 credits or equivalent.

Objectives

On the completion of the course the students should be able to:

- account for the fundamental background of Density Functional Theory (DFT).
- understand the difference between DFT and other many-body approaches.
- account for what physical properties can be calculated with DFT.
- explain how electron correlations are approximated within DFT.
- explain the difference between different functionals such as LDA,GGA-PBE, B3LYP.
- understand the limitations of DFT.
- work with DFT codes such as Wien2k, SIESTA, VASP, NRLMOL to calculate the electronic structure of simple solids.

Content

Introduction to many-electron problems

- Hartree-Fock (HF) theory.
- Configuration Interaction (CI).
- Practical difficulties in solving many-electron problems.

Foundation of DFT

- The Thomas-Fermi model: precursor to modern DFT.
- Functional and functional derivatives, Euler-Lagrange equation.
- Hohenberg-Kohn Theorem.
- N and v-representability of densities, and non-uniqueness of potentials.

Kohn-Sham (KS) Equation

- Effective exact single particle method to the many-body problem.
- Exchange and correlation energies.
- Interpretation of KS eigenvalues: Koopman's theorem, Ionization energy, Fermi surface, band gap.
- KS equation for spin-polarized systems.

Approximation to Functionals

- Local approximation: local density approximation (LDA).
- Semilocal approximation: generalized gradient approximation (GGA).
- Non-local approximation: hybrid functional.
- Self-interaction correction.

Introduction to time dependent DFT

- Runge-Gross Theorem.
- Time-dependent Kohn-Sham equation.

Practical implementation of DFT methods

- General scheme for solving Kohn-Sham equation.
- Full potential and pseudo potential methods.
- Basis functions: Gaussian, LAPW, Numerical.
- Application of DFT methods for molecules and solids.

Type of Instruction

The teaching consists of lectures and tutorials.

Students can also register for the "distance" version of the course and follow the course live via the internet. The recorded lectures will also be posted on course homepage.

Examination

The course is assessed with the grades A, B, C, D, E, Fx or F.
The grade A constitutes the highest grade on the scale and the remaining grades follow in descending order where the grade E is the lowest grade on the scale that will result in a pass. The grade F means that the student's performance is assessed as fail (i.e. received the grade F).

Assessment of student performance is made through the presentation of assignments and a written test.

Re-examination will be offered within six weeks under the regular semester periods.

Course Evaluation

During the course or in close connection to the course, a course evaluation is to be carried out. The result and analysis of the course evaluation are to be communicated to the students who have taken the course and to the students who are to participate in the course the next time it is offered. The course evaluation is carried out anonymously. The

compiled report will be filed at the Faculty.

Other

Grade criteria for the A–F scale are communicated to the student through a special document. The student is to be informed about the grade criteria for the course by the start of the course at the latest.

Required Reading and Additional Study Material

Reference Literature

1. Density-Functional Theory of Atoms and Molecules by Robert G. Parr and Yang Weitao, Publisher: Oxford University Press (1994), ISBN-13: 978-0195092769.
2. Density Functional Theory: An Advanced Course by Eberhard Engel and Reiner M. Dreizle, Publisher: Springer, 2011 edition, ISBN-13: 978-3642140891.
3. Electronic Structure: Basic Theory and Practical Methods by Richard M. Martin, Publisher: Cambridge University Press; 1 edition (2008), ISBN-13: 978-0521534406.
4. Density Functional Theory: A Practical Introduction by David Sholl and Janice A Stecke, Publisher: Wiley-Interscience; 1 edition (2009), ISBN-13: 978-0470373170.
5. Selected notes/papers.