



LUND
UNIVERSITY

Faculty of Science

FYST27, Physics: Electron Structure of Solids and Surfaces, 7.5 credits

*Fysik: Elektronstrukturen hos fasta ämnen och ytor, 7,5
högskolepoäng*

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2012-09-03 and was last revised on 2012-09-03. The revised syllabus applies from 2012-09-03, autumn semester 2012.

General Information

The course is an elective course for second-cycle studies for a Master or Bachelor of Science degree in Physics. It can also be taken as a freestanding course.

Language of instruction: English

Main field of studies

Physics

Depth of study relative to the degree requirements

A1F, Second cycle, has second-cycle course/s as entry requirements

Learning outcomes

The aim of the course is that, on completion of the course, the student should have acquired the following knowledge and skills:

Knowledge and understanding

On completion of the course, the student should:

- Be able to give the background of and explain the practical application of theoretical methods and models that are used for a quantitative description of the electron structure of crystalline materials.
- Show ability of being able to profit by the main contents of the original articles that are published in the magazines.

Skills and abilities

On completion of the course, the student should:

- In simpler cases be able to use and interpret the results of several of the program packages for electronic structure calculations that are available in research society today.

Course content

The course consists of the following parts:

1. Based on Many-Particle Theory, an explanation of the relevance of one-particle equations and of the concepts of exchange and correlation is given.
2. The main concepts within density functional theory of ground state properties of molecules and solid bodies. The simplest approximations and their qualities are described.
3. The concepts of quasi particles and their eigenenergies are reviewed, and used to describe photo emission. We present simple approximations for eigenenergies, and we discuss the precision of the approximations.
4. Different methods to solve one-particle equations are used, such as:
 - Bloch's theorem, reciprocal space, Brillouin zones in two and three dimensions, rotational symmetries, classifications and matrix elements.
 - Plane waves and pseudopotentials.
 - Linear methods for the band problem, mainly LAPW and the LMTO method.
 - Single-particle Green's functions, Slater-Koster for impurities and adsorbates, and surface states.

Course design

Teaching consists of lectures combined with practical exercises.

Assessment

The course is examined through an oral test and a number of individual written assignments. The student should furthermore participate in the compulsory parts of the course. Students who do not pass the regular exam are offered a re-examination shortly after the regular exam.

Subcourses that are part of this course can be found in an appendix at the end of this document.

Grades

Marking scale: Fail, Pass, Pass with distinction.

To pass the entire course a passed test, passed individual written assignments, and participation in all compulsory parts are required. The final grade is determined by weighing the results of the different required elements of the examination.

Entry requirements

For admission to the course, FYSN17 Quantum Mechanics and FYSC13 Solid State Physics, or the equivalent, are required. Some experience in programming is recommended.

Subcourses in FYST27, Physics: Electron Structure of Solids and Surfaces

Applies from H12

1201 Electron Structure of Solids and Surfaces, 7,5 hp
Grading scale: Fail, Pass, Pass with distinction