MH2426 Quantum Engineering Computations for Nanosystems 7.5 credits

Kvantmekaniska datorberäkningar för nanosystem

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for MH2426 valid from Spring 2011

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Materials Science and Engineering

Specific prerequisites

IF1621 Kvantmekanik I, or similar like:

- Quantum mechanics or quantum physics, introductory level.
- Solid state physics or semiconductor physics, introductory level
- Numerical methods, introductory level

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

When you have finished this course, you will be able to perform DFT calculations of certain simpler materials properties (e.g., density, bulk modulus, band gaps). You will also be able to analyze the results of your calculations, and understand the limitations of DFT calculations. In order to do that, you will have to integrate your computer skills (Matlab, Linux) with your knowledge of quantum mechanics, atomic physics, numerical methods and solid state physics. You will also know about several state-of-the-art applications of DFT calculations.

Course contents

Repetition of basic quantum mechanics and solid state physics (operators, Schrödinger equation, expectation values, atomic orbitals, solving the Schrödinger equation in spherical coordinates, variational calculus, Bloch's theorem, Bravais lattice, reciprocal space, band structure, k-points). Electron-electron interaction. Exchange. Correlation. Single-particle model. Effective potential. Homogenous electron gas. Thomas-Fermi model. Functional derivative. Theoretical foundations of DFT. Kohn-Sham equation. DFT model for the helium atom, and solving this model numerically (in Matlab) using finite differences. Calculation and analysis of simpler materials properties using a DFT program package. Assessment of the quality of the calculations. The concepts self-consistency and convergence in DFT calculations. Limitations of DFT calculations. State-of-the-art applications of DFT calculations.

Course literature

Jos Thijssen, "Computational Physics", Cambridge University Press, 2007.

Richard M. Martin "Electronic Structure, Basic Theory and Practical Methods", Cambridge University Press, 2004.

Examination

- HEM1 - Home Assignments, 2.0 credits, grading scale: P, F
- TEN1 - Examination, 4.0 credits, grading scale: A, B, C, D, E, FX, F
- NÄR1 - Attendance, 1.5 credits, grading scale: P, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Other requirements for final grade

Passed all the home assignments and computer exercises. Attendance at the guest lectures. Written exam at the end of the course.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.