



MH2425 Simulation and Modelling on the Atomic Scale 6.0 credits

Simulering och modellering på atomär skala

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

Establishment

Grading scale

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

Education cycle

Second cycle

Main field of study

Materials Science, 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.

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). DFT model for the helium atom. 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.

Disposition

Lectures 8 h (i.e. 4 lectures 2 h each)

Computer exercises 40 h (i.e. 10 computer exercises 4 h each)

Course literature

- Richard M. Martin “Electronic Structure, Basic Theory and Practical Methods” Cambridge University Press, 2004.
- J.M. Thijssen, “Computational Physics”, Cambridge University Press, 2007

A general text book in solid state physics is also very useful, e.g., Ashcroft and Mermin, “Solid State Physics”.

A general text book in quantum mechanics is also very useful, e.g., P. W. Atkins “Molecular Quantum Mechanics”.

Equipment

We will provide access to all necessary software (Matlab, DFT code, Linux environment)

Examination

- TENA - Examination, 4.0 credits, grading scale: A, B, C, D, E, FX, F
- LABA - Laboratory work, 2.0 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.

Completing all the home assignments and computer exercises. Written exam at the end of the course.

Other requirements for final grade

Grade E: All HA and CE have been completed and handed in on time.

In order to get a higher grade (A-D) you will need to do the written exam.

The grade Fx is given if the requirements for grade E have not been fulfilled.

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.