



BB2340 Theoretical Materials Design 7.5 credits

Teoretisk materialdesign

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

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

Establishment

Course syllabus for BB2340 valid from Autumn 2007

Grading scale

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

Education cycle

Second cycle

Main field of study

Biotechnology

Specific prerequisites

1. Three years at the School of Chemistry, Chemical Engineering and Biotechnology, KTH, or equivalent.
2. Courses in Quantum Mechanics, Quantum Chemistry and Molecular Modeling are helpful.
3. Some basic experience with computers.

Language of instruction

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

Intended learning outcomes

To gain some understanding of basic properties of molecules and materials. To rationalize properties with chemical concepts like chemical bonds, polarity and electronic structure. How to perform a rational design in order to achieve certain macroscopic properties of a material. To learn some basic concepts in modeling of properties, like optical, electronic and magnetic properties and how these properties connect to various experimental techniques used to characterize materials. To obtain some practical experience in computation of parameters related to the various materials properties.

Course contents

Electric and magnetic fields interacting with molecules and materials.

Basic techniques for evaluation of molecular properties.

Optical techniques: Optical absorption, fluorescence, phosphorescence and dichroism.

X-ray techniques: X-ray diffraction and X-ray spectroscopies.

Magnetism from the molecular perspective: magnetizability and molecular magnets.

Magnetic resonance techniques: nuclear magnetic resonance and electron paramagnetic resonance properties.

Molecular electronics: Basic properties of molecular electronic devices.

Relations between microscopic and macroscopic properties.

Materials with periodic symmetries; polymers and crystals.

Materials without periodic symmetries; amorphous solids and biomolecules.

Nanomaterials and nanoparticles

Understanding structure-property and structure-function relationships.

Some thumb rules for rational design of materials

Overview of modern modeling methods for prediction of properties.

Course literature

1. Course book - "Molecular Materials with Specific Interactions"

W.A. Sokalski, ISBN-10: 1-4020-5371-1. Distributed Notes.

2. Instructions to computer exercises.

Examination

- TEN1 - Examination, 6.0 credits, grading scale: A, B, C, D, E, FX, F
- ÖVN1 - Exercises, 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.

Other requirements for final grade

1. Written exam.
2. Written report for the computer exercises.

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.