



# 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.

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

## Establishment

Course syllabus for MH2425 valid from Spring 2009

## 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

## Language of instruction

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

## Intended learning outcomes

Acquire knowledge of modern methods in computer simulations techniques relevant for nanotechnology and nano- materials research. Acquire practical skills in how to use and implement such computational methods, and learn about their possible applications and limitations. The course gives an introduction to research topics in the field, through practical exercises.

## Course contents

Density functional theory and molecular dynamics, and how these methods are implemented numerically. Quantum mechanics and atomic physics relevant for understanding how the computational methods work. Solving practical exercises using C++. Addressing and analyzing a research problem in nanoscience using state-of-the-art research simulation software.

## Course literature

Lecture notes will be distributed during the course. A good place for learning C++ is [www.cplusplus.org/doc/tutorial](http://www.cplusplus.org/doc/tutorial). A recommended book is Numerical Recipes, the Art of Scientific Computing, by W. H. Press, S.A. Teukolsky et al. which will be used in some exercises. Free simulation software home pages: ABINIT [www.abinit.org](http://www.abinit.org) and SIESTA [www.uam.es/departamentos/ciencias/fismateriac/siesta](http://www.uam.es/departamentos/ciencias/fismateriac/siesta).

## Examination

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

## 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.

