



CB2070 Molecular Quantum Mechanics 7.5 credits

Molekylär kvantmekanik

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

This courseplan is valid from Fall 2021.

Grading scale

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

Education cycle

Second cycle

Main field of study

Engineering Physics

Specific prerequisites

Completed course in Quantum Mechanics

Language of instruction

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

Intended learning outcomes

The course aims to provide fundamental knowledge and introduce selected tools needed to perform quantum mechanical calculations at the molecular level. It addresses students in physics and applied mathematics as well as mathematical- and physical-oriented chemists. It primarily addresses students with a basic understanding of quantum mechanics.

After completed course you should be able to:

- form and use wave functions and operators for many-electron systems
- characterise the symmetry of wave functions and thereby understand spectroscopic selection rules
- explain strong covalent bonds in terms of wave functions
- explain the correlated motions of electrons
- perform calculations of approximate wave functions with help of computers

Course contents

Hamiltonian operators, Pauli principle, Born–Oppenheimer approximation, potential energy surfaces, electronic structure theory, wave functions, electron densities, molecular orbitals, Slater determinants, Hartree–Fock, orbital energy and Koopmans' theorem, group theory and symmetry, spin for many-electron systems, electron correlation, configuration interaction, Møller–Plesset perturbation theory.

Examination

- LAB1 - Laboratory work, 2.5 credits, grading scale: P, F
- TEN1 - Written exam, 5.0 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.

The examiner, in consultation with the KTH Disability Coordinator (Funka), decides on any adapted examination for students with documented permanent impairment.

In group exercises, all group members share a collective responsibility for the work.

Laboration reports can be complemented

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.