



FCB3202 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

Course syllabus for FCB3202 valid from Spring 2022

Grading scale

P, F

Education cycle

Third cycle

Language of instruction

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

Intended learning outcomes

After completion of the course the student shall be able to

- demonstrate in-depth knowledge and analytical ability in molecular quantum mechanics adequate for the level of educational level of the course, and critically review others- work in the field

- demonstrate good ability to explain and analyze complex concepts in molecular quantum mechanics based on relevant research literature, and in a pedagogical way communicate the knowledge in writing and orally
- be able to reflect on and describe how scientific issues in the field's research can contribute to sustainable societal development

Course contents

The course's theoretical content includes Hamiltonian operators, Pauli principle, Born-Oppenheimer approximation, 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, potential-energy surfaces, structure optimization, transition states and reactions, normal coordinates and vibrational motion, time-dependent perturbation theory and light-matter interaction.

The practical content of the course includes computer exercises based on the course's subject focus and an individual project related to the course's theoretical foundations. The project is based on a research question and is based on selected research articles. The project has a clear goal that requires the development of a module in the programming language Python. The theoretical basis for the research question must be obtained and a project plan must be prepared before the design and implementation phase begins. Concluding numerical simulations form the basis for answering the research question.

Specific prerequisites

Eligible for studies at the third-cycle level.**

Examination

- LAB1 - Laboratory work, 1.5 credits, grading scale: P, F
- PRO1 - Project, 6.0 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.

Grading criteria are specified in the course PM.

Other requirements for final grade

Required for final grade: 90% attendance at lectures, written critical reflection for selected scientific articles, approved written project report and completed oral project presentation (PRO1); and attendance on computer exercises and completed exercise reports (LAB1).

Transitional regulations

If the examination form is changed, the student will be examined according to the examination form that applied when the student was admitted to the course. If the course is completed, the student is given the opportunity to be examined on the course for another two academic years.

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.