

## Computational Quantum Chemistry (C004148)

**Course size** *(nominal values; actual values may depend on programme)*

**Credits** 8.0

**Study time** 210 h

### Course offerings and teaching methods in academic year 2024-2025

A (semester 2)

English

Gent

lecture

seminar

### Lecturers in academic year 2024-2025

Bultinck, Patrick

WE06

lecturer-in-charge

Acke, Guillaume

WE06

co-lecturer

### Offered in the following programmes in 2024-2025

[Master of Science in Teaching in Science and Technology\(main subject Chemistry\)](#)

**crdts**

8

**offering**

A

[Master of Science in Chemistry\(main subject Materials and Nano Chemistry\)](#)

8

A

### Teaching languages

English

### Keywords

quantum chemical programming, software development, method development

### Position of the course

This course follows up on a thorough introduction to molecular quantum mechanics and aims to familiarize the students with the implementation of quantum chemical methods, which are theoretically elaborated in the course 'Advanced Quantum Chemistry'. The emphasis in this course is on method development and not on molecular modeling.

### Contents

- - Modern software development: Linear algebraic software packages, Collaboration tools, Version control, Testing and code coverage, Continuous integration, Documentation, Building systems, Software design.
- Quantum Chemical Integrals: Obara-Saika, Libint.
- Hartree-Fock: RHF, UHF, DIIS.
- Perturbation theory on Hartree-Fock: MP2.
- Correlated Quantum Chemical Methods: CEPA0, CCD, CCSD, CIS, CISD, FCI.
- Response theory: CPHF, TDHF, CCLR.
- Orbital optimization.

### Initial competences

An excellent training in quantum chemistry is required, amounting at least 12 ECTS credits in previous exposure to quantum chemistry, quantum mechanics and related fields. The course on Advanced Quantum Chemistry is heavily relied on and is highly advised to be taken alongside this course..

### Final competences

- 1 The student obtains a highly advanced knowledge of modern quantum chemical methods.
- 2 The student is able to bring a theoretical method from the stage of model description to an effective implementation.
- 3 The student is able to carry out large scale computational experiments on modern advanced computational infrastructure.
- 4 The student masters the area of software development in computational chemistry.

**Conditions for credit contract**

Access to this course unit via a credit contract is determined after successful competences assessment

**Conditions for exam contract**

This course unit cannot be taken via an exam contract

**Teaching methods**

Seminar, Lecture

**Extra information on the teaching methods**

On campus lecture, online project and online tutorials with support through Ufora and MS Teams.

**Study material**

Type: Handouts

Name: Advanced Quantum Chemistry Handout

Indicative price: Free or paid by faculty

Optional: no

Language : English

Number of Pages : 200

Available on Ufora : Yes

Online Available : Yes

Available in the Library : No

Available through Student Association : No

Usability and Lifetime within the Course Unit : one-time

Usability and Lifetime within the Study Programme : one-time

Usability and Lifetime after the Study Programme : not

**References**

- "Molecular Electronic-structure theory" T. Helgaker, P. Jorgensen & J. Olsen, Wiley, ISBN 0-471-96755-6

**Course content-related study coaching**

Interactive support through Ufora 'Discussions'. Individual guidance by teachers / assistants: by electronic appointment via MS Teams.

**Assessment moments**

continuous assessment

**Examination methods in case of periodic assessment during the first examination period**

Oral assessment

**Examination methods in case of periodic assessment during the second examination period**

Oral assessment

**Examination methods in case of permanent assessment**

Assignment

**Possibilities of retake in case of permanent assessment**

not applicable

**Extra information on the examination methods**

- 1 The students gradually develop their own codes through first implementing methods of increasing complexity. Each implementation is separately marked and used as part of the non-periodic evaluation.
- 2 The final exam is the independent implementation of a quantum chemical method on a highly advanced computational infrastructure with focus on the efficiency of the program written in a modern programming language. After evaluation of the algorithm, the student is interviewed on the method and its implementation during an oral exam.

**Calculation of the examination mark**

85% of the end score is based on the non-periodic evaluation. 25% is based on the evaluation of the reports for the implementation of methods during the seminars. 60% is based on the evaluation of the final and independent implementation of a method on a highly advanced computational infrastructure with focus on the efficiency of the program written in a modern programming language. Failure to submit the reports within the deadline set, renders a zero score for each

report.

The remaining 15% of the score is earned based on the oral exam on the implemented method and its implementation.