GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2023-2024

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 2023-2024

A (semester 2)	English	Gent	lecture
			seminar

Lecturers in academic year 2023-2024

Bultinck, Patrick	WE06	lecturer-in-charge
Acke, Guillaume	WE06	co-lecturer

Offered in the following programmes in 2023-2024	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Chemistry)	8	A
Master of Science in Chemistry(main subject Materials and Nano Chemistry)	8	A
Exchange Programme in Chemistry (master's level)	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. Because of COVID19, changed working methods can be rolled out if this proves necessary.

Learning materials and price

An integrated course is offered via Ufora, where course notes and assignments from tutorials are supplemented with web lectures and knowledge clips. Each student must have their own computer with a webcam and microphone.

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.