GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2023-2024

Advanced Quantum Chemistry (C004147)

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

Credits 4.0 **Study time** 115 h

Course offerings in academic year 2024-2025

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	**crdts**	**offering**
Master of Science in Teaching in Science and Technology (main subject Chemistry)	4	A
Master of Science in Chemistry (main subject Materials and Nano Chemistry)	4	A
Exchange Programme in Chemistry (master's level)	4	A

Teaching languages

English

Keywords

electronic structure theory, electron correlation, ab initio methods

Position of the course

This course follows up on a thorough introduction to molecular quantum mechanics and aims to familiarize the students with modern electronic structure methods based on wave functions. This course provides the necessary theoretical background for the course 'Computational Quantum Chemistry'.

Contents

- Quantum chemical building blocks: Basis sets, Integrals, Spin
- Hartree-Fock theory: Self-consistent field, Roothaan-Hall, Pople-Nesbett
- Second quantization: Algebra of creation and annihilation operators, Wick's theorem, Kutzelnigg-Mukherjee and diagrammatic notation
- Modern electronic structure methods: Configuration interaction, Coupled cluster, Multiconfiguration self-consistent field, Many body perturbation theory
- Response theory: Molecular properties, Orbital relaxation

Initial competences

This course builds further on certain final competences of the courses:
- Mathematics: basic concepts
- Electronic structure
- Symmetry and spectroscopy

Final competences

1 Being able to judge the quality of published computational studies.
2 Being able to select the proper methods for a problem at hand.
3 Being able to develop new methdos independently.

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

Lecture, independent work

Extra information on the teaching methods

Students are taught the basics of quantum chemical methods during the classes and need to extend this knowledge via flipped classroom teaching and guided self study.

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: 978-1118531471
- "Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory", I. Shavitt, R. J. Bartlett (Cambridge University Press), ISBN: 978-0521818322
- "Second Quantized Approach to Quantum Chemistry: An Elementary Introduction", P. R. Surjan (Springer Berlin Heidelberg), ISBN: 978-3642747571
- "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", A. Szabo, N. S. Ostlund (Dover Publications), ISBN: 978-0486691862

Course content-related study coaching

On campus lecture, independent work with support through Ufora and MS Teams. Because of COVID19, changed working methods can be rolled out if this proves necessary.

Assessment moments

continuous assessment

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

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

Examination methods in case of permanent assessment

Assignment

Possibilities of retake in case of permanent assessment

examination during the second examination period is possible in modified form

Extra information on the examination methods

The students write a report in which they critically approach a published method by means of a theoretical analysis that is detailed enough to start an implementation of that method.

Calculation of the examination mark

Assignments: 100%