

## Advanced Quantum Chemistry (C004147)

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

**Credits 4.0** **Study time 115 h**

**Course offerings and teaching methods in academic year 2026-2027**

A (semester 2)	English	Gent	independent work lecture
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**Lecturers in academic year 2026-2027**

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

**Offered in the following programmes in 2026-2027**

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 methods 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**

#### **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.

#### **Study material**

Type: Other

Name: Lecture material'

Indicative price: Free or paid by faculty

Optional: no

Additional information: 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.

#### **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%