GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2024-2025

Electronic Structure (C003972)

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

Credits 5.0 **Study time 135 h**

Course offerings and teaching methods in academic year 2026-2027

A (semester 1)	Dutch	Gent	seminar
			lecture

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	crdts	offering
Bachelor of Science in Chemistry	5	A
Linking Course Master of Science in Chemistry(main subject Materials and Nano Chemistry)	5	A
Preparatory Course Master of Science in Chemistry(main subject Materials and Nano Chemistry)	5	A

Teaching languages

Dutch

Keywords

Quantum chemistry, quantum mechanics, theoretical chemistry

Position of the course

This course continues the theoretical approach to chemistry and is part of the physical chemistry training. It highlights the role of quantum mechanics in chemistry and how it can be used to solve atomic and molecular problems using approximation methods. The focus lies on fundamental insight in the theories and methods with emphasis on Single Slater determinant methods that are studied in detail.

Contents

- Approximation methods for non-exactly solvable problems
- Many-electron atoms: the central field approximation
- Coupling of angular momenta in atoms
- Many-electron atoms: advanced approximations
- Matrix representations of operators and Clebsch-Gordan coefficients
- Molecules: the Born-Oppenheimer approximation
- Diatomic molecules: quantum numbers and wave functions
- Single Slater determinant methods: Hartree-Fock theory
- Many Slater determinant methods: Configuration Interaction

Initial competences

This course builds further on certain final competences of the courses:
- General chemistry
- Chemical structures
- Mathematics: basic concepts
- Mathematics: advanced techniques
- Physics: mechanics
- Physics: waves, optics and thermodynamics

This course requires the knowledge of the matter taught in Chemical Structures (C003964) and mathematics courses (C004113 and C004114). It is essential that the student has taken these courses prior to taking the Electronic Structure course.

Final competences

1 The student has gained a much deeper insight and knowledge of the fundamental aspects of modern chemistry.
2 The student understands the limitations and range of applicability for electron structure methods.
3 The student is able to design electronic structural models for chemical systems and interpret the subsequent solutions.

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

Study material

Type: Syllabus

Name: Bachelor's quantum theory
Indicative price: € 20
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

References

- "Molecular Quantum Mechanics, 5th edition", P. W. Atkins en R. S. Friedman (Oxford University Press), ISBN: 978-0199541423
- "Quantum Chemistry, 2nd edition", D. A. McQuarrie (University Science Books), ISBN: 978-1891389504
- “Introduction to quantum mechanics, 2nd edition”, B.H. Bransden en C.J. Joachain (Longman Scientific), ISBN: 978-0582356917

Course content-related study coaching

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

Assessment moments

end-of-term assessment

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

Oral assessment, Written assessment with open-ended questions

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

Oral assessment, Written assessment with open-ended questions

Examination methods in case of permanent assessment

Possibilities of retake in case of permanent assessment

not applicable

Extra information on the examination methods

The evaluation evaluates the theoretical part (oral examination with a written preparation) as well as the exercises (written examenation). The evaluation evaluates (1) the insight in electronic structural methods (2) the capacity to apply them to chemical problems and (3) the interpretation of the results obtained for applications on real chemical problems.

Calculation of the examination mark

The exam comprises two parts. The theory part that counts for 10 out of 20 points and the exercise part that also counts for 10 of the 20 points. The theory part consists of one question that can be prepared on paper and is examined in an oral

defense and one question that is answered in a purely written fashion. Students must participate in both parts of the exam or else cannot pass. Failure to participate in one of both parts or failure to reach a mark of at least 4/10 results in a no-pass end score irrespective of the grand score on 20.