

Quantum View on Chemistry (C004360)

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

Credits 4.0

Study time 120 h

Course offerings in academic year 2024-2025

Lecturers in academic year 2024-2025

Bultinck, Patrick

WE06

lecturer-in-charge

Hens, Zeger

WE06

co-lecturer

Offered in the following programmes in 2024-2025

	crdts	offering
Linking Course Master of Science in Chemistry (main subject (Bio)Organic and Polymer Chemistry)	4	A
Linking Course Master of Science in Chemistry (main subject Analytical and Environmental Chemistry)	4	A
Linking Course Master of Science in Chemistry (main subject Materials and Nano Chemistry)	4	A
Preparatory Course Master of Science in Chemistry (main subject (Bio)Organic and Polymer Chemistry)	4	A
Preparatory Course Master of Science in Chemistry (main subject Materials and Nano Chemistry)	4	A

Teaching languages

Dutch

Keywords

atoms and molecules, spatial structure, electronic structure, chemical bond, quantum mechanics, stereochemistry, conformation

Position of the course

This is a course within the 'general chemistry' learning track.

It provides a thorough knowledge of the spatial structure and electronic structure of molecules, and the relationship between the two. This includes a thorough introduction to the basic principles of quantum mechanics, and its use in describing and understanding of electronic structure and the chemical bonding.

The emphasis is on teaching general knowledge with more specialized learning can build on.

The course makes use of skills in modeling and simulation.

Contents

- Functions and vectors; operators and matrices
- The Schrödinger equation
- Chemical two-state systems
- Time-dependent systems
- More electrical systems
- Wave mechanics - exactly solvable problems
- Wave mechanics - spherical potentials
- Quantum mechanical description of atomic systems
- Quantum mechanical description of molecules

Initial competences

No specific requirements

Final competences

- 1 The student understands the description of atoms, molecules and chemical bonding and is familiar with the language and the related interpretations of the concepts at its base.
- 2 The student has insight into the way in which the above leads to the composition and structure of the Periodic Table.
- 3 The student has gained insight into the different types of chemical bonds and can recognize and describe them correctly.
- 4 The student is familiar with the concept of resonance and the precise meaning and application; he / she can derive the relevant resonance structures
- 5 The student can recognize, describe and name the different types of isomerism.
- 6 The student is able to recognize and name the major functional groups of organic molecules and name.
- 7 Derive the IUPAC name of simple inorganic and organic compounds and from the IUPAC name derive the associate structure formula.
- 8 Analyze the symmetry of a molecule and apply the insight in predicting physical properties, crystal forms and orbitals.
- 9 The student is familiar with the concept of conformation and can perform simple conformational analysis and explain from this the dynamic behavior of molecules.
- 10 The student understands the basic principles of quantum mechanics and to apply them within the context of two-level systems.
- 11 The student has insight into the electronic structure of atoms and the quantum mechanical description thereof.
- 12 The student understands the chemical bond and the quantum mechanical description thereof.
- 13 The student is able to solve problems of chemical structure by reasoning from a quantum mechanical context.

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, seminar

Learning materials and price

- English course notes and English reference material.
- Background texts and links on Ufora.
- Each student disposes of their own computer.

References

- Leonard Susskind and Art Friedman, Quantum Mechanics, the theoretical minimum. Penguin Books, UK, 2015. ISBN 9780141977812 (about 15 EUR) - optional.
- Colleges (video) from this book, iTunes or YouTube (free) - required viewing.

Course content-related study coaching

Assessment moments

end-of-term assessment

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

Written assessment with open-ended questions

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

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 exam includes both a theory and an exercises part.

Calculation of the examination mark

The theory part accounts for 40%, while exercises account for 60%.

