

## Molecular Structure (E021560)

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

**Credits 3.0** **Study time 90 h**

**Course offerings in academic year 2025-2026**

A (semester 2) Dutch Gent

**Lecturers in academic year 2025-2026**

Van Speybroeck, Veronique TW17 lecturer-in-charge

**Offered in the following programmes in 2025-2026**

	crdts	offering
<a href="#">Bachelor of Science in Engineering(main subject Biomedical Engineering)</a>	3	A
<a href="#">Bachelor of Science in Engineering(main subject Chemical Engineering and Materials Science)</a>	3	A
<a href="#">Bridging Programme Master of Science in Chemical Engineering</a>	3	A

**Teaching languages**

Dutch

**Keywords**

Quantum Mechanics, Molecular symmetry, Spectroscopy

**Position of the course**

This basic course provides more in-depth insight in phenomena at the atomic and molecular scale.

The principles of quantummechanics are introduced such as the Schrödinger equation, wavefunction and postulates of quantum mechanics. These concepts are applied on atomic and molecular systems, with the aim to obtain the solutions of hydrogenic like atoms and to understand rovibrational spectra of simple molecules. The importance of symmetry for explaining spectroscopic properties and chemical bonding are introduced.

**Contents**

- Wave-particle duality, uncertainty principle of Heisenberg
- Schrödinger equation: dynamic and stationary wave equation; probability distribution and wavefunction
- Postulates of quantum mechanics
- 1-dimensional potential problems: infinite potential well, harmonic oscillator
- 3-dimensional central potential: orbital momentum, spherical harmonics
- Hydrogen atom: energy spectrum and wave functions
- Symmetry groups in molecules and spectroscopy; introduction of point groups to identify molecular symmetry
- Rationalization of rotational and vibrational spectroscopy by means of the harmonic oscillator and rigid rotor and concepts of symmetry
- Importance of symmetry to rationalize the formation of the chemical bond

**Initial competences**

This course builds upon certain final competences from Physics I and Physics II.

**Final competences**

- 1 Understand the importance of a quantummechanical approach to describe phenomena at the atomic and molecular scale.
- 2 Master basic concepts of quantummechanics: particle-wave duality, Schrödinger equation, probability distribution, postulates of quantummechanics.
- 3 Solve the Schrödinger equation for basic potential problems (1D or central or

problems where separation of variables is possible).

- 4 Master basic concepts to correctly solve a central problem at the quantum mechanical level, such as the orbital angular momentum and spherical harmonics.
- 5 Master the quantum mechanical description of the hydrogen atom.
- 6 Understand the importance of symmetry for spectroscopy and formation of the chemical bond.

#### **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

#### **Study material**

Type: Syllabus

Name: Moleculaire structuur

Indicative price: € 5

Optional: yes

Language : Dutch

Number of Pages : 150

Available on Ufora : No

Online Available : No

Available in the Library : No

Available through Student Association : No

Additional information: The course material for the course Quantum Mechanics II consists of a syllabus and slides. The slides will be posted on Ufora during the academic year and there is the possibility to purchase the syllabus

Type: Slides

Name: Slides

Indicative price: Free or paid by faculty

Optional: no

Language : Dutch

Available on Ufora : Yes

Online Available : Yes

Available in the Library : No

Available through Student Association : No

#### **References**

- J. Michael Hollas, Modern Spectroscopy John Wiley & Sons
- B. H. Bransden and G. J. Joachain, Introduction to Quantum Mechanics, Longman 1989

#### **Course content-related study coaching**

Lecturer and assistants are available before and after lectures or by appointment.

#### **Assessment moments**

end-of-term assessment

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

Written assessment

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

Written assessment

#### **Examination methods in case of permanent assessment**

#### **Possibilities of retake in case of permanent assessment**

not applicable

#### **Extra information on the examination methods**

- Written theory exam, closed book.
- Written exercise exam, closed book.
- A formulary is provided during the exam.

