GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2024-2025

Atomic and Molecular Physics (C004222)

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

Credits 5.0 **Study time 150 h**

Course offerings and teaching methods in academic year 2024-2025

A (semester 2)	Dutch	Gent	lecture	25.0h
			seminar	10.0h
B (semester 2)	Dutch	Gent	seminar	
			lecture	

Lecturers in academic year 2024-2025

Joos, Jonas	WE04	lecturer-in-charge
Vrielinck, Henk	WE04	co-lecturer

Offered in the following programmes in 2024-2025	crdts	offering
Bachelor of Science in Physics and Astronomy	5	A
Master of Science in Teaching in Science and Technology(main subject Mathematics)	6	A, B
Master of Science in Mathematics	6	A, B
Preparatory Course Master of Science in Physics and Astronomy	5	A
Preparatory Course Master of Science in Physics and Astronomy	5	A

Teaching languages

Dutch

Keywords

Quantum modeling of electronic and molecular structure, electronic spectroscopy, vibrational spectroscopy.

Position of the course

This course unit belongs to the learning pathway Structure of matter in the bachelor program Physics and Astronomy.
The goal of this course is to apply the principles of quantum mechanics to atoms and molecules. Analytical and numerical computing techniques are applied to obtain wave functions and energy eigenvalues for atoms and molecules. From these, physical observables will be extracted such as the molecular structure of ground and excited states, electronic and vibrational spectra. Theoretical results will always be checked with experimental observations. This course unit bridges fundamental theoretical physics with more applied domains such as photonics, solid state physics and chemistry.

Contents

- Hydrogen atom: recap analytical solution (eigen functions and energy eigenvalues); fine structure, hyperfine structure.
- Helium atom: ground state; excited states and spectrum; Pauli principle.
- Polyelectronic atoms and ions: central field approximation; Slater determinant; Hartree-Fock theory; electron shell model and systematics: quantum mechanical origin of the periodic table.
- Excited states of atoms: perturbative treatment of electronic Coulomb repulsion and spin-orbit coupling in the Russell-Saunders and jj coupling schemes; configuration interaction and electron correlation.
- Atomic spectroscopy: interaction between matter and radiation; absorption and emission; selection rules; lasers; atoms in external electric and magnetic fields.

- Molecular Hamiltonian: Born-Oppenheimer approximation; non-adiabatic terms.
- Molecular orbital theory: symmetry classification of molecules; linear combinations of atomic orbitals (LCAO); Hückel theory for pi electron, ligand field theory for d electrons.
- Vibrational spectroscopy of molecules: normal modes, overtones and combination modes; selection rules; infrared and Raman spectra; rotational energy levels.
- Electronic spectroscopy of molecules: Franck-Condon transitions; selection rules, fluorescence and phosphorescence; nonradiative decay.

Initial competences

Nonrelativistic quantum mechanics (angular momentum algebra, hydrogen atom, perturbation theory) electromagnetism, group and representation theory. This corresponds to the final competences of the courses Quantum Mechanics 2, Relativity and Electromagentism and Groups and Representations.

Final competences

1 Knowing, understanding and being able to apply key concepts of physics and basic methods of atomic and molecular physics.
2 Having a thorough basic knowledge of general physics domains (such as quantum mechanics, wave theory, optics and electromagnetism), needed to study atomic and molecular physics.
3 Having a broad knowledge of mathematics, including group and representation theory, and being able to apply it to solve physical problems.
4 Being able to argue under what conditions physical and mathematical approximations can be correctly used.
5 Being able to interpret atomic and molecular spectra.
6 Having advanced knowledge of the electronic structure of matter and the spectroscopy of atoms and molecules, enabling one to initiate advanced experimental and theoretical studies in this or related domains.
7 Begin able to correctly use physics terminology in Dutch and English.

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: Atomic and molecular physics
Indicative price: Free or paid by faculty
Optional: no
Language : English
Number of Pages : 216
Available on Ufora : Yes
Online Available : No
Available in the Library : No
Available through Student Association : Yes

References

- M. Weissbluth, Atoms and Molecules, 1st edition, Academic Press 2012 (ISBN 978-0323142946), price €59.90; 730 pages.
- P.W. Atkins en R.S. Friedman, Molecular Quantum Mechanics, 5th edition, Oxford 2011 (ISBN 978-0199541423), price €74.89; 537 pages.
- B. O. Roos, R. Lindh, P. A. Malmqvist, V. Veryazov, P.-O. Widmark, Multiconfigurational Quantum Chemistry, 1st edition, Wiley 2016 (ISBN 978-0470633465), price €115; 240 pages.
- M. S. Dresselhaus, G. Dresselhaus, Group Theory: Application to the Physics of Condensed Matter, Springer 2010 (ISBN 978-3642069451), price €53.49; 597 pages.

Course content-related study coaching

Interactive support via Ufora (forums), e-mail or personal contact with teacher (after making an appointment).

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

- Theory: oral exam with written preparation, closed book.
- Exercises: written, open book.

Calculation of the examination mark

- 5/20 points: theory
- 15/20 points: exercises