

Atomic and Molecular Physics (E025010)

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

Credits 6.0 **Study time** 180 h **Contact hrs** 60.0 h

Course offerings and teaching methods in academic year 2016-2017

A (semester 1)	lecture	30.0 h
	seminar: coached exercises	30.0 h
B (semester 1)	seminar: coached exercises	30.0 h
	guided self-study	30.0 h

Lecturers in academic year 2016-2017

Van Speybroeck, Veronique	TW17	lecturer-in-charge
Vrielinck, Henk	WE04	co-lecturer

Offered in the following programmes in 2016-2017

	crdts	offering
Bridging Programme Master of Science in Engineering Physics	6	A
Master of Science in Electromechanical Engineering (main subject Control Engineering and Automation)	6	A
Master of Science in Electromechanical Engineering (main subject Electrical Power Engineering)	6	A
Master of Science in Electromechanical Engineering (main subject Maritime Engineering)	6	A
Master of Science in Electromechanical Engineering (main subject Mechanical Construction)	6	A
Master of Science in Electromechanical Engineering (main subject Mechanical Energy Engineering)	6	A
Master of Science in Photonics Engineering	6	A
European Master of Science in Nuclear Fusion and Engineering Physics	6	A
European Master of Science in Nuclear Fusion and Engineering Physics	6	A
Master of Science in Engineering Physics	6	A
Master of Science in Engineering Physics	6	B

Teaching languages

Dutch, English

Keywords

Atomic and molecular spectra, quantum modeling of atoms and molecules

Position of the course

The aim of this course is to build the quantum-mechanical formalism required for the theoretical interpretation of the atomic and molecular spectra.

Contents

- One-electron atoms : Fine structure and hyperfine structure: Spin-orbit interaction, Darwin term, Selection rules for electric dipole transitions, Hyperfine structure and isotope shifts
- Interaction of one-electron atoms with external electric and magnetic field: Stark effect, Zeeman effect, Strong fields ? Paschen-Back effect
- The atomic and molecular Hamiltonian: The molecular Hamiltonian, Atomic Units, Born-Oppenheimer approximation

- Two electron atoms: The Schrodinger equation for two electron atoms, He in the independent particle model (IPM), Time independent perturbation correction to IPM, Effective nuclear charge, Hartree-Fock for He, Electron correlation, Spin wave function Pauli exclusion principle, Statistics of indistinguishable particles, Level scheme of two-electron atoms
- Many electron atoms: Central field approximation, Pauli exclusion principle and Slater determinants, Labeling Atomic States, Configuration, term, level and state, Hund's Rules, The Hartree-Fock approximation, Corrections to the central field approximation (L-S and j-j coupling)
- Interaction of many electron atoms with electromagnetic radiation
- Molecular structure: General nature of molecular structure ? Molecular spectra, Diatomic molecules - Symmetry properties ? Molecular Term Symbols- The hydrogen molecular ion - Correlation Diagrams, The Molecular orbital idea, Bonding and antibonding molecular orbitals, Molecular orbital theory for homonuclear diatomics, Molecular hydrogen within LCAO approximation, Photoelectron spectrum : experimental proof for MOs, Heteronuclear molecules, Molecular Symmetry - Point Groups, Polyatomic molecules, Vibration-Rotation spectroscopy

Initial competences

Non-relativistic advanced quantum mechanics and perturbation theory (stationary and time dependent) - electromagnetism

Final competences

- 1 To be able to model atoms and molecules with quantum mechanical methods and to interpret atomic and molecular spectra.
- 2 Application-oriented reflecting on new insights obtained by modeling of atoms and molecules.
- 3 Dispose of enough knowledge and comprehension to critically evaluate the results of complex calculations of atoms and molecules.
- 4 Be able to apply prior quantummechanical knowledge in a creative, targeted and innovative way to solve molecular and atomic many body problems.

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

Guided self-study, lecture, seminar: coached exercises

Extra information on the teaching methods

Classroom lectures; Classroom problem solving sessions

Learning materials and price

Syllabus 2016

B. H. Bransden & Joachain, Physics of Atoms and Molecules ISBN 0582 35692

Second Edition published 2003

References

- B. H. Bransden & Joachain, Physics of Atoms and Molecules, ISBN 0582 35692, Second Edition published 2003
- J. M. Hollas, Modern Spectroscopy, ISBN 0-471-93076-8

Course content-related study coaching

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

Evaluation methods

end-of-term evaluation

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

Written examination, open book examination, oral examination

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

Written examination, open book examination, oral examination

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

Theory and exercise exam
Theory : Oral open-book exam, written preparation
Exercise : written open-book exam - problems

Calculation of the examination mark