

## 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 Slaterdeterminants, 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**