CH-244

Quantum chemistry

Drabbels Marcel

Cursus	Sem.	Type
Chemistry and chemical engineering	BA3	Obl.
HES - CGC	H	Obl.

Language of teaching	English
Credits	6
Session	Winter
Semester	Fall
Exam	Oral
Workload	180h
Weeks	14
Hours	**6 weekly**
Courses	4 weekly
Exercises	2 weekly
Number of positions	

Summary

Introduction to Quantum Mechanics with examples related to chemistry

Content

- Introduction and historical perspective
- The Time Independent Schrödinger equation and applications to simple systems
- Measurements in quantum mechanical systems
- Operator formulation of the Schrödinger Equation
- Postulates of quantum mechanics
- Time dependent Schrödinger equation
- The harmonic oscillator
- Three dimensional systems
- Angular momentum
- The hydrogen atom
- Approximation methods
- Many electron atoms
- Electron spin and the Pauli principle
- Term symbols and coupling of angular momentum
- Quantum mechanical treatment of molecules
- Electronic structure calculations

Learning Outcomes

By the end of the course, the student must be able to:

- Formulate quantum mechanical concepts
- Derive quantum mechanical operators
- Solve eigen value equations
- Solve the Schrodinger equation for simple systems
- Apply quantum mechanical concepts to simple problems
- Use approximation methods
- Formulate the relation between spin and the Pauli Exclusion principle and discuss the implications for chemistry

- Derive term symbols for atoms and molecules
- Discuss the principles of molecular bonding

Teaching methods

Ex Cathedra with excersise sessions

Expected student activities

Work on the exercises at home

Supervision

Office hours	Yes
Assistants	Yes

Resources

Bibliography

Primary Reference:

- D. A. McQuarrie, *Quantum Chemistry*

Secondary References:

- P. W. Atkins, *Molecular Quantum Mechanics*
- Cohen-Tannoudji, Diu, and Laloë, *Quantum Mechanics*
- B.H. Bransden and C.J. Joachain, *Introduction to Quantum Mechanics*

Ressources en bibliothèque

- Quantum mechanics / Bransden
- Molecular quantum mechanics / Atkins
- Quantum chemistry / McQuarrie
- Quantum mechanics / Cohen-Tannoudji

Moodle Link

- http://moodle.epfl.ch/course/view.php?id=2381

Prerequisite for

Chimie physique expérimentale