

CH-244

Quantum chemistry

Drabbels Marcel

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

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|----------------------------|-----------------|
| 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

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](#)
- [Quantum mechanics / Cohen-Tannoudji](#)
- [Quantum chemistry / McQuarrie](#)
- [Molecular quantum mechanics / Atkins](#)

Prerequisite for

Chimie physique expérimentale