CH-353

Introduction to electronic structure methods

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Cursus	Sem.	Type
Biocomputing minor	H	Opt.
Chemistry	BA5	Opt.
Computational science and Engineering	MA1, MA3	Opt.
HES - CGC	H	Opt.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	During the semester
Workload	120h
Weeks	14
Hours	**4 weekly**
Courses	3 weekly
Exercises	1 weekly
Number of positions	

Summary

Repetition of the basic concepts of quantum mechanics and main numerical algorithms used for practical implementions. Basic principles of electronic structure methods:Hartree-Fock, many body perturbation theory, configuration interaction, coupled-cluster theory, density functional theory.

Content

Short repetition of the basic concepts of quantum mechanics and the main numerical algorithms used for practical implementions. Basic principles of electronic structure methods: Hartree-Fock, many body perturbation theory, configuration interaction, coupled-cluster theory, density functional theory. Overview of computational molecular modelling techniques.
Application of these techniques in a practical research project.

Learning Outcomes

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

- Manage basic theoretical concepts of electronic structure methods-
- Carry out simple electronic structure calculations.

Transversal skills

- Plan and carry out activities in a way which makes optimal use of available time and other resources.
- Evaluate one's own performance in the team, receive and respond appropriately to feedback.
- Make an oral presentation.
- Write a scientific or technical report.

Teaching methods

Ex cathedra and exercices on computers

Assessment methods

Ongoing controls as follow:
1/3 of final grade = 1 written exam in the middle of the semester
1/3 of final grade = 1 oral exam at the end of the semester
1/3 of final grade = average of the grades obtained on the weekly reports and questions asked on these reports.

Resources

Ressources en bibliothèque

- Molecular modelling / Leach
- Modern quantum chemistry / Szabo