CH-351

Molecular dynamics and Monte-Carlo simulations

Röthlisberger Ursula

Cursus	Sem.	Type
Chemistry	BA6	Obl.
Computational science and Engineering	MA2, MA4	Opt.
HES - CGC	E	Opt.

Language of teaching	English
Credits	2
Session	Summer
Semester	Spring
Exam	During the semester
Workload	60h
Weeks	14
Hours	**2 weekly**
Courses	1 weekly
Exercises	1 weekly
Number of positions	

Summary

Introduction to molecular dynamics and Monte-Carlo simulation methods.

Content

- Time-dependent Schrödinger equation
- Statistical mechanics
- Short introduction to statistical mechanics
- Molecular Dynamics simulation
- Monte Carlo simulation

Learning Outcomes

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

- Manage basic theoretical concepts of Molecular Dynamics and Monte Carlo methods.
- Carry out simple Molecular Dynamics and monte Carlo simulations.

Transversal skills

- Take feedback (critique) and respond in an appropriate manner.
- Use both general and domain specific IT resources and tools
- Write a scientific or technical report.