

CH-351

Molecular dynamics and Monte-Carlo simulation

Röthlisberger Ursula

Cursus	Sem.	Type
Chemistry	BA6	Obl.
Computational science and Engineering	MA2, MA4	Opt.
Computational science and engineering minor	E	Opt.
HES - CGC	E	Opt.
Minor in Quantum Science and Engineering	E	Opt.
Quantum Science and Engineering	MA2, MA4	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.

Assessment methods

control continue with 2 written exams and grades for exercise reports (each 1/3 written exam 1, written exam 2 and exercises)

Resources

Moodle Link

- <https://go.epfl.ch/CH-351>