

CH-351

**Molecular dynamics and Monte-Carlo simulations**

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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
<b>Hours</b>	<b>2 weekly</b>
Courses	1 weekly
Exercises	1 weekly
<b>Number of positions</b>	

**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.

**Supervision**

Office hours	No
Assistants	Yes
Forum	No

**Resources**

**Websites**

- [http://scgc.epfl.ch/telechargement\\_cours\\_chimie](http://scgc.epfl.ch/telechargement_cours_chimie)