

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.