

CH-420

Understanding advanced molecular simulation

Smit Berend

Cursus	Sem.	Type
Chimiste	MA2, MA4	Opt.
Computational science and Engineering	MA2, MA4	Opt.
Computational science and engineering minor	E	Opt.

Language of teaching	English
Credits	4
Session	Summer
Semester	Spring
Exam	During the semester
Workload	120h
Weeks	14
Hours	3 weekly
Lecture	2 weekly
Project	1 weekly
Number of positions	

Summary

This course introduces advanced molecular simulation techniques such as Monte Carlo and Molecular dynamics in different ensembles, free energy calculations, rare events, Configurational-bias Monte Carlo etc.

Content

The course will be given in five blocks, each covers a topic and ends with an assignment to carry out some simulations.

- [Weeks 1-3] Computational Carpentry and Statistical Thermodynamics
- [Weeks 4-5] Basic Monte Carlo and Molecular Dynamics
- [Weeks 6-9] Monte Carlo and Molecular dynamics in different ensembles
- [Week 7] semester break
- [Weeks 10-13] Free energy calculations and rare events
- [Weeks 14-15] Special topics

Keywords

molecular simulation, molecular dynamics, Monte Carlo simulation

Learning Prerequisites**Recommended courses**

knowledge on statistical thermodynamics, some basic programming skills

Assessment methods

The mark will be a: assignments given during the course (60%) and reports + oral presentation of 2 blocks (40%)

Resources**Bibliography**

D. Frenkel and B. Smit, *Understanding Molecular Simulations: from Algorithms to Applications*, 2nd ed. (Academic Press, San Diego, 2002)

Ressources en bibliothèque

- [Understanding molecular simulation : from algorithms to applications / Frenkel](#)

Moodle Link

- <https://go.epfl.ch/CH-420>