CH-420

Understanding advanced molecular simulation

Smit Berend

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

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