CH-452

Computational methods in molecular quantum mechanics

Bonella Sara

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.
Chimiste	MA1, MA3	Opt.
Computational science and Engineering	MA1, MA3	Opt.
Minor in Quantum Science and Engineering	H	Opt.
Quantum Science and Engineering	MA1, MA3	Opt.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	Oral
Workload	120h
Weeks	14
Hours	**3 weekly**
Lecture	2 weekly
Exercises	1 weekly
Number of positions	

Summary

This course will discuss the main methods for the simulation of quantum time dependent properties for molecular systems. Basic notions of density functional theory will be covered. An introduction to simulating nuclear quantum effects for adiabatic and non adiabatic dynamics will be provided.

Content

Short repetition
Introduction to classical molecular dynamics simulations for molecular systems
Density Functional theory, basic theorems

Advanced topics
Time dependent Schroedinger equation for a system of nuclei and electrons. The coupled channels equation
Integration methods for first principles molecular dynamics with classical ions.
Adiabatic and non adiabatic molecular dynamics: approximate methods for numerical solution
Nuclear quantum effects.

Keywords

simulation and modelling of materials
quantum systems

Learning Prerequisites

Required courses

Basic quantum mechanics

Learning Outcomes

By the end of the course, the student must be able to:

- Prove the basic theorems of DFT
- Interpret input and output of typical community codes for classical and ab initio molecular dynamics
- Discuss the evolution of the different electronic structure methods for electronic excited states
- Discuss basic equations for quantum evolution of nuclei and electrons

Transversal skills

- Evaluate one's own performance in the team, receive and respond appropriately to feedback.
- Summarize an article or a technical report.

Expected student activities

Weakly summary (three point bullet list) of lecture material + question
Development (in team) of small research project, computational or based on literature
Oral presentation of research project

Assessment methods

1/4 Evaluation of weakly summaries
1/2 Development and presentation of research project
1/4 Oral exam on course topics

Resources

Moodle Link

- https://go.epfl.ch/CH-452