CH-452

Computational methods in molecular quantum mechanics

Bonella Sara

Cursus	Sem.	Type
Chimiste	MA1, MA3	Opt.
Computational 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**
Courses	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 and of its time dependent version will be covered in the context of adiabatic and non adiabatic dynamics.

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
Representing excited electronic states, Time dependent density functional theory
Adiabatic and non adiabatic molecular dynamics: approximate methods for numerical solution
Nuclear quantum effects.

Learning Prerequisites

Important concepts to start the course

Basic concepts of quantum mechanics
basic knowledge of a programming language (C, fortran, Matlab)

Learning Outcomes

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

- Solve theoretical problems in quantum chemistry and physics
- Decide which theoretical method is more appropriate to perform quantum molecular dynamics simulations
- Prove the basic theorems of DFT and TDDFT
- Sketch excited state reaction paths of photoexcited molecular systems
- Justify the selection of a computational scheme for the solution of a given problem on excited state dynamics
- Derive different solutions for the combined electron-nuclear dynamics
- Discuss the evolution of the different electronic structure methods for electronic excited states
- Assess / Evaluate the range of application of different approximate methods for excited states quantum molecular dynamics

Transversal skills

• Use a work methodology appropriate to the task.
• Make an oral presentation.

Teaching methods

Blackboard and coding excercises

Expected student activities

Solution of take home problem sets
Development (in team) of small research project, computational or based on literature
Oral presentation of research project

Assessment methods

1/3 Midterm take home exam
1/3 Presentation of research project
1/3 Oral exam on course topic

Supervision

Office hours	Yes
Assistants	Yes
Others	Office hours to be determined by appointment via email

Resources

Bibliography

- D. J. Tannor, «Introduction to quantum mechanics. A time-dependent prospective», Univ. Science Books.
- D. Marx, J. Hutter, «Ab-inito molecular dynamics », Cambridge University Press
and lecture notes.

Ressources en bibliothèque

• Ab Initio Molecular Dynamics : Basic Theory and Advanced Methods / Marx
• Introduction to quantum mechanics / Tannor

Notes/Handbook

Lecture notes