UE Molecular modelling

ECTS
3 credits

Component
UFR Chimie-Biologie

Semester
Tous les ans

- **Teaching language(s):** English
- **Open to exchange students:** Yes
- **Code d'export Apogée:** YAX9CH18

Presentation

Description

Course outline:

Common modelling methods based on classical (MM, MD) and quantal (HF, DFT) approaches are addressed and their application are illustrated during lectures. Three computational labs are made to make students familiar with the application of these methods.

Details:

I. Lect1- Introduction: The potential energy surface
II. Lect2- Molecular Mechanics, Forcefield methods
III. Lab1- Forcefield methods, exploration of a potential energy surface
IV. Lect3- Ab initio methods, the self-consistent field, basis sets, density functional theory and applications
V. Lab2- ab initio methods: electron structure, reactivity
VI. Lect4- Molecular Dynamics simulations
VII. Lab3- Molecular Dynamics Simulations

Course parts

CM	Lectures (CM)	12h
UE Molecular modelling - TP	Practical work (TP)	9h

Recommended prerequisites

Prerequisites:

Basic electronic structure of atoms and molecules (bachelor program in chemistry, CHI110, CHI504 and CHI607 in Grenoble)

Period : Semester 9

Skills

Skills:

basic knowledge about the usual modelling methods in chemistry in order to be able to apprehend a theoretical work and collaborate with theoretical chemists.

Useful info

Contacts

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Place

Grenoble

Campus

Grenoble - University campus