

UE Molecular modelling



Niveau d'étude
Bac +5



ECTS
3 crédits



Composante
UFR de Chimie
et de biologie



Période de
l'année
Toute l'année

Diplômes intégrant cet élément

- Master Chimie

- › **Langue(s) d'enseignement:** Anglais
- › **Ouvert aux étudiants en échange:** Oui
- › **Code d'export Apogée:** YAX9CH18

Présentation

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

Heures d'enseignement

CM	CM	12h
TD	TD	9h

Pré-requis recommandés

Prerequisites:

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

Période : Semestre 9

Compétences visées

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.

Infos pratiques

Contacts

Responsable pédagogique

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