Computational chemistry 2

ECTS
3 crédits

Etablissement(s)
UFR Chimie, UFR des Sciences fondamentales et biomédicales

Volume horaire
24h

Période de l'année
Semestre 2

En bref

- **Langue(s) d'enseignement:** Anglais
- **Forme d'enseignement :** Cours magistral & Travaux pratiques
- **Ouvert aux étudiants en échange:** Non

Présentation

DESCRIPTION

This module aims to provide the students with advanced concepts in numerical and data driven chemistry which are necessary in advanced molecular modeling and simulation. In particular the module will cover the formalisms and applications of density functional theory (DFT) including the performance and systematic improvement of exchange correlation functionals. The molecular environment will be taken into account both implicitly with continuum methods and explicitly by hybrid quantum mechanics/ molecular mechanics frameworks. The principle of classical and ab initio MD simulation will be also tackled with a special emphasis on the inference of structural and electronics properties from simulation trajectory, using also artificial intelligence based techniques for the reduction of dimensionality

- Introduction to DFT theory et Kohn-Sham approximation
- Definition of Exchange Correlation functionals and their systematic improvement (Jakob Ladder)
- Modeling solvation through implicit polarizable continuum methods,
- Describing the environment using hybrid QM/MM methods. Electrostatic and polarizable effects and QM/MM frontier
- Molecular dynamics simulations in complex systems
- Analysis of trajectories, unsupervised artificial intelligence for clustering and identification of collective movements.

HEURES D'ENSEIGNEMENT

Computational chemistry 2	Cours Magistral	16h
Computational chemistry 2	Travaux Pratiques	8h

PRÉ-REQUIS OBLIGATOIRES

Computational Chemistry 1

En bref

CONTACTS

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LIEU(X)

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