

# Modélisation moléculaire



## En bref

- › Langue(s) d'enseignement: Français
- › Ouvert aux étudiants en échange: Oui

## Présentation

### Description

- › Choice of the theoretical model to answer a molecular problem – 7.5h CM
  - # Available theoretical methods and their limitations.
  - # The problem of electronic correlation.
  - # Choosing calculations parameters.
  - # The potential energy surface of the excited states and the spectral modeling.
  - # The importance of vibronic coupling.
  - # Simple and advanced approaches to model reactivity
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- .› Setting up a strategy adapted to a problem – 7.5h CM and 10h TP
  - # Study of an experimental problem (article).
  - # Choice of a calculation strategy and its limits.
  - # Choice of a problem to study and practice.
  - # Simulation of the absorption and emission properties of complex molecules.

### Objectifs

The theoretical calculation of the absorption and emission properties of UV-visible light, as well as the modelling of organic reactivity, are now widely available with *ab initio* methods. The objective of this course is to train informed users capable of choosing, independently and with a critical eye, a calculation method to model the ground state and excited states of complex molecules. The first part of this teaching covers and deepens the problems related to the calculation methodology while the second part is dedicated to the practice of modelling optical spectra (absorption, emission) and is mainly carried out in the form of project work.

## Heures d'enseignement

CM - Modélisation moléculaire	Cours magistral	15h
TP - Modélisation moléculaire	Travaux pratique	10h

## Pré-requis obligatoires

# Choosing the right theoretical model to answer a problem related to the reactivity or the UV-visible spectroscopy properties of a complex molecule.

# Exploit judiciously and rigorously the results of molecular calculations.

# Analyze and summarize data for exploitation.

# Conduct an innovative approach that takes into account the complexity of a situation by using information that may be incomplete or contradictory.

# Give an oral account of his/her work.

## Infos pratiques

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### Lieu(x)

> Angers