

Molecular Modelisation



SCHOOL

Faculty of Science



CAMPUS

Belle-Beille



LEVEL

2nd year Master's degree



OPEN TO EXCHANGE STUDENTS

Yes



SEMESTER

Fall (S1)

> **Degree course:** Light, Molecules, Matter

> **Teaching unit:** UE2

> **Course language:** English

> **Duration (hours):** 25

> **ECTS:** 2

> **Teacher(s):** Thomas CAUCHY

> **Assessment:**

Continuous assessment

Final exam

> **Teaching methods:**

Lecture course 15 hours

Tutorial course hours

Practical work 10 hours

Case study

Project

COURSE DESCRIPTION

Choice of the theoretical model to answer a molecular problem - 7.5 lecture hours

- 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 modelling.
- The importance of vibronic coupling.
- Simple and advanced approaches to model reactivity.

Setting up a strategy adapted to a problem ? 7.5 lecture hours and 10 tutorial hours.

- 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.

OBJECTIVES

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.