

CH-431

**Physical and computational organic chemistry**

Corminboeuf Clémence

Cursus	Sem.	Type
Chimiste	MA2, MA4	Opt.

Language of teaching	English
Credits	2
Session	Summer
Semester	Spring
Exam	Oral
Workload	60h
Weeks	14
<b>Hours</b>	<b>2 weekly</b>
Courses	2 weekly
<b>Number of positions</b>	

**Summary**

This course introduces modern computational electronic structure methods and their broad applications to organic chemistry. It also discusses physical organic concepts to illustrate the stability and reactivity of organic molecules.

**Content****Computational Methods**

- Electronic structure approaches for organic chemistry
- Overview of density functional theory and post-Hartree-Fock methods
- Introduction to machine learning methods for chemistr

**Fundamentals of physical organic chemistry**

- Thermodynamic stabilities
- Stabilizing effects
- Computation of reaction mechanisms
- Radicals, diradicals, carbenes and spin multiplicity
- Kinetic isotope effects
- (Organic reactions dynamics)

**Special topic in computational/physical organic chemistry**

- Aromaticity
- Molecular Strain
- Linear free energy scaling relationships
- Machine learning models for catalysis

**Selected article for presentation****Keywords**

Computational organic chemistry, DFT, reaction mechanisms, chemical concepts

**Learning Outcomes**

By the end of the course, the student must be able to:

- Choose an appropriate computational method to address a given chemistry problem
- Estimate the uncertainties associated with the use of a given computational approach

- Assess / Evaluate the (de)stabilizing effects of a molecule
- Elaborate orbital energy diagrammes
- Interpret the forbidden/allowed nature of a chemical reaction
- Specify the type of kinetic isotope effects
- Identify the main message of an article

### Transversal skills

- Communicate effectively, being understood, including across different languages and cultures.

### Expected student activities

resolve the mini and maxi quiz  
read, understand and present a scientific article

### Assessment methods

1/3 présentation; 2/3 oral exam

### Resources

#### Ressources en bibliothèque

- [Modern Physical Organic Chemistry / Anslyn](#)
- [Computational Organic Chemistry / Bachrach](#)

#### Websites

- [http://scgc.epfl.ch/telechargement\\_cours\\_chimie](http://scgc.epfl.ch/telechargement_cours_chimie)

#### Moodle Link

- <http://moodle.epfl.ch/course/view.php?id=15018>