CH-431

Physical and computational organic chemistry

Corminboeuf Clémence

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Obl.
Chimiste	MA2, MA4	Opt.

Language of teaching	English
Credits	2
Session	Summer
Semester	Spring
Exam	During the semester
Workload	60h
Weeks	14
Hours	**2 weekly**
Courses	2 weekly
Number of positions	

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

Moodle Link

- https://go.epfl.ch/CH-431