

ChE-609(1)

Computational methods in Chemistry and Chemical Engineering-Computational Carpentry and online materials

Lecturers (see below), Smit Berend

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Obl.

Language of teaching	English
Credits	1
Session	
Exam	Project report
Workload	30h
Hours	21
Courses	7
Exercises	14
Number of positions	

Frequency

Every year

Remark

Next time May 4-8 2020 This course as three modules that can each be followed separately.

Summary

This course will have three components: Molecular Simulation, Electronic Laboratory Notebooks, and Machine learning. The focus of the course is applications to microporous materials (metal organic frameworks, zeolites, covalent organic frameworks) and is aimed at non-computational chemists.

Content

This introduction level course ChE -609(1) "Computational methods in Chemistry and Chemical Engineering – Computational Carpentry and online materials" is an online (graduate) course that introduces computational methods for those that would like to gain some knowledge on how these techniques are used.

The methods we discuss are general but the illustrations are from our research on porous materials. The course is particularly aimed at those that because of the lock-downs of many experimental labs have their course/lab-program disrupted. All the teaching material will be made available through EPFL's Moodle site. Participation from outside EPFL is encouraged.

We set up the computational environment and learn the basics of the Python programming language and Bash. This module is taught in flipped classroom format. You will find a quiz at the end of the section to test your knowledge and you will need this knowledge to work on the other modules, of this course.

Exam : Project report (passed or failed)

Prior knowledge:

We do not expect any prior knowledge of programming beyond the level of a typical Matlab-like introduction. We do start the course we present some of the computer science tools that we will use throughout.

Other blocks.

This course has three coming units to which you may enroll separately

• ChE-609(2) Molecular Simulation of Adsorption

In this module we learn how to use molecular simulations to understand and predict adsorption in porous materials. (1 ECTS = Project report)

• ChE-609(3) Machine Learning

In this module we learn how to use machine learning to predict the gas adsorption in porous materials.
(1 ECTS = Project report)

• **ChE-609(4) Data in Chemistry and Electronic Lab Notebooks**

In this module we show how electronic lab notebooks can be used to organize data of open science publication and make them accessible for machine learning.

(1 ECTS = Project report)

Most of the block are in the form of a flipped class room in which the theory lectures are recorded and there will be a Zoom session for discussion.

Keywords

machine learning, molecular simulation, electronic laboratory notebooks

Learning Prerequisites

Required courses

Learning Prerequisites:

basic thermodynamics and some basic knowledge on computational methods (e.g., Matlab or programming)

Learning Outcomes

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

- Apply and to understand some of the computational methods discussed in the course.

Resources

Bibliography

To be provided