ChE-609(3)

Computational method in Chemistry and Chemical Engineering-Machine Learning

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Obl.

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

Frequency

Every year

Remark

Starting May 18-22 2020 This course as two other 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

ChE-609(3) = course unit entitled "Machine Learning"
we learn how to use machine learning to predict the gas adsorption in porous materials.

ChE-609(3) 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.

Exam : Project report on "Machine Learning"

Prior knowledge:
The introduction course ChE-609(1) "Computational methods in Chemistry and Chemical Engineering – Computational Carpentry" and online materials.
In this module, 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.

Keywords

machine learning

Learning Prerequisites

Required courses

ChE-609(1) entitled Computational methods in Chemistry and Chemical Engineering - Computational Carpentry and online materials

+ have 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 to understand and apply some of the computational methods discussed in the course