CH-315

Modeling lab

Smit Berend

Cursus	Sem.	Type
Chemical Engineering	BA5	Obl.
Chemistry	BA5	Obl.

Language of teaching	English
Credits	3
Withdrawal	Unauthorized
Session	Winter
Semester	Fall
Exam	During the semester
Workload	90h
Weeks	14
Hours	**4 weekly**
Project	4 weekly
Number of positions	

It is not allowed to withdraw from this subject after the registration deadline.

Summary

In this course we give a hands-on introduction on the use of modeling and data in chemistry. After an introduction in the different tools used by computational chemists, we discuss three topics in more detail molecular simulation of adsorption, data in chemistry, and machine learning.

Content

Introduction

In this course we give a hands-on introduction on the use of modeling and data in chemistry. After an introduction in the different tools used by computational chemists, we discuss three topics in more detail. We start with the course with an example of molecular simulation, which we use to predict the adsorption isotherms of materials that are used for carbon capture. Next, we are addressing the question on how to store chemical data electronically. The main idea here is how to create an open science infrastructure for chemistry. With an open science infrastructure, we will have access to large amounts of data, which can be processed using Machine Learning, which will be our last topic.

Content

The course has an introduction and three separate modules:

1. Computational Carpentry: In this part, we introduce the computational environment. We show you how to install the required packages on your computer and you will learn some very basic Python and Bash
2. Molecular Simulation of Adsorption: In this module we show how one can predict an adsorption isotherm from the crystal structure of a material.
3. Data in Chemistry: In this module we discuss data in chemistry. Open science is becoming the norm for scientific research. This implies that we have to think about how to make data publicly available. In this module, we show how to store chemical data and how to make data available in electronic format using standard protocols and formats through the systematic use of electronic laboratory notebooks.
4. Machine Learning in Chemistry: In this module we discuss the use of Machine Learning (ML) in Chemistry. ML is a technique to discover correlations in very large data sets. We show how ML can be used to analyze the data from the adsorption simulation.

Keywords

Molecular simulation, Machine Learning, Electronic Laboratory Notebooks, data

Learning Prerequisites

Required courses

The course assumes elementary knowledge of:

- computer programming in Phython (see Information, Computation, Communication CS-119(k))
- Thermodynamics of adsorption (see Physical chemistry of interfaces CH-341)

Learning Outcomes

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

- Formulate whether or not machine learning will be useful approach for a particular problem
- Carry out a simple machine learning study
- Formulate how to compute thermodynamic and transport properties from molecular simulation
- Carry out a molecular simulation based screening study
- Formulate how to best store data
- Carry out storage of chemical data in well-defined formats

Transversal skills

- Use both general and domain specific IT resources and tools
- Collect data.
- Write a scientific or technical report.
- Use a work methodology appropriate to the task.

Teaching methods

The course will be carried out completely online. All modules are taught in *flipped classroom* format. Details can be found on the Moodle page. There will also be a Slack channel dedicated for the course where the TAs are available for support. Each module consists of three parts:

1. Preparation: We have recorded all the theory in the form of a sequence of 10-20 min YouTube videos. Each video is followed by a quiz and you can only go to the next video if you have answered 80% of the questions correctly. We expect that these videos and quizzes will be completed before the module starts.
2. Instructions: (day 1) this will be hands-on exercises there will be joined Zoom sessions in which the material will be discussed. Students are expected to submit results before each of these Zoom sessions.
3. Project: (day 2) the methodology of the theme will be used in the form of a project. This project will be done in collaboration and a report is expected.

Expected student activities

The students are expected:

- to watch the videos and carry out the test **before** the modules start
- for each joined Zoom session prepare at least one question
- submit (partial) results during the instruction sessions
- to collaborate on the projects and write a report

Assessment methods

The mark will be: 50% Zoom participation (submission of intermediate results during the Zoom sessions) and 50% reports of the projects.

Supervision

Office hours	No
Assistant.e.s	Yes
Forum	Yes

Resources

Moodle Link

- https://go.epfl.ch/CH-315