CHEM-E4225 Computational Chemistry II 2023

This course will cover computational chemistry methods, including post-Hartree-Fock methods, DFT, time dependent DFT and constrained DFT. We will investigate the solvation methods and modelling of solid-liquid interphase. Also the modelling of chemical reaction and electrochemical systems are discussed. Most of the quantum chemistry computations will be done with Orca software and the ML with python codes.

The last part will focus on Machine Learning. There we investigate both supervised learning and clustering methods.

There will be no exam but the course is completed by doing assignments and writing reports on them. I will also give points of the exercises. You will **25 % form exercises and 75 % from the assignments**.

There is not a clear text-book for the course but a lot of the material can be found form

C.J. Cramer: Essentials of Computational Chemistry (2 ed) Wiley

Lectures 24 h
Exercises 12 h
Assignments 30 h
Other independent studying 54 h