CHM1453 Density Functional Theory (Fall 2022)

Time: Wednesdays, 12 pm - 2 pm

Location: in-person at rm.1084, Sidney Smith Hall, 100 St. George, + Zoom also provided

Instructor: Prof. Alex Voznyy o.voznyy@utoronto.ca

Course Summary

The goal of this course is to introduce the basics of computational quantum chemistry, specifically the density functional theory (DFT), and high-performance computing to students with primarily experimental background. It aims to provide students with the necessary computational knowledge and hands-on experience in running DFT calculations to complement their ongoing lab-based research projects. The course will cover organic molecules and periodic inorganic systems, calculations for geometry relaxation, formation energies, and electronic structure, and will cover the tools to run and analyze the results. It will discuss the main numerical methods used, as well as the capabilities and limitations of DFT.

Topics

- UNIX command line and access to computational cluster
- Software: VASP, CP2K, SIESTA, Gaussian, Discovery Studio
- Visualizing the structures and wavefunctions
- Basics of FORTRAN and Python for post-processing the results
- High-throughput materials screening
- Quantum mechanics recap (Schroedinger equation in matrix form, variational method)
- What is DFT
- Exchange-correlation functionals
- Pseudopotentials
- Plane-wave vs. orbital basis sets
- Reciprocal space (k-space) and Bloch theorem
- Energy levels, projected density of states, wavefunctions
- Reaction thermodynamics, formation energies
- Kinetic barriers, nudged elastic band method
- Molecular dynamics
- Phonons and vibrations
- Optical properties
- Numerical methods for matrix diagonalization, energy optimization

Grading

- Presentation on one of the DFT concepts/methods – 25%
- Computational results for your own research project – 50%
- Presentation or report on your own DFT project – 25%