CHM1441HF Mathematical Methods (Fall 2019)

Hands-on Density Functional Theory for your research

Time: Mondays or Wednesdays TBD, 10 am -12 pm

Location: St.George or UTSC, depending on the number of students; alternating every week is possible; Skype/Zoom will be provided

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

Slack channel will be provided

Office: UTSC EV564

Course Summary

The goal of this course is to teach you the basics of density functional theory (DFT) and high-performance computing, and find the way to apply it to your ongoing research project. The course will cover molecules, periodic systems and other topics as needed based on your project needs, and will provide you with the tools to calculate and analyze the results, and will discuss capabilities and limitation 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
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- 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

Text: wiki-style manual will be provided https://dft-uoft.slite.com

(Register here

https://slite.com/organization/join-link/dft-uoft/6ct5NzFGreNtPPApdDuLnf/default)

Grading

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