

### CHM1453 Density Functional Theory (Fall 2024)

**Time:** Wednesdays, 11 am - 1 pm

**Location:** in-person at FE328, 371 Bloor Street, + Zoom also provided

**Instructor:** Prof. Alex Voznyy [o.voznyy@utoronto.ca](mailto: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%

### ***COURSE POLICIES***

Each member of this course is expected to maintain a:

- (i) professional and respectful attitude during all course activities, including classes, laboratories, tutorials, and other online activities.
- (ii) personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
- (iii) collection of notes recorded independently based on concepts covered in course activities (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation)
- (iv) familiarity with the university policy on Academic Integrity

The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. The CHM1453 Teaching team will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and we wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment, and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our [Equity Offices](#).

### **INSTITUTIONAL POLICIES AND SUPPORT**

#### ***ACADEMIC INTEGRITY***

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously.

The [University of Toronto's Code of Behaviour on Academic Matters](#) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see [www.academicintegrity.utoronto.ca/](http://www.academicintegrity.utoronto.ca/)).

#### **COPYRIGHT**

If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited. More information regarding this is available here: <https://teaching.utoronto.ca/ed-tech/audio-video/copyright-considerations/>

### ***ACCESSIBILITY NEEDS***

Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact [Accessibility Services](#) as soon as possible.

### ***ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES***

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor before the session/assignment date to arrange accommodations.

### ***ADDITIONAL SERVICES & SUPPORT***

The following are some important links to help you with academic and/or technical service and support:

- School of Graduate Studies' [Policies and Guidelines](#)
- Full library service and resources on conducting online research through University of Toronto Libraries [University Libraries Research](#)
- Resources on academic support from the [Academic Success Centre](#)
- Learner support at the [Writing Centre](#)
- Information for [Technical Support/Quercus Support](#)

### ***ACKNOWLEDGEMENT OF TRADITIONAL LANDS***

We wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.