The University *of* Western Ontario
Department of Chemistry

Chemistry 9575

Density-Functional Computations

Fall 2025

Course Information

(TENTATIVE)

Instructor: Prof. Viktor N. Staroverov
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Lectures and Tutorials: Tuesday, 10:00 am – 11:15 am, CHB 115
Wednesday, 3:00 pm – 4:15 pm, CHB 115

First class: Tuesday, October 28
Last class: Wednesday, December 3

Course web site: `https://westernu.brightspace.com`

Prerequisite(s): Open to all registered graduate students. For undergraduate students, a minimum mark of 80% in Chemistry 2284B or similar course is required.

Course Description

This course provides a practical introduction to the use of computational density-functional theory (DFT) methods in chemical research. Emphasis is on developing a clear understanding of key concepts and best practices, including the selection of appropriate functionals, basis sets, integration grids, solvation models, and other computational parameters. Students will acquire hands-on experience with DFT by performing and analyzing density-functional calculations of molecular orbitals, molecular structures, chemical reactivity, thermochemistry, vibrational and electronic spectra, and materials.

Course Objectives

1. Explain the principles of density-functional theory (DFT) and the role of exchange-correlation functionals.
2. Know how to select appropriate density-functionals approximations, basis sets, and computational settings.
3. Perform and interpret DFT calculations of molecular orbitals, molecular structures, reaction energies, optical and vibrational spectra, and other properties using software packages, e.g., *Gaussian*.
4. Evaluate the limitations and accuracy of DFT methods in different chemical contexts.
5. Carry out a computational project using DFT tools.
6. Communicate research findings effectively in the form of written reports and oral presentations.

Course Topics

1. Overview of electronic structure methods. Theoretical foundations of DFT.
2. Types of density-functional approximations (LDA, GGA, meta-GGA, hybrid, double hybrid functionals). How to choose an appropriate functional.
3. Basis sets. Pseudopotentials and effective core potentials.
4. Computational setup. Integration grids, convergence criteria. Reproducibility.
5. Software and tools. Common DFT packages. *Gaussian* input file preparation, job submission, and output interpretation. Visualization tools for molecular orbitals, electron densities, etc.
6. Applications to molecular systems. Geometry optimization and energy calculations, thermochemistry and reaction mechanisms, vibrational analysis and IR spectra, transition state searches and reaction pathways, implicit solvation models.
7. Time-dependent DFT (TDDFT) for excited states.
8. Dispersion and noncovalent interactions. Limitations of standard DFT for weak interactions, empirical dispersion corrections.
9. Frontiers, challenges, and current trends in DFT. Benchmarking DFT methods.
10. Best practices. Data management, writing computational reports.

Course Materials

1. D. S. Sholl and J. A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley & Sons, Inc., Hoboken, New Jersey), 2009. Available online at Western Libraries.
2. W. Koch, M. C. Holthausen, *A Chemist's Guide to Density Functional Theory*, 2nd edition (Wiley-VCH Verlag GmbH, Weinheim), 2001. Available on the internet and at Western Libraries.

Methods of Evaluation

Assignments (3 in total)	60 %
Computational project	40%

Use of electronic devices. Any electronic devices are allowed.

Use of generative artificial intelligence. Use of generative artificial intelligence (AI) tools is permitted, provided that the student explains how they were used (e.g., to polish the writing, to analyze data, to answer a question, etc.) Work prepared using AI tools without such disclosures will receive no credit.

Scholastic offences. Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following website: `https://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_offences.pdf`

Western Academic Policies require that all graduate course outlines contain the following statement: "Western is committed to reducing incidents of gender-based and sexual violence (GBSV) and providing compassionate support to anyone who is going through or has gone through these traumatic events. If you are experiencing or have experienced GBSV (either recently or in the past), you will find information about support services for survivors, including emergency contacts at the following website: `https://www.uwo.ca/health/student_support/survivor_support/get-help.html` To connect with a case manager or set up an appointment, please contact support@uwo.ca."