Chemistry
UNIVERSITY OF TORONTO

CHM 1449H: Machine Learning and Physics Based View on Chemical Compound Space (Chem Comp Space)

Room: UC244
Day/Time: Thursday 11 am - 1 pm
Course Syllabus: Winter 2024

I TEACHING TEAM

INSTRUCTOR
Name: Anatole von Lilienfeld
Email: anatole.vonlilienfeld@utoronto.ca
Office: Lash Miller Chemical Laboratories, CPTG, LM420F
Student hours: upon appointment

Prof. von Lilienfeld is the inaugural Clark Chair in Advanced materials at University of Toronto and at the Vector Institute. He is also a Canada CIFAR AI Chair at the Vector Institute. Previously he has held professorships at various European universities (Physics, University of Vienna (2020-2022); Physical Chemistry, University of Basel (2013-2020); Computational Chemistry, University of Brussels (2016)). He is also affiliated with the Machine Learning group at the Technical University of Berlin. Over the years he has been teaching undergraduate courses on `Introduction to physical chemistry', `Physical chemistry IV: Electronic structure', `Physical Chemistry I: Thermodynamics', `Quantum chemistry: Density Functional Theory', and `Theoretical Physics I: Classical Mechanics'. Research in his lab deals with first principles based studies of chemical compound space using quantum mechanics, statistical mechanics, and machine learning. Recordings of some of his research presentations and teaching playlists can be found at his youtube channel Prof von Lilienfeld - YouTube. Personal postings (mostly related to academic research and teaching activities) can be found at Anatole von Lilienfeld (@ProfvLilienfeld) / Twitter

II COURSE OVERVIEW

COURSE DESCRIPTION:
Chemical compound space, historically an elusive concept in the atomistic sciences, is gaining increasing attention as it becomes relevant for virtual design and discovery of novel chemicals and processes, as well as for a deepened physics based understanding of quantitative structure property relationships. This is an advanced course on this topic which deals with the underlying physics in terms of relevant quantum and statistical mechanics in combination with modern computer simulation and machine learning tools. This is a new course in the graduate curriculum of relevant departments such as Chemistry, Materials Science & Engineering, Physics, Chemical Engineering, and Computer Science.

The course is continuously updated and very research oriented (Master and PhD students attending should have interests in computational and theoretical chemistry/physics/materials). It has been developed by the instructor over the last decade and is biased towards his lab's research output but findings and insights contributed by others will also be mentioned.

STUDENT LEARNING OUTCOMES:
By the end of this course, students will have developed and strengthened a quantitative and physics based understanding of chemical compound space. They will also increase their technical programming and development skill sets for computationally dealing with machine learning and atomistic simulations.

PREREQUISITE COURSE(S):
This course assumes you have a basic understanding of elementary physics and physical chemistry. The language used is mathematical and involves multivariable calculus.
Prerequisites include undergraduate knowledge in terms of:
-statistical mechanics
-computer programming
-quantum mechanics
-applied mathematics (linear algebra, differential equations, optimization)
-atomistic simulation

READINGS:
Recommended: Popular undergraduate and graduate textbooks on quantum chemistry, statistical mechanics, applied mathematics (e.g. numerical recipes, https://numerical.recipes/), and machine learning.

Further reading could include:

- Chapter 'Towards the Computational Design of Compounds from First Principles', O. Anatole von Lilienfeld, in book 'Many-Electron Approaches in Physics, Chemistry and Mathematics A Multidisciplinary View', Book, Editors: Volker Bach, Luigi Delle Site; First book bridging disciplines for the many-electron problem Written by researchers at the cutting edge in their respective fields. Great care is taken to make each chapter accessible for people with different backgrounds (computer science, chemistry, mathematics, physics). Published in Mathematical Physics Studies (2014), Springer.
- Book `Machine learning meets quantum physics', edited by Kristof T Schütt, Stefan Chmiela, O Anatole Von Lilienfeld, Alexandre Tkatchenko, Koji Tsuda, Klaus-Robert Müller. Published in Lecture Notes in Physics (2020), Springer.
- Ab initio machine learning in chemical compound space, B Huang, OA Von Lilienfeld, Chemical reviews 121 (16), 10001-10036 (2021)
- Retrospective on a decade of machine learning for chemical discovery, OA von Lilienfeld, K Burke, Nature communications 11 (1), 4895 (2020)
- Exploring chemical compound space with quantum-based machine learning, OA von Lilienfeld, KR Müller, A Tkatchenko, Nature Reviews Chemistry 4 (7), 347-358 (2020)

- Quantum machine learning in chemical compound space, OA Von Lilienfeld, Angewandte Chemie International Edition 57 (16), 4164-4169 (2018)
- Machine learning, quantum chemistry, and chemical space, R Ramakrishnan, OA von Lilienfeld, Reviews in computational chemistry 30, 225-256 (2017)
- First principles view on chemical compound space: Gaining rigorous atomistic control of molecular properties, OA Von Lilienfeld, International Journal of Quantum Chemistry 113 (12), 1676-1689 (2013)

III COURSE ORGANIZATION

This course consists predominantly of classes. Students are expected to attend all classes, and work through their homework.

The outline of the course consists of the following five chapters:

1) Introduction to chemical compound space
2) First principles view on chemical compound space
3) Machine learning in chemical compound space
4) Optimization in chemical compound space
5) Examples

IV EVALUATION/GRADING SCHEME

OVERVIEW:
Marked Problem sets (x5): 100%

ASSESSMENT DATES & MARK BREAKDOWN:
Five homework problems (each up to 20%): To be uploaded via Quercus **before** the subsequent lecture begins.

Students who are absent from class for any reason (e.g., COVID-19 illness, other illness or injury, family situation) and who require consideration for missed academic work should report their absence through the online absence declaration. The declaration is available on ACORN under the “Profile and Settings” menu. A student who misses any form of evaluation must additionally contact both, instructor and tutor, via email with a screenshot of their ACORN absence declaration WITHIN ONE WEEK to discuss their situation. This is a requirement to receive consideration for the missed evaluation. For students missing the homework for valid reasons, the corresponding grade will be interpolated as the average of the other homework grades.

IMPORTANT: if an unexpected technical issue occurs with a university system (e.g., Quercus services, network outage) that affects availability or functionality, it may be necessary to revise the timing or weighting of the marked problem sets.

V COURSE POLICIES

- Students are strongly encouraged to take notes using pen and paper. The use of any mobile devices such as laptops, tablets, calculators, or cell-phones is strictly prohibited during class.
- Each member of this course is expected to maintain a:

(i) professional and respectful attitude during all course activities, including classes, laboratories, tutorials and online activity.

(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 (overleaf)

- 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 Course Instructor will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and 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.
- Communication with instructor: Preferably during class or office-hours. If in person communication is impossible for whatever reason one can send an email. The email will be answered within 48 hrs. on weekdays. The subject line must begin with ''CHM328:" …
- Privacy language and appropriate use of course materials: For additional information, see the syllabus "Copyright" section.
- Policy for late submissions: Solutions to homework that are handed in too late (i.e. after the corresponding tutorial explaining the solutions started) will be graded as a fail.

VI TECHNOLOGY REQUIREMENTS

- Students are strongly encouraged to make use of computers and literature when working on problem sets and when revisiting their notes taken. Consequently, technical issues are possible. When working on a piece of academic work, students are responsible for scheduling enough time to allow for reasonable delays due to technical difficulties to be overcome, so such issues will not be acceptable grounds for deadline extension. Particularly, maintaining an up-to-date independent backup copy of your work is strongly

recommended to guard against hard-drive failures, corrupted files, lost computers, etc.

- Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here: https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/
- Advice for students more broadly regarding online learning is available here: https://onlinelearning.utoronto.ca/getting-ready-for-online/

VII INSTITUTIONAL POLICIES & 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 (governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

On term tests:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com) to post term test questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**
2. Looking and copying someone else's answers or collaborating/discussing answers for homework problems.
3. Misrepresenting your identity.

In general academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

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/).

COPYRIGHT
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The unauthorised use of any form of device to audiotape, photograph, video-record or otherwise reproduce lectures, course notes or teaching materials provided by instructors is covered by the Canadian Copyright Act and is prohibited. Students must obtain prior written consent to such recording. In the case of private use by students with disabilities, the instructor's consent must not be unreasonably withheld.

Students may not create audio or video recordings of classes with the exception of those students requiring accommodation for a disability, who should speak to the instructor prior to beginning to record lectures. Students creating unauthorized audio recording of lectures violate an instructor's intellectual property rights and the Canadian Copyright Act. Students violating this agreement will be subject to disciplinary actions under the Code of Student Conduct.

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.

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:

- General student services and resources at Student Life
- Full library service through University of Toronto Libraries

- Resources on conducting online research through University Libraries Research
- Resources on academic support from the Academic Success Centre
- Learner support at the Writing Centre
- Information for 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.