SPECIAL TOPICS IN CHEMISTRY II:
MACHINE LEARNING FOR CHEMICAL APPLICATIONS
(CHEMISTRY 420)
Fall 2021

Instructor: Dr. Konstantinos (Kostas) Vogiatzis
Office: Bu 319
Office Hours: Monday 10:10 – 11:00 am
Wednesday 3:00 – 4:00 pm
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Lectures:

Monday	9:15 – 10:05 am,	TBD
Wednesday	9:15 – 10:05 am,	TBD
Friday	9:15 – 10:05 am,	TBD

Course Description: Artificial intelligence (AI) rapidly changes many aspects of chemical sciences, from drug discovery, material design, and the discovery of new reactions and molecules till the acceleration of computer sciences and robotics for chemical applications. This course will cover the key aspects of AI and modern chemoinformatics and how they are applied on chemical sciences.

Textbook: *Chemoinformatics: Basic Concepts and Methods* Edited by Engel and Gasteiger, (Wiley-VCH Verlag GmbH & Co., 2018).

Additional Resources:
A. *Practical Chemoinformatics* by Karthikeyan, Vyas, (Springer, 2014)
B. *An Introduction to Chemoinformatics* by Leach, Gillet (Springer, 2007)
C. *Machine Learning in Chemistry* by Janet, Kulik (ACS in Focus, 2020)

Grading:

Computational Exercises:	40%
Final Project + Presentation:	60% (30% + 30%)
Attendance	Bonus

Computational Exercises: Computational exercises will complement the learning objectives of the course and will provide a deeper understanding of machine learning applications in chemistry. Notes on introduction to Python, Jupyter notebooks, and machine learning and chemoinformatics packages will be provided. Every computational task will include a step-by-step guide that will help you complete the assignment.

Final Project: Each student should complete a final project that utilizes the knowledge that is covered during the semester and includes a topic of their interest. The topic of the project will be chosen by the student with the help of the instructor. A list of tentative projects will be provided to all students. A written document should be submitted before the end of the semester that contains the following:

1. Scope of the project
2. Literature background
3. Computational assessment
4. Results
5. Conclusions

Final Presentation: At the end of the semester, each student should prepare a 10-minute presentation where they will present the final project to the class. Each presentation will be evaluated based on the following rubric:

	Excellent 8-10	**Good 5-7**	**Needs Improvement 0-4**
Understanding of the topic	Ideas are clearly explained and follow-up comments indicate a thorough understanding of the topic.	Ideas are clearly explained for the most part. Few challenges exist in the explanations, but the presenter shows that understands the main ideas of the topic well.	There is confusion on the topic and its concepts. The presenter lacks understanding of the ideas and this is evident on lack of explanations or limited explanations or inaccurate explanations and clarifications.
Quality of the presentation	The presentation materials are professional, well designed, readable, and support the observer's and reader's understanding.	Most of the materials are clear and well designed. Occasional errors do not interfere with understanding. The overall presentation for the most part is professionally designed.	The materials are poorly developed or there are errors that affect understanding. The presentation resources are challenging to read and the presentation is not professionally designed.
Results	A well-justified computational procedure was followed, and the results are clearly presented.	The computational procedure is not fully justified, it contains a few logical errors, and the results are not clear to the audience.	The computational procedure has significant flaws, it contains logical errors, and the results are not presented in a very clear manner.
References	All resources when used are cited and the citation is according to ACS guidelines.	Some of the resources are cited and the citation follows ACS with some errors.	There is no reference or the reference includes several errors.
Connection with the course content	The presentation connects with the course and expands the presenter's and observers' understanding of the content.	There is some connection with the course content.	There is no connection with the course content.
Answers to questions	The presenter clearly and accurately articulates responses to questions.	Most of the responses are clear and accurate without avoiding to answer what is asked.	The presenter avoids to answer questions or does not answer them when asked.
Time	The presentation is within the provided time frame.	The presentation exceeds the allotted time by 5 minutes.	The presentation exceeds the allotted time more than 10 minutes.
Total			

Learning Objectives: The planned coverage for *CHEM420: Special Topics in Chemistry – Machine Learning for Chemical Applications* includes the topics listed below.

Topic	Description
1. Intro to Python:	Learn how to use Jupyter notebook, download basic packages, simple Python commands
2. Basic Concepts:	Molecular representations, computer processing of chemical structure information, representation of chemical reactions
3. Chemical Databases:	Databases and data resources in chemistry, chemical structure search
4. Data Collection:	Molecular mechanics, molecular dynamics, empirical methods, ab initio methods, density functional theory
5. Inductive Learning Methods:	Modeling and prediction of properties (QSPR/QSAR), descriptors, multivariate analysis, neural networks,
6. Bioinformatics:	Sequence databases, protein families
7. Quantum Machine Learning:	Machine learning potentials for atomistic simulations, machine learning for *ab initio* and density function theory methods

Grading Scale:

80 and above: **A-** and **A**
60-80: **B-**, **B**, **B+**
45-60: **C-**, **C**, **C+**
30-45: **D-**, **D**, **D+**
Below 30: **F**

***Note**: These letter grade assignments are subject to change, but only in the direction beneficial to the students.*

Academic Dishonesty: An act of academic dishonesty may lead to such penalties as reduction of grade, probation, suspension, or expulsion from the University.

Honor Statement: *An essential feature of The University of Tennessee is a commitment to maintaining an atmosphere of intellectual integrity and academic honesty. As a student of the University, I pledge that I will neither knowingly give nor receive any inappropriate assistance in academic work, thus affirming my own personal commitment to honor and integrity.*

Disability Services: Any student who feels he or she may need an accommodation based on the impact of a disability should contact the Office of Disability Services (ODS) at 865-974-6087 in 2227 Dunford Hall to document their eligibility for services. ODS will work with students and faculty to coordinate reasonable accommodations for students with documented disabilities.

Other General Policies:	Please include your full name and section number in all of the emails you send. You should always include a subject which starts with CHEM420. Always bring your student ID to all lectures, discussions, lab meetings, and exams. Keep your cell phone off during lectures, discussions, lab meetings, and exams.

ADDITIONAL NOTES:

1. The instructor reserves the right to revise, alter or amend this syllabus as necessary. Students will be notified in writing / email of any such changes.
2. Also, in case that the University stays closed due to inclement weather, please access the course online as we may complete the class online. An announcement will be sent to assure that participants are aware.
3. **The instructor of this class owns the copyright to the syllabus, handouts, assignments, quizzes, and exams associated with the class.** All presentations developed by the instructor, as well as the instructor's lectures, are also protected by copyright, whether these presentations are delivered live in-class, shared through *Zoom* or other videoconference platforms, or uploaded to *Canvas* or similar sites.
4. Sharing any of this material without the written permission of the instructor is a violation of copyright law, and is therefore also a violation of the University's policy on acceptable use of information technology resources (UT policy number IT0110). That policy states that students will not commit copyright infringement, "including file sharing of video, audio, or data without permission from the copyright owner" and that file sharing is a violation of the university's student code of conduct. I will report all such violations to the Office of Student Conduct and Community Standards.