

AI in Chemistry – CHM 4930 Syllabus

CHM 4930, **Spring 2024**, Tues:1:55 – 2:45 pm (T7); Thurs 7-8: 1:55-3:50 pm (R7-8)

Room: Lectures scheduled for synchronous delivery on Canvas

Instructor: Mingjie Liu, mliu@chem.ufl.edu, Office: LEI 240C;

Course Description.

Course Coverage.

- Course Goals.**
- Handle and visualize different types of datasets common in Chemistry.
 - Process data for use in machine learning approaches.
 - Identify the suitability of different ML approaches to answer chemical questions based on data.
 - Use standard ML python pipelines to train models.
 - Assess the quality of the models and their predictive power.
 - Recognize different applications of ML in Chemistry.
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Tentative Schedule of Classes:

Data handling

Introduction to the course. Python notebooks.
Type of data in Chemistry and Biochemistry
Chemical data and chemical descriptors
Molecular similarity
RDKit python library for chemical data
Databases of materials and chemical data
Processing data: analysis and visualization of data

Classical machine learning

Scikit-learn, machine learning in Python
Dimensionality reduction: embedding space
Classification: supervised and unsupervised methods
Unsupervised learning: clustering methods
Unsupervised learning: kernel methods and support vector machines (SVM)
Supervised learning: inference models, model training and evaluation
Linear and non-linear classification models
Decision trees and random forest approaches (RF)
Probabilistic methods

Neural Networks and beyond

Neural networks and deep learning
Processing sequential data: recurrent neural networks (RNN)
Processing graph data: graph neural networks (GNN)
Machine learning Interatomic potential (ANN)

Required Textbooks:

No required textbooks.

Recommended Textbooks:

TBD

Canvas Website. All students will have access to the Canvas website: <https://ufl.instructure.com/>

You will login with your Gatorlink account username and password. This is where you will find general class information, important news, office hours, handouts, class notes, and keys. This is also where you will be able to find out your point totals and histograms.

Class Requirements:

- 1) Three homework (10 points each = 30 points)
 - 2) In-class Lab (30 points)
 - 2) Final project (15 points)
 - 3) Project presentation (15 points)
 - 4) Attendance and in-class participants (10 points)
- = 100 points total**

Homework (In-Class Lab). Homework (In-Class Lab report) due date is posted on the class calendar. Late homework (if it is turned in on the same day, but after the deadline) will have a 20% deduction on the grade. The day after, the solutions will be posted, and no more homework will be accepted for grading.

Final Projects. Students will use the techniques they have acquired to simulate their systems of interest and prepare a report.

Presentation. The final projects results will be presented at the end of the semester with 15min + 5min Q&A.

Grading. Grades will be curved based on points earned out of 100.

85-100 A
75-85 B+
65-75 B
60-65 B-
< 60 C

Assignment Regrading. If you have a question concerning the grading of an assignment, you may submit the entire assignment for complete regrading. The assignment must be submitted for regrading by the next class meeting after the date the assignment was returned to the class.

Office Hours. Wednesday 1-3 pm, LEI 240C by email appointment.

TA: Jirui Jin

TA Office Hours.

Accommodations for students with disabilities. Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the instructor when requesting accommodation.

Course Evaluations. “Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.”

UF Honor Code: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

On all work submitted for credit by students at the university, the following pledge is either required or implied: **“On my honor, I have neither given nor received unauthorized aid in doing this assignment.”** “The university requires all members of its community to be honest in all endeavors. A fundamental principle is that the whole process of learning and pursuit of knowledge is diminished by cheating, plagiarism and other acts of academic dishonesty. In addition, every dishonest act in the academic environment affects other students adversely, from the skewing of the grading curve to giving unfair advantage for honors or for professional or graduate school admission. Therefore, the university will take severe action against dishonest students. Similarly, measures will be taken against faculty, staff and administrators who practice dishonest or demeaning behavior.”

Cheating and Plagiarism. Cheating and/or plagiarism will not be tolerated. The minimum penalty will be an automatic zero on the assignment in question. Suspension from the University may also result. Do not risk it. It is not worth it. Plagiarism consists of passing off as one’s own the ideas, words, writings, etc. that belong to someone else. You are committing plagiarism if you copy the work of another person and turn it in as your own, even if you have that person’s permission. See: <https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>

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Counseling. The University of Florida provides counseling services for students, staff, and faculty.

U Matter, We Care: If you or someone you know is in distress, please contact umatter@ufl.edu, 352-392-1575, or visit U Matter, We Care website to refer or report a concern and a team member will reach out to the student in distress.

Counseling and Wellness Center: Visit the Counseling and Wellness Center website or call 352-392-1575 for information on crisis services as well as non-crisis services.

Student Health Care Center: Call 352-392-1161 for 24/7 information to help you find the care you need, or visit the Student Health Care Center website.

University Police Department: Visit UF Police Department website or call 352- 392-1111 (or 9-1-1 for emergencies).

UF Health Shands Emergency Room / Trauma Center: For immediate medical care call 352- 733-0111 or go to the emergency room at 1515 SW Archer Road, Gainesville, FL 32608;