

Course Syllabus
CHEM 4630/5630: Programming for data analysis in the physical sciences

Chemistry Department, College of Liberal Arts and Sciences, University of Colorado Denver

Instructors: Emilie Guidez	Term: Spring 2025
Office: Science Building 4128B	Class meeting days: Friday
Phone: 303-315-7691	Class meeting times: 10am-10:50am
Email: emilie.guidez@ucdenver.edu	Class location: NORTH 3004
Office hours: MW 10:00am-11:00am	

1. Welcome!

Welcome to programming for data analysis in the physical sciences. In this course, you will learn to write python scripts to process and interpret data. Writing code to process and analyze data has become a valuable skill in all STEM fields. This course will provide some basic foundations and hopefully encourage you to keep learning on your own.

2. Course overview

This course will be taught using live coding format (the instructor will code live in the classroom with the students). In this course, you will learn to process data using python scripts that you will write. Data include for example absorption spectra, coordinate files... You will also learn how to use Python libraries and write functions (for example to create high resolution graphs). Finally, you will learn best coding practices, how to keep track of different versions of your code and share your code using Github.

3. Learning objectives.

By the end of this course you will be able to:

- a) Use basic Python commands
- b) Extract and analyze data from molecular modeling simulation files or spreadsheets
- c) Plot and analyze spectroscopic data.
- d) Keep track of different versions of your code and share your code on Github

4. Course pre-requisites and co-requisites.

Pre-requisites: General chemistry I (CHEM 2031), General Chemistry II (CHEM 2061)

Recommended: Organic chemistry I (CHEM 3411)

5. Course credits

1 credit hour

6. Required text and materials.

Required text: None

Required additional materials and skills:

- This course requires the use of computer (mac or PC). If you do not own a laptop, you can use one from the chemistry department.

7. Course schedule

The course schedule is shown below. Week assignments are tentative and may be adjusted depending on the pace of the class.

Week	Topics
1	Basic tools for data analysis
2	Basic tools for data analysis
3	Basic tools for data analysis
4	Extracting and processing molecular properties from molecular modeling simulations
5	Extracting and processing molecular properties from molecular modeling simulations
6	Extracting and processing molecular properties from molecular modeling simulations
7	Extracting and processing molecular properties from molecular modeling simulations
8	Processing and analyzing spectroscopic data
9	Processing and analyzing spectroscopic data
10	Processing and analyzing spectroscopic data
11	Processing and analyzing spectroscopic data
12	Code sharing and version control
13	Code sharing and version control
14	Code sharing and version control
15	Fall break
16	Code sharing and version control
17	Finals week

8. Graded Assignment

Final exam

The final exam will be a final project due the Friday before finals week (May 6th).

Undergraduate students will be expected to turn in a script that will process experimental/computational data and produce a specific output (graph and/or table). The code must be appropriately commented.

Graduate students will be given a similar assignment but they will be expected to share their code on Github and write an appropriate documentation.

Homework assignments

Three homework assignments will be given in this course. Each assignment will be worth 20 points. For each homework assignment, each student will turn in a python script that can be executed to perform a specific task. All homework assignments are due at the end of the semester, the Friday before finals week (May 6th). You may resubmit homework assignments as many times as you like for a regrade.

9. Basis for final grade.

Assessment	Points per occurrence	Number of occurrences	Points possible
Homework	20	3	60
Final	100	1	100
Total			160

10. Grading scale.

The grading scale is based on percentage, which is shown below.

94-100	A
90-93	A-
87-89	B+
84-86	B
80-83	B-
77-79	C+
74-76	C
70-73	C-
67-69	D+
64-66	D
60-63	D-
0 - 59	F

The instructor may or may not curve the accumulated grades, depending on the overall performance of the class. The curving may or may not improve your grade, but it will not lower your grade.

11. Grade Dissemination

Your grades of the quizzes and exams can be found via the course's Canvas course shell. You can access your scores at any time within the Canvas Gradebook.

12. Course Procedures

Course Policies: Grades

In order to receive full credit for homework assignments and exam, you will need to turn in your script(s) online. The script(s) must produce the correct output and be appropriately commented.

Attendance Policy

Students are expected to attend classes and actively participate in the class discussions. UC Denver Student Attendance and Absences Policy can be found at http://www.ucdenver.edu/faculty_staff/employees/policies/Policies%20Library/OAA/StudentAttendance.pdf

Late Work Policy

No late assignments will be accepted. They will be given zero.

Extra Credit Policy

No other extra credit will be given.

Grades of "Incomplete"

The current university policy concerning incomplete grades will be followed in this course. Incomplete grades are given only in situations where unexpected emergencies prevent a student from completing the course and the remaining work can be completed the next semester. The instructor is the final authority on whether you qualify for an incomplete. Incomplete work must be finished by the end of the subsequent semester or the "I" will automatically be recorded as an "F" on your transcript.

Rewrite/Resubmit Policy

No rewrites or resubmission will be accepted.

13. Course Policies: Technology and Media

Email

One of the requirements for this course is that you maintain an email address, check it regularly for messages, be sure it is working, and notify the instructor in time if you change your email address. Official university communication is only sent via a student's university email address. Normally, you are responsible for any messages the instructor sends to you via email 24 hours prior. You may contact the instructor via email, in addition to phone calls and seeing the instructor during office hours. The instructor will answer emails as quick as possible (usually within 24 hours), but delays may be expected during weekends and breaks, when the instructor is traveling or on sick leave, and in other special situations (e.g. the university email server is down).

While email is a convenient tool, please do not abuse it. Please limit the contents to stuff related to this course and to academic purpose. **Please indicate explicitly your name, student ID, and the course title in the email**, which will help the instructor to quickly locate the necessary information when replying. The instructor may request you to meet in person if your questions are difficult to answer via email (e.g. your question requires extensive discussion). According to the University's interpretation of the Family Education Rights and Privacy Act (FERPA), your instructors are not allowed to discuss grades via email, as it is not considered a secure means of communication.

However, I am able to discuss your grades via email if you include the following disclaimer (or some similar statement) in your email to me:

"I understand that email is not a secure means of communication and give you permission to discuss my grade via email."

Canvas

This course will make use of the Canvas course management system. You should automatically be registered for access to the course site. You should check your Canvas account regularly. The syllabus for the course is listed there. Your grades will be posted to your personal page, so you will know your standing and can correct any clerical errors with ease. The instructor may also post notes and assignments on Canvas.

You can log into Canvas at <https://ucdenver.instructure.com/login>. If you have any problems with the online system, please contact the Help Desk immediately. The instructor does not have any authority in managing your account.

Laptop and Mobile Device Usage

Each student must bring a laptop to class.

Library-supplied online databases and collections

If you need to use the library for further information (e.g., dictionaries and references), please contact the library staff. The Auraria library website is at <http://library.ucdenver.edu/>.

Classroom Response Clickers

This course does not use student response devices such as clickers. However, you are expected to actively participate in the classroom discussion.

14. Course Policies: Student Expectations

Student grievances

Student complaints about this course or instructor should be communicated directly to the instructor in a face-to-face meeting (unless this course is an online course). If the issues cannot be resolved, you should meet with the chairperson of the Chemistry Department. Contact 303-315-7650 to arrange a meeting. If meeting with chairperson does not resolve the issues, you may appeal to the Associate Dean of Student Success in the Office of the CLAS Dean (NC 5014, 303-315-7000). The decision of the Associate Dean is final. You may also meet with the CU Denver Ombudsman to ask for assistance. For additional information, please see the CLAS policy “Procedures for Student Grievances about Courses or Faculty” available from the Office of the CLAS Dean.

Civility

Everyone must be treated with respect and courtesy both in class and after class. Everyone must commit to create a climate for learning characterized by respect for each other.

Professionalism

Disruptive behavior is not tolerated; this includes foul language, cell phone use in class, talking loudly on things irrelevant to the course during the lecture, etc. Anyone who disrupts the class will be asked to leave the classroom immediately.

Late Arrivals, Early Departures, Absence

Students are expected to attend class on time.

Auraria Library

The Auraria Library offers many services, research databases, and collections. A list of specific librarian contact and/or library subject expert web page can be found at <http://library.auraria.edu/services/researchhelp/specialists>.

Writing Center

The Writing Center website is

<http://www.ucdenver.edu/academics/colleges/CLAS/Centers/writing/Pages/TheWritingCenter.aspx>

Tutoring & Student Assistance

The Learning Resources Center offers free drop-in (“open lab”) tutoring as well as scheduled small-group tutoring. “Open lab” tutoring does not require an appointment; see the posted schedule for available times. Scheduled tutoring requires that you sign up with the LRC. Spaces are available on a first-come-first-served basis and often fill up early in the semester. For more information about the LRC, see their website at www.ucdenver.edu/lrc. Tutoring is not provided directly by the instructor or the course teaching / learning assistants.

15. University policies

Disability and Access:

The University of Colorado Denver is committed to ensuring the full participation of all students in its programs, including students with disabilities. If you have a disability or think you have a disability and need accommodations to succeed in this course, I encourage you to contact Disability Resources and Services (DRS) and/or speak with me as soon as you can. (DRS is located in Academic Building 1, Suite 2116, and at disabilityresources@ucdenver.edu.) I am committed to providing equal access as required by federal law, and I am interested in developing strategies for your success in this course.

Link to University policies on service animals

<http://equity.ucdenver.edu/wp-content/uploads/2017/02/Service-Animal-Policy-FINAL-DRAFT-2016-11-30.pdf>

Students Called for Military Duty

If you are a student in the military with the potential of being called to military service and /or training during the course of the semester, you are encouraged to contact your school/college Associate Dean or Advising Office immediately.

Other deadlines and procedures:

For relevant university deadlines and procedures (such as the last day to withdraw from a course) as well as academic support sites, please see this website https://clas.ucdenver.edu/faculty-staff/sites/default/files/attached-files/student_services_and_calendar.pdf. ”

16. Academic Dishonesty and CLAS Academic Ethics Policy

Students are expected to know, understand, and comply with the ethical standards of the University. A university's reputation is built on a standing tradition of excellence and scholastic integrity. As members of the University of Colorado Denver academic community, faculty and students accept the responsibility to maintain the highest standards of intellectual honesty and ethical conduct.

Academic dishonesty is defined as a student's use of unauthorized assistance with intent to deceive an instructor or other such person who may be assigned to evaluate the student's work in meeting course and degree requirements.

Examples of academic dishonesty include, but are not limited to, the following:

A. Plagiarism: Plagiarism is the use of another person's distinctive words or ideas without acknowledgment. Examples include:

1. Word-for-word copying of another person's ideas or words;
2. The mosaic (the interspersing of one's own words here and there while, in essence, copying another's work);
3. The paraphrase (the rewriting of another's work, yet still using their fundamental idea or theory);
4. Fabrication of references (inventing or counterfeiting sources);
5. Submission of another's work as one's own;
6. Neglecting quotation marks on material that is otherwise acknowledged

Acknowledgment is not necessary when the material used is common knowledge.

B. Cheating: Cheating involves the possession, communication, or use of information, materials, notes, study aids or other devices not authorized by the instructor in an academic exercise, or communication with another person during such an exercise. Examples include:

1. Copying from another's paper or receiving unauthorized assistance from another during an academic exercise or in the submission of academic material;
2. Using a calculator when its use has been disallowed;
3. Collaborating with another student or students during an academic exercise without the consent of the instructor

C. Fabrication and Falsification: Fabrication involves inventing or counterfeiting information, i.e., creating results not obtained in a study or laboratory experiment. Falsification, on the other hand, involves the deliberate alteration of results to suit one's needs in an experiment or other academic exercise.

D. Multiple Submissions: This is the submission of academic work for which academic credit has already been earned, when such submission is made without instructor authorization.

E. Misuse of Academic Materials: The misuse of academic materials includes, but is not limited to, the following:

1. Stealing or destroying library or reference materials or computer programs;
2. Stealing or destroying another student's notes or materials, or having such materials in one's possession without the owner's permission;
3. Receiving assistance in locating or using sources of information in an assignment when such assistance has been forbidden by the instructor;
4. Illegitimate possession, disposition, or use of examinations or answer keys to examinations;
5. Unauthorized alteration, forgery, or falsification;
6. Unauthorized sale or purchase of examinations, papers, or assignments

F. Complicity in Academic Dishonesty: Complicity involves knowingly contributing to another's acts of academic dishonesty. Examples include:

1. Knowingly aiding another in any act of academic dishonesty;
2. Allowing another to copy from one's paper for an assignment or exam;
3. Distributing test questions or information about the materials to be tested before the scheduled exercise;
4. Taking an exam or test for someone else;
5. Signing another's name on attendance roster or on an academic exercise

Students who fail to comply with the UC Denver CLAS Academic Ethics Policy are subject to disciplinary action as set forth by the College policy. For more information regarding the Academic Ethics Committee policies and procedures, please refer to

<https://clas.ucdenver.edu/faculty-staff/policies-procedures/handling-academic-dishonesty>

An act of Academic Dishonesty may lead to sanctions including a reduction in grade (up to and including a permanent F for the course).

17. CLAS and Chemistry Department Withdrawal Policy for Spring 2019

CLAS withdrawal policy

Deadlines and Procedures for Dropping Courses (Notes 1 and 2)	
through 7 th day	electronic or manual course drops, no faculty or administrative approvals required, tuition refunded, no course notation on student's transcript
8 th to 12 th day - Census day	electronic or manual course drops, no faculty or administrative approvals required, no course notation on student's transcript, and \$100 drop fee is assessed
After census through 10 th week	dropping for poor academic performance allowed, manual course drops using SAF only, faculty signature required on SAF. On-Line Courses Only – email from faculty (University email address) may substitute for faculty signature. Course notation on student's transcript with a W grade. No tuition adjustment.
11 th through 12 th week	faculty option to extend drop deadline for academic reasons, faculty signature is required on SAF, associate dean/designee's signature required, 12 th week deadline treated as an <i>absolute</i> deadline, SAF processed by 5:00 pm on deadline. On-Line Courses Only – email from faculty (University email address) may substitute for faculty signature
after 12 th week	dropping for poor academic performance is not allowed, student with verifiable special circumstances may complete the petition process on reverse side

1. Dates are for full-semester, 16-week courses. Exact dates for a particular semester or term are provided by the UC Denver Registrar, www.ucdenver.edu
Click on Current Students>Academic Resources>Academic Calendars links.
2. Drop deadlines for courses not starting at the beginning of the semester are established by the UC Denver Registrar.

Chemistry Department Policy for Withdrawals

- Students who wish to withdraw from a chemistry course beginning Monday of the 11th week through Friday of the 14th week of the semester will be allowed to do so. Students must follow the CLAS Late Withdrawal Policy which requires the signature of the instructor and a CLAS advisor or dean.
- Beginning Monday of the 11th week through Friday of the 14th week of the semester, students can drop a course that serves as a co-requisite for another course without having to drop both courses. That is, *the Chemistry Department will allow co-requisites to be broken after the 10th week of the semester is completed.* This applies to all co-requisite courses (listed below) in the chemistry department.

Chemistry Courses requiring a co-requisite course:

- Course CHEM 2038 has the co-req CHEM 2031 or CHEM 2081
- Course CHEM 2068 has the co-req CHEM 2061 or CHEM 2091
- Course CHEM 2088 has the co-req CHEM 2031 or CHEM 2081
- Course CHEM 2098 has the co-req CHEM 2061 or CHEM 2091
- Course CHEM 3011 has the pre-req/co-req CHEM 3421 or CHEM 3491
- Course CHEM 3018 has the pre-req/co-req CHEM 3011
- Course CHEM 3118 has the co-req CHEM 3111 or CHEM 3481
- Course CHEM 3418 has the co-req CHEM 3411 or CHEM 3481
- Course CHEM 3428 has the co-req CHEM 3421 or CHEM 3491
- Course CHEM 3481 has the co-req CHEM 3418 or CHEM 3488
- Course CHEM 3488 has the co-req CHEM 3411 or CHEM 3481
- Course CHEM 3498 has the co-req CHEM 3421 or CHEM 3491

- Course CHEM 4121 has the co-req CHEM 4128 for chem majors
- Course CHEM 4128 has the co-req CHEM 4121
- Course CHEM 4511 has the pre-req/co-req MATH 3511 or CHEM 4500 (effective Spring 2018)
- Course CHEM 4518 has the co-req CHEM 4511
- Course CHEM 4521 has the pre-req/co-req MATH 3511 or CHEM 4500 (effective Spring 2018)
- Course CHEM 4538 has the co-req CHEM 4521
- Course CHEM 4548 has the pre-req/co-req CHEM 4511 and CHEM 4521
- Course CHEM 4810 has the pre-req/co-req CHEM 3421 or CHEM 3491 (effective Spring 2018)
- Course CHEM 4815 has the co-req PHYS 2020 or PHYS 2331

**Questions? Ask Lynx Center – ucdenver.edu/lynxcenter
Student Commons 1st floor - 303-315-5969 - lynxcenter@ucdenver.edu**

STUDENT SUPPORT

CARE Team is there for you
Call 303-352-3579 if you
or a classmate needs extra help
Submit a concern at
www.ucdenver.edu/life/services/CARE

Call 911 in case of emergency
Auraria Campus Police: 303-556-5000

CAREER CENTER

ucdenver.edu/careercenter - Tivoli 267
303-315-7315 - careercenter@ucdenver.edu

COUNSELING CENTER

ucdenver.edu/counselingcenter - Tivoli 4th floor
303-315-7270

DISABILITY RESOURCES & SERVICES

ucdenver.edu/disabilityresources - Student Commons 2116
303-315-3510 - disabilityresources@ucdenver.edu

OFFICE OF EQUITY

equity.ucdenver.edu - Lawrence Street Center 12th floor
303-315-2567 – equity@ucdenver.edu

PHOENIX CENTER AT AURARIA

24/7 Free and Confidential Helpline: 303-556-2255
Info on interpersonal violence, referrals, options, & next steps
www.thepca.org - Tivoli 259 - 303-556-6011- info@thepca.org

FREE TUTORING

Contact these services for academic
assistance throughout the semester

LEARNING RESOURCES CENTER

ucdenver.edu/lrc - Student Commons 2105
303-315-3531 - tutorialservices@ucdenver.edu

MATH EDUCATION RESOURCE CENTER

MERC Lab North Classroom 4015
math.ucdenver.edu/~mkawai/MERC - 303-315-1712

WRITING CENTER

North Classroom 4014 | Campus Village | Auraria Library
writingcenter.ucdenver.edu

UNDERGRADUATE ACADEMIC ADVISING

ucdenver.edu/undergradadvising

*Graduate students: contact your graduate program
directly for advising information*

ACADEMIC SUCCESS ADVISING CENTER (ASAC)

Student Commons 1113
303-315-1940 - asac@ucdenver.edu

ARCHITECTURE AND PLANNING (CAP)

CU Building 2000
303-315-1000 - cap@ucdenver.edu

ARTS AND MEDIA (CAM)

Arts Building 177
303-315-7400 - camadvising@ucdenver.edu

BUSINESS SCHOOL

15th and Lawrence Street, 4th floor
303-315-8110 – undergrad.advising@ucdenver.edu

EDUCATION AND HUMAN DEVELOPMENT (SEHD)

Lawrence Street Center 701
303-315-6300 - education@ucdenver.edu

ENGINEERING AND APPLIED SCIENCES (CEAS)

North Classroom 2605
303-315-7510 - CEASstudentservices@ucdenver.edu

LIBERAL ARTS AND SCIENCES (CLAS)

North Classroom 1030
303-315-7100 – clas_advising@ucdenver.edu

SCHOOL OF PUBLIC AFFAIRS (SPA)

Lawrence Street Center 525
303-315-2228 - spa@ucdenver.edu

Plan Ahead! Review Important Dates & Deadlines at
ucdenver.edu/registrar >> CU Denver Registrar >> Academic Calendar