San José State University, Department of Chemistry
Chem 270, Introduction to Computational Chemistry, Spring 2022

Course and Contact Information

Instructor:	Gianmarc Grazioli, Ph.D. Preferred names: Dr. Grazioli or Dr. G
Email:	gianmarc.grazioli@sjsu.edu
Class Days/Time:	T/R, 6:00pm - 7:15pm
Office Hours **(a.k.a. student hours)**	Thursdays 4:10pm – 5:30pm Fridays 10:30am – 11:30am or by appointment
Classroom:	Online – Canvas: https://sjsu.instructure.com/courses/1478995
Prerequisites:	CHEM 160 or CHEM 161A/161B, MATH 30, MATH 31 (or equivalent course with a grade of "C" or better; "C-" not accepted), or instructor consent.

Course Description

Students will be introduced to theories and methodologies used in computational chemistry, with a focus on molecular simulation methods and cheminformatics. Students will learn via a combination of project-based learning, lectures, and student presentations on topics from the computational chemistry literature. Prior programming experience is not required, but a willingness to learn to code in Python is required.

Textbook

Essentials of Computational Chemistry: Theories and Models - 2nd Edition
By Christopher J. Cramer

Used paperback versions of this book can be found for under $40 online, new are around $50. The University of Cincinnati has also posted a PDF of **the book for free:** https://www.eng.uc.edu/~beaucag/Classes/AdvancedMaterialsThermodynamics/Books/Essentials%20of%20Computational%20Chemistry.pdf

Recommended Free Python Training to Complete Prior to Taking this Course
https://education.molssi.org/python_scripting_cms/

Course Goals and Learning Objectives

Course Learning Outcomes (CLO)

(1) To become conversant in methodologies from computational chemistry used in research and industry for analyzing the dynamic structure and function of molecules; (2) to develop the skill of teaching one's self to write computer code and use new software tools to solve chemical problems; (3) to read and critique multiple journal articles from the scientific literature; (4) to improve written and verbal communication skills as applied to topics in computational chemistry.

Classroom Protocol

- Students are expected to keep up with all of the coding projects, tutorials, videos, presentations, and readings listed on the course Canvas page. Each week will be organized as a separate module with all materials and assignments for the week. Projects that require multiple weeks to complete will be posted in the Canvas module for the week when they are introduced, and due dates will be given in the Canvas module.

- Graded materials will include coding projects, student presentations, and oral exams. The exact point breakdown will be given on the Canvas page, but will be roughly 40% coding projects, 40% student presentations, and 20% oral exams.

- Students are encouraged to work together on coding projects, so please share ideas with each other openly as you collaborate (i.e. students turning in similar codes will not be considered cheating). The philosophy behind the oral exams is that you need to be able to explain to me how the code you wrote for the coding projects works (see student learning outcome on being *conversant*). So, if your friend helps you with a coding project, make sure you understand **why** you wrote what you wrote because you will need to be able to explain it later!

- Students are encouraged to make use of my office hours. Office hours are also known as student hours because this is time that I have put aside to help you the students with any course material that you are having difficulty with. If you need help but are unable to meet with me via Zoom during my scheduled office hours, please email so that we can set up a meeting at some other time. Another thing to note is that, similar to a math course, new material in this course will build heavily onto previously covered concepts. This means that, if you are having trouble with a concept, do not wait to talk to me about it because you will probably need to understand it in order to be successful with future material. Again, please make the most of student hours!
- Students are expected to be respectful toward the instructor and other members of the course, and not engage in behaviors that show disrespect for or distract from others' learning. You are adult learners, and professionalism is expected. This extends to all forms of communication used in this course, including but not limited to Zoom chat, discussion boards, email, etc.

- Success in this course is based on the expectation that students will spend, for each unit of credit, a minimum of 45 hours over the length of the course (normally three hours per unit per week) for instruction, preparation/studying, or course related activities, including but not limited to internships, labs, and clinical practica. Other course structures will have equivalent workload expectations as described in the syllabus.

Email Communication:

In addition to the Canvas interface, it is your responsibility to keep up with class announcements sent via your SJSU email address. I will also work to keep up with emails I receive from you, and I aim to respond to your emails within 24 hours or less during the week, or by the following Monday for emails received during the weekend. Professors get a ton of email, so if I send you a very short response, it is only because I wanted to respond in a timely manner and did not have time to write something more formal. For questions related to this course, I prefer that you contact me through the Canvas messaging app, as it helps me ensure that I don't miss your message in my email inbox.

Late and Incomplete Work

Assignments are typically due at 11:59PM on their respective due dates (unless otherwise specified. The bulk of the points in this course are allotted to projects that will require about 4 weeks each to complete. If you make steady progress each week, you will have plenty of time to complete each project, so the need for an extension should be extremely rare. Nonetheless, if you have an extenuating circumstance where you feel you need an extension, please let me know. Do not expect to be able to turn in assignments late and receive full credit.

Chemistry and the Computer, Spring 2022
Tentative Course Schedule

I tailor the pace and content of this course to best serve the needs of the students and the class. Consequently, all readings, assignments, and due dates are subject to change. All due dates will be listed in our Canvas page, and any changes will be announced via Canvas announcement or email. Please stay up-to-date on Canvas.

Course Schedule

Week	Date	Topics	Graded Materials
1	Jan 27 (Thurs)	Overview and Getting Started with Python	
2	Feb. 1 (Tues)	Definition of Terms, Potential Energy Surfaces (PESs) and Conservative Fields	
2	Feb. 3 (Thurs)	Python basics	Begin First Python Programming Project

Week	Date	Topics	Graded Materials
3	Feb. 8 (Tues)	Taylor Series and Fourier Series	
3	Feb. 10 (Thurs)	Python applications for PESs and other concepts	
4	Feb. 15 (Tues)	Optimization, Energy Minimization, and Model Fitting	
4	Feb. 17 (Thurs)	Python Programming Q&A Session (to help you with your programming project)	Finish the First Python Programming Project
5	Feb. 22 (Tues)	Asynchronous class on running a Lennard-Jones Fluid Simulation	Complete the Lennard-Jones Fluid Simulation Lab, and Start Working on Explaining How my Lennard-Jones Fluid Simulation Code works
5	Feb. 24 (Thurs)	Class Discussion on Lennard-Jones (LJ) Fluid Simulation Code	
6	Mar. 1 (Tues)	Presentation by Dr. Sara Capponi	One Page Reflection Paper on Dr. Capponi's Talk
6	Mar. 3 (Thurs)	Student Presentations on Different Functions from the Lennard-Jones Fluid Simulation Code	Student Presentations on Different Functions from the Lennard-Jones Fluid Simulation Code
7	Mar. 8 (Tues)	Optimization, Energy Minimization, and Model Fitting	Writing an MCMC sampler in Python for a 2-well 1D Potential
7	Mar. 10 (Thurs)	Force Fields and Molecular Modeling	
8	Mar. 15 (Tues)	Small Molecule Docking	
8	Mar. 17 (Thurs)	Simulations of Molecular Ensembles	Students should start thinking about what their presentation topic
9	Mar. 22 (Tues)	1:1 Meetings to Review Progress on Student Presentations	

Week	Date	Topics	Graded Materials
9	Mar. 24 (Thurs)	1:1 Meetings to Review Progress on Student Presentations	
10	Mar. 29 (Tues)	SPRING BREAK NO CLASS	SPRING BREAK NO CLASS
10	Mar. 31 (Thurs)	SPRING BREAK NO CLASS	SPRING BREAK NO CLASS
11	Apr. 5 (Tues)	Simulations of Molecular Ensembles	Start writing a time correlation function calculator for the LJ fluid simulation code
11	Apr. 7 (Thurs)	Applied statistical mechanics and calculating observables from simulations	
12	Apr. 12 (Tues)	Applied statistical mechanics and calculating observables from simulations	Build a canonical NVT ensemble from the LJ fluid simulation code
12	Apr. 14 (Thurs)	In-class Python coding session	
13	Apr. 19 (Tues)	In-class Python coding session	
13	Apr. 21 (Thurs)	In-class Python coding session	Finish up your coding projects
14	Apr. 26 (Tues)	Machine learning applications in chemistry	Work on your presentations!
14	Apr. 28 (Thurs)	Machine learning applications in chemistry	Work on your presentations!
15	May 3 (Tues)	STUDENT PRESENTATIONS	STUDENT PRESENTATIONS
15	May 5 (Thurs)	STUDENT PRESENTATIONS	STUDENT PRESENTATIONS
16	May 10 (Tues)	STUDENT PRESENTATIONS	STUDENT PRESENTATIONS
16	May 12 (Thurs)	STUDENT PRESENTATIONS	STUDENT PRESENTATIONS
Final Exam	Thurs. May 19 5:15-7:30 PM	RESPONSE PAPER TO STUDENT PRESENTATION	RESPONSE PAPER TO STUDENT PRESENTATION

Grading Scale:

Grade	*Percentage*
A plus	*96 to 100%*
A	*93 to 95%*
A minus	*90 to 92%*
B plus	*86 to 89 %*
B	*83 to 85%*
B minus	*80 to 82%*
C plus	*76 to 79%*
C	*73 to 75%*
C minus	*70 to 72%*
D plus	*66 to 69%*
D	*63 to 65%*
D minus	*60 to 62%*
F	*59 to 0%*

SJSU Student Resources:

CAPS
It is estimated that 1 in 4 people will have a mental health struggle in their life. There are campus resources available for free to help:
https://www.sjsu.edu/counseling/

Academic Advising
https://www.sjsu.edu/aars/index.html

Canvas Student Support
https://www.sjsu.edu/ecampus/teaching-tools/canvas/index.html

UndocuSpartan Student Resource Center
The UndocuSpartan Student Resource Center (USRC) is invested in creating educational opportunities that will further the success of UndocuSpartans at SJSU. The center works alongside undocumented/AB 540 students and allies to create a campus community that is welcoming and inclusive of all students regardless of their immigration status.
https://www.sjsu.edu/undocuspartan/

Spartan Food Pantry
The Spartan Food Pantry is a walk-in, full-service, staffed, food assistance program offering non-perishable goods, fresh produce, and refrigerated items to eligible students.
https://www.sjsu.edu/sjsucares/get-assistance/spartan-food-pantry.php

SJSU Cares Housing Insecurity Assistance Request Form
https://cm.maxient.com/reportingform.php?SanJoseStateUniv&layout_id=12

ADDENDUM TO ALL CHEMISTRY DEPARTMENT GREENSHEETS
(Except Chem 291 Sections)
Revised August 2018

University Policy

Per University Policy S16-9, university-wide policy information relevant to all courses, such as academic integrity, accommodations, etc. will be available on the Office of Graduate and Undergraduate Programs' Syllabus Information Web Page at http://www.sjsu.edu/gup/syllabusinfo/

CHEMICAL SAFETY – ***all courses***

Chem 120S is a required course for all chemistry majors and minors and a prerequisite for all Chem 180/298 research.

EMERGENCIES AND EVACUATIONS – ***all courses***

If you hear a continuously sounding alarm, or are told to evacuate by Emergency Coordinators (colored badge identification), walk quickly to the nearest stairway (end of each hall). Take your personal belongings, as you may not be allowed to immediately return. Follow instructions of Emergency Coordinators. Be quiet so you can hear. Once outside, move away from the building. Do no return to the building unless the Police or Emergency Coordinators announce that you may.

STUDENTS REGIESTERED WITH THE ACCESSIBLE EDUCATION CENTER – ***all courses***

Campus policy in compliance with the Americans with Disabilities Act: "If you need course adaptations or accommodations because of a disability, or if you need special arrangements in case the building must be evacuated, please make an appointment with me as soon as possible, or see me during office hours. Presidential Directive 97-03 requires that students with disabilities requesting accommodations must register with DRC to establish a record of their disability."

ACADEMIC INTEGRITY STATEMENT – ***all courses*** (from the Office of Student Conduct and Ethical Development):

"Your own commitment to learning, as evidenced by your enrollment at San José State University, and the University's Academic Integrity Policy requires you to be honest in all your academic course work. Faculty members are required to report all infractions to the Office of Student Conduct and Ethical Development. The policy on academic integrity can be found at http://sa.sjsu.edu/student_conduct