San José State University
College of Science, Department of Chemistry
CHEM 101 - Chemistry and the Computer
Sections 01 and 02, Fall 2021

Course and Contact Information

Instructor(s):	Gianmarc Grazioli, Ph.D. (he/him) Preferred names: Dr. Grazioli or Dr. G
Email:	gianmarc.grazioli@sjsu.edu
Office Hours (aka Student Hours):	Tues. 2:00 pm – 3:10 pm and Thurs. 2:00 pm – 3:10 pm or by appointment Zoom link available in Canvas
Class Days/Time:	Activity: Tues and Thurs. 9:30 am - 10:20 am Seminar: Tues. and Thurs. 10:45 am - 11:35 am
Classroom:	Online: Canvas/Zoom
Prerequisites:	Chem 55, Math 030 or 030P with grades of "C" or better; "C-" not accepted.

Course Description: Analysis of chemical problems. Spreadsheets, mathematical software packages, computer programming, computational chemistry methods.

Technology Intensive Online Course Notification:

This is a technology intensive fully online course that will require students to have access to a computer, with internet connectivity, onto which they can install and use software such as Microsoft Excel and various tools for writing and executing Python code (the free Anaconda distribution of Python is ideal - https://www.anaconda.com/products/individual). Nonetheless, *no prior experience in computer programming or Excel is required for this course*. Although official class days/times have been scheduled (above), the course will be conducted asynchronously as much as possible. The course also has no required textbook. Each week, you will have a new module to complete in Canvas (readings, video lectures, tutorials, etc.), which must be completed by the end of the week (11:59PM Fridays).

Student Learning Outcomes

- Students will develop foundational knowledge and computer skills that will allow them to explore career paths at the interface of chemistry and scientific computing.

- Students will learn to become self-guided practitioners in applying scientific computing methods toward solving problems in chemistry. With all the great free resources that can be found on the internet, learning to code is one of the most accessible skills that can be learned via self-study.

Course Outcomes

- One of my top priorities as the instructor for this course is to teach you how to teach yourself to implement computational tools into your work in the field of chemistry.

- Although we will devote some time to learning about the concepts that underpin some of the computational techniques used in chemistry, there is no substitute for "getting your hands dirty" by applying the methods. The final goal is then to **learn by doing** with project-based learning.

Classroom Protocol

- Students are expected to keep up with all of the tutorials, videos, 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.

- The scheduled quizzes will be based on the material covered in the Canvas modules ranging from the date of the previous quiz up to the date of the present quiz (not including material introduced the same day as the quiz). The quizzes are meant to ensure that you are learning the skills needed to complete the 3 projects, which comprise the bulk of your grade.

- Given the fact that this course is being taught remotely and mostly asynchronously, it is extremely important to your learning that you 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 Google Chat 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. 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

Late and Incomplete Work

All assignments are due at 11:59PM on their respective due dates listed below, 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.

Chem 101 / Chemistry and the Computer, Fall 2021, Tentative Course Schedule

All readings, assignments, and due dates are subject to change to best serve the needs of the students and course. Any changes will be announced via email or Canvas announcement.

Course Schedule

Week	Date	Broad Topics	Specific Topics	Graded Materials
1	Aug 19 (Thurs)	Basics of Computers and Microsoft Excel	Examples of how computers are used in different fields of chemistry, along with fundamentals on how computers work.	
2	Aug 24 (Tues)	Display of Quantitative Information/Data Visualization	Data import and export, graphing to scientific standards, scaling, formatting, dealing with different number formats, Data types in programming: Boolean, integer, float, string, etc.,	Pretest **(10 points)** Note: graded on completion only, not on the accuracy of your answers

Week	Date	Broad Topics	Specific Topics	Graded Materials
2	Aug 26 (Thurs)	Display of Quantitative Information I Textual	Installing Anaconda, Number formatting, significant figures and symbols. Table formatting. Display of units. Equation editor. Install Pymol, and basic Pymol visualizations	Quiz 1 **(10 points)**
3	Aug 31 (Tues)	Basic Chemical Calculations	Chemical functions: plots to extract information: Gas Laws, solubility, pH and complexation.	
3	Sep 2 (Thurs)	Generalized Multivariate Least Squares Regression	Theory and application of univariate and multivariate least squares analysis using Excel	Quiz 2 **(10 points)**
4	Sep 7 (Tues)	Programming in Python	Loading data from Excel files into Python, using Spyder, Jupyter, defining functions, loops, logic operations, other syntax	Begin Work on Project 1
4	Sep 9 (Thurs)	Programming in Python	Loading data from Excel files into Python, using Spyder, Jupyter, defining functions, loops, logic operations, other syntax	
5	Sep 14 (Tues)	Statistical Calculations	Excel exercises in statistics: Descriptive aspects mean, median, mode, standard deviation, confidence tests. Data Modeling by Regression	
5	Sep 16 (Thurs)	Propagation of Random Uncertainty: Simulation and Theory	Discrete distributions generated by variable input variables. Differential error propagation methods	Quiz 3 **(10 points)**
6	Sep 21 (Tues)	Monte-Carlo Methods	Error propagation by extrema and by random number generation. Calibration curve examples.	

Week	Date	Broad Topics	Specific Topics	Graded Materials
6	Sep 23 (Thurs)	Spectral Fitting	Multivariate Linear and Non-linear regression	
7	Sep 28 (Tues)	Smoothing Methods	Smoothing functions, moving average, triangular, Gaussian.	
7	Sep 30 (Thurs)	Discrete Fourier Analysis	Basic concepts and theorems, issues attending discrete signal processing (Nyquist theorem, aliasing etc.) signal recovery, smoothing	Project 1 is due (**100 points**)
8	Oct 5 (Tues)	Molecular Visualizations	Using Pymol to make movies of molecular structures	Begin Work on Project 2
8	Oct 7 (Thurs)	Monte Carlo Molecular Simulations	Demonstration of Monte Carlo Simulations on low dimensional models	
9	Oct 12 (Tues)	Molecular Dynamics Simulations	Demonstration of Monte Carlo Simulations on low dimensional models	
9	Oct 14 (Thurs)	Molecular Dynamics Simulations	Full scale molecular simulations via Chem Compute	Quiz 4 **(10 points)**
10	Oct 19 (Tues)	Molecular Dynamics Simulations	Full scale molecular simulations via Chem Compute	
10	Oct 21 (Thurs)	Analysis of Simulation Data	Python Data Analysis tutorial from MolSSI	
11	Oct 26 (Tues)	Analysis of Simulation Data	Python Data Analysis tutorial from MolSSI	
11	Oct 28 (Thurs)	Analysis of Simulation Data	Python Data Analysis tutorial from MolSSI	Project 2 is due (**100 points)**
12	Nov 2 (Tues)	Machine Learning in Chemistry	Overview of machine learning and examples of applications	Begin Work on Project 3
12	Nov 4 (Thurs)	Machine Learning in Chemistry	Supervised Learning	Quiz 5 **(10 points)**

Week	Date	Broad Topics	Specific Topics	Graded Materials
13	Nov 9 (Tues)	Machine Learning in Chemistry	Unsupervised Learning	
13	Nov 11 (Thurs)	Machine Learning in Chemistry	Machine learnable data structures for chemical data	Quiz 6 **(10 points)**
14	Nov 16 (Tues)	Machine Learning in Chemistry	k-means clustering of configurations from molecular simulation data	
14	Nov 18 (Thurs)	Machine Learning in Chemistry	Fitting a model to clustering data	
15	Nov 23 (Tues)			Project 3 is due **(100 points)**
15	Nov 25 (Thurs)	Happy Thanksgiving!	No Class	
16	Nov 30 (Tues)	Quantum Computing	q-bits, quantum annealing, quantum logic gates	
16	Dec 2 (Thurs)	Review for Final		
Final Exam	Dec. 9 9:45-12:00	Online Final Exam		Final Exam **(30 points)**

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.