Research in Chemistry
(CHEM 3950/4160/4170/4950)
Course Syllabus – Fall 2024

Instructor: Samer Gozem
E-mail: sgozem@gsu.edu

Instruction mode: This is a **hybrid** course. Given the computational nature of our research, research could equally well be performed at home or online. However, the course includes some in-person events such as individual or group meetings.

Software required for this course: The following software is required for this course:

Required Software:

- IQmol (http://iqmol.org)
- PuTTY (Only if you are using a Windows operating system: https://www.putty.org)

Optional software:

- An SFTP client, E.g., WinSCP for Windows or free version of CyberDuck for Mac.
- For writing the report, I recommend using Grammarly, which is free for GSU students: (https://technology.gsu.edu/technology-services/it-services/training-and-learning-resources/grammarly/

Course Prerequisites: Prior discussion with the instructor. Other pre-requisites are not strictly required, although Chem 4120 (quantum mechanics) is recommended for understanding some of the concepts in this research course. Students in this course will also learn how to work on a Bash Unix environment, so any programming experience is a plus.

Course Description: Students will learn how to use computational chemistry tools and software to solve a chemical problem. At the end of this course, each student must write an ACS-style report on their results and findings and discuss their results in the context of existing literature.

Course Objectives: To learn how to conduct scientific research in computational chemistry. This includes learning how to conduct literature search, data collection, data analysis, and to draw conclusions from the data.

Specific Learning Outcomes: The learning outcomes depend on the details of the research project agreed on after discussion with the instructor. A few typical learning outcomes are listed below.

1. Learn how to use a molecular editor and visualization package to build molecules and run quantum mechanical calculations.
2. Become familiar with working on a high-performance computing environment, including getting used to UNIX commands and vim text editor, enough to write and modify input files and extract information from output files generated by a quantum mechanical software package.
3. Learn how to run quantum chemical calculations (or hybrid quantum mechanical / molecular mechanical calculations) to compute the properties of chemical or biological systems.
4. Perform a literature search of experimental data against which to validate computational results.
5. Discuss results of calculations considering existing computational and experimental research.

Grading: The grade scheme is as follows:

Criteria		%
Participation		**30**
Progress of the research project		**30**
Written Report (breakdown of grades below)		**40**
Scientific creativity and merit	5	
Introducing the problem	10	
Data and Data analysis	10	
Discussion of results	10	
Report format, clarity, referencing	5	

Grade	Points
A+	98-100
A	93-98
A-	90-93
B+	87-90
B	80-87
B-	75-80
C+	70-75
C	65-70
C-	60-65
D	50-60
F	< 50

Participation: At the start of the semester, each student will agree with the course instructor on a format for meetings and communication throughout the semester. This could be in the form of online or face to face group meetings or individual project meetings. The participation grade will depend on the student's attendance and participation during those meetings.

Research Project: During a meeting at the start of the semester (or before that), the student and instructor will discuss and agree on a research project to be carried out during the semester. Typically, such a meeting is a pre-requisite for taking the course in the first place. During this and subsequent meetings, the details of the research project are discussed, and next steps agreed on. The "progress of the research project" grade is determined by the student's effort on the research project, their communication of their questions and results to the instructor, and their ability to overcome obstacles standing in the way of the completion of the research project.

Written Report: At the end of the semester, each student will write a report reflecting the work they did during the semester. The report should be submitted on iCollege by **Monday, December 13th, 2024**. The report should be approximately 10-15 pages long (double spaced, 12-sized font, 1-inch margins, including figures and references). The referenced ACS-style report should provide context, introduce the goal of the project, and present data and results, and discuss the results in context of existing literature, when available. The report must represent your **individual effort**, even if your work was part of a bigger collaborative project.

Course Evaluation: Your constructive assessment of this course plays an indispensable role in shaping education at Georgia State. Upon completing the course, please take the time to fill out the online course evaluation.

Accommodations: Students who wish to request accommodation for a disability may do so by registering with the Access and Accommodation Center. Students may only be accommodated upon issuance by the Access and Accommodation Center of a signed **Accommodation Plan** and are responsible for providing a copy of that plan to instructors of all classes in which accommodations are sought.

Student Integrity Policy: Information about the GSU policy on academic policy can be found at this link: https://deanofstudents.gsu.edu/student-conductpolicy-on-academic-honesty/

Last day to withdraw is **Tuesday, October 15th, 2024**
The University requires faculty, on a date set by the Provost after the mid-point of the course,
1. to give a WF to all those students who are on their rolls but no longer taking the class, and
2. to report the last day the student attended or turned in an assignment.