

**Chemical Research
(CHEM 4160)
Course Syllabus – Fall 2021**

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Instruction mode during COVID-19: Assignments will be posted on iCollege. The discussion forum will be the primary form of communication, to encourage collaboration and ongoing discussion. We may decide to have meetings, as needed.

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

Required Software:

- IQmol (<http://iqmol.org>)
- PuTTY (Only for Windows operating systems: <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: CHEM 4160 is a chemistry research course. In this section, 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:

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 use time-dependent density function theory (TD-DFT) calculations to:
 - a. obtain molecular geometries and vibrational frequencies
 - b. simulate the spectral properties of organic dyes. Use color theory to make deductions about the color of these dyes in solution.
 - c. predict the solvatochromic shifts of these dyes in different solvents.
 - d. design and carry out a proposed independent mini computational project.
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.

Assignment: During the first half of the course, there will be one assignment due on iCollege every 1-2 weeks. Keep in mind, as this is a research course, you are strongly encouraged to explore the methods and tools that you learn well beyond the minimum required to complete the assignments. Each student will be individually assigned one dye to use for that part of the course. During the second half of the course, the students must come up with their own mini project through discussions with the instructor.

Written Report: Each student will write a report reflecting the work they did during the semester. The report should be emailed to me as a pdf file by **Monday, December 6th, 2021**. 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, 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.

Grading: The grade scheme is as follows:

Criteria	%
Participation	20
Accurate and timely completion of assignments	40
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

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: Tuesday, October 12th, 2021

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.