Chemical Research
(CHEM 4160)
Course Syllabus – Summer 2021

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Instruction mode: Assignments will be posted on iCollege. The discussion forum will be the primary form of communication, to encourage collaboration and ongoing discussion.

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

Required Software:

- Webex (https://technology.gsu.edu/technology-services/it-services/collaboration-tools/webex/)
- IQmol (http://iqmol.org)
- PuTTY (Only for Windows operating systems: https://www.putty.org)
- An SFTP client, E.g., WinSCP for Windows or free version of CyberDuck for Mac.

Optional software:

- 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. While other prerequisites are not strictly required, please note that part of this research does rely on advanced concepts in physical chemistry, so a strong background in physical chemistry is highly recommended. Specifically, I suggest completing Chem 4110 (thermodynamics) with a grade of at least a B before taking this section of Chem 4160. Taking Chem 4120 (quantum mechanics) is also recommended for understanding some of the concepts. Students who have not yet taken those courses or are not interested in physical chemistry research are recommended to seek other sections of Chem 4160. Students in this course will learn how to work on a Bash Unix computing 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 Expectations: The assignments set a minimum pace for student progress in the course. Typically, student researchers spend at least 6-8 hours a week on research. Please note that part of this course requires students to use asynchronously recorded lectures and tutorials to learn how to work on a Bash Unix environment, so being interactive, asking questions when stuck, and self-motivation are critical to succeeding in this course.

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 in light of existing computational and experimental research.

Assignment: **During the first half of the course, there will be one assignment due on iCollege every week**. 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.

Written Report: Each student will write a report on their research. The report should be emailed to me as a pdf file by **Friday, July 23rd, 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

Last day to withdraw: **Friday, July 2nd, 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.