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Goals

Our group uses computational chemistry tools to develop explanatory and predictive models for chemical reactions. We are experts at studying reactions that may seem “messy” and revealing the simple chemical rules governing them. The chemical rules that we uncover should be testable by experimentalists and should improve the efficiency of the reactions we study. Thus, we seek practical and tangible solutions to chemical problems.

Guiding Principles

- We use rigorous and robust computational approaches when tackling all research projects.
- We present our approach, data, and results clearly and completely to audiences within and beyond the theoretical and computational chemistry fields.
- We embrace research collaborations with experimentalists.
- We take pride in a research environment where all voices are heard, all ideas are taken seriously, and all group members feel supported.

Learning Outcomes

The students in my research group acquire computational chemistry skills that they will use to explore the chemical factors that govern molecular structure and chemical reactions that have economic, environmental, and medicinal importance.

Core computational chemistry skills: They will be able to:

- generate conformational ensembles of molecular systems using molecular mechanics force field methods,
- compute geometries at ground and transition states on reaction coordinates, and
- analyze the electronic properties of these geometries to answer questions related to molecular stability, chemical reactivity, and catalysis.

Software proficiencies: The typical student researcher will learn how to use:

- *Schrödinger Macromodel* and *Gaussian* for molecular mechanics and quantum mechanics calculations,
- *Gaussview* and *PyMOL* for molecular visualization,
- extensive spreadsheet use for data analysis,
- *Python* scripts developed by the research advisor to process large datasets from their computations and,
- if they choose, they may build programming skills along the way.

Communication skills: Students will have several opportunities to present their work, both orally and in writing, to audiences within and beyond the chemistry community, thus developing critical skills transferable to any industry.

Getting Started

As you begin conducting research in my group, you will be asked to conduct the following:

1. **Schedule and attend weekly 1:1 project discussion meetings.** During these meetings, we will discuss research topics, review and discuss literature, and sharpen your project goals.
2. **Prepare a one- to two-page research proposal (with my guidance).** With my close guidance, you will develop a proposal document containing your project's motivation, specific aims, and research plan, including the proposed timeline for completion and

deliverables (e.g., internal and external presentations, contributions to publications, capstone requirements, etc.).

Group Meetings (Research Days)

As a research group member, you are expected to attend and actively participate in weekly meetings that last for an hour. The timing of these meetings will be determined based on the availability of the students in the group. During these meetings, each student will present their research updates in a fully developed presentation format on a rotating schedule. Your presentation should be at most 15 minutes, allowing for 10-15 minutes of discussion. You will present your research at least once every month. Before the start of the group meeting, you will be required to submit your research presentation slide deck as a PDF to the appropriate assignment portal on Canvas. Feedback on these presentations will be provided, and you will be expected to incorporate this feedback in time for your next presentation.

Group Meetings (Literature Days)

We will organize a literature group meeting after a few cycles in the research presentation schedule. Before the meeting, I will provide you with a published paper that you must read carefully and thoroughly. Additionally, you will receive a Canvas quiz consisting of a series of questions related to the paper. You will be expected to answer these questions before the meeting. During the meeting, each student will lead the discussion on a particular sub-section of the paper. You can expect to participate in a literature group meeting at least once a semester.

Time Commitment

You are expected to dedicate a certain amount of time to your research project, depending on the number of CHEM 150, CHEM 151, or CHEM 152 credits you have signed up for or the agreement from an externally funded grant. If you plan on enrolling in CHEM 150/151/152, please be aware of the time commitment required by the research group. To make significant progress in your research, it is recommended that you sign up for two CHEM 150/151/152 credits each semester. It is important to note that chemistry majors are required to satisfactorily complete 4 to 6 credit hours of CHEM 151-152. Students who have elected the Joint Major in Chemistry and Biology are required to satisfactorily complete 6 credit hours of CHEM 151-152 or BIO 193-194.

# Credits	Total # Hours	Average # of Hours per Week (14 weeks)
1	56	4
2	112	8
3	168	12

Notes on time commitment:

- You are expected to record your research activities, including dates, time spent, and a list of activities. Submit this as a weekly update to the research group's Canvas portal.
- It's okay to spend more or less time on research than the average time mentioned above. Adjust your research time each week based on the demands of your coursework, which should be your top priority in college.

- You should not work more than 19 hours a week on research. Please get in touch with me if you are nearing that limit.

Weekly Research Hours

You are expected to spend most of your time conducting research in the lab room, which includes literature reviews, preparing and submitting computational jobs, data analysis, developing figures, and writing manuscripts.

To ensure progress in your research project, it's important to schedule time blocks for research work in the lab room at least two days per week. You should discuss your preferred time slots with the research advisor at the beginning of each semester to finalize them.

During your research time in the lab room, we will have multiple conversations to discuss your progress and plan. Please ensure you have all the raw and interpreted data you want to discuss, any questions you may have, and any issues you have encountered. This will help you stay on track with your research project.

End-Of-Semester Check-In

We will schedule a one-on-one meeting within the last two weeks of each semester. In this meeting, we will discuss your research project progress, including your participation and engagement in group meetings and discussions.

End-Of-Semester Evaluation

I will provide you with an assessment of the following evaluation items:

- You have attended all your research lab hours, and during these meetings, you have demonstrated progress on your research project.
- You have actively participated in all research group meetings unless your research advisor has excused you otherwise.
- You have incorporated feedback from your research advisor into all subsequent presentations.

Evaluation	Description	Outcome
Satisfactory	All 4 of the evaluation items above were achieved	Continuation of CHEM 150/151/152 (or grant funded) research
Concern	1-2 of the evaluation items were not achieved	Probationary period next semester. Continuation of CHEM 150/151/152 (or grant funded) research.

Unsatisfactory	1-2 evaluation items above were not achieved during a probationary period	Discontinuation of CHEM 150/151/152 (or grant funded) research.
	OR	
	3-4 evaluation items above were not achieved	

Note: If there are any issues with your research progress, your P.I. will bring it up during the semester. A **“Concern”** or **“Unsatisfactory”** evaluation is uncommon.

Post-College Preparation

One of my primary responsibilities is to help you move forward in your academic or professional journey. Depending on your goals, this could mean applying to graduate school, professional school, or the workforce. Regardless of your choice, we must ensure that you are well-prepared and competitive. Here are some general guidelines that we will adjust to fit your individual needs:

- You should schedule a meeting with me one year before graduation to discuss your career goals.
- You should create a timeline for preparing your application materials during your final year of college.
- I will review and provide feedback on your statements and essays as part of your application packet.
- You should meet with Career Services to explore job and internship opportunities.
- Finally, I will serve as one of your referees and provide a recommendation letter tailored to your applications.

Lab Electronic Access

All research group materials are available on Canvas. The Canvas site will be the primary repository of all lab documents and resources, presentation submissions, feedback, discussions, and announcements.

Wellness

College students often experience issues that may interfere with academic success, such as academic stress, sleep problems, juggling responsibilities, life events, relationship concerns, or feelings of anxiety, hopelessness, or depression. If you or a friend is struggling, I strongly encourage you to seek support. Helpful, effective resources are available on campus at no charge.

- Check-in with an academic dean if you are struggling with courses or unsure what educational resources are available at HMC by emailing academicdeans@g.hmc.edu.
- Contact [The Office of Health and Wellness](#) to discuss options by emailing wellness@hmc.edu.
- [Monsour Counseling and Psychological Services \(MCAPS\)](#) provides crisis support services 24/7/365. Students can call us at 909-621-8202 and press “1” at the prompt to speak with a crisis counselor. Other prompt options are available for those not in crisis.