Chem 4050/5050
Computational Problem Solving in the Chemical Sciences

FL2024

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Lecture Time:	M-W-F 11:00A-11:50A
Recitation Time:	R 11:30A-12:50P
Lecture Room:	Lopata Hall 103
Recitation Room:	Eads 212

Contents

1 Course Description

Have you ever wondered how molecular interactions shape the world around us? Why do certain materials exhibit unique properties? How can we predict and manipulate chemical reactions at the atomic level? These are the mysteries at the heart of chemistry, where understanding the unseen world of atoms and molecules can unlock groundbreaking advances in science and technology. However, one needs specialized numerical methods and computational chemistry skills to explore these questions. This course is designed to bridge this gap. It provides a comprehensive introduction to the mathematical and computational skills necessary to model chemical phenomena at the atomic level. We start by building a strong foundation in mathematical representations of chemical problems, utilizing open-source software tools for problem-solving, data interpretation, and visualization of materials and molecular structures. In the second part of the course, we delve into the fascinating world of atomic-level computer modeling. You'll learn various methodologies, such as Monte Carlo and molecular dynamics. We'll analyze static (thermodynamic and structural) and dynamic properties and their statistical errors. Don't worry if you're new to coding – we'll cover the basics of Python programming in the first few lectures, setting you up for success. By the end of this course, you will be proficient in using computational tools, understanding atomic interactions, and approaching chemical problems with a structured and strategic thought process. Join us to unlock the secrets of the molecular world and transform the way you see chemistry!

1.1 Prerequisites

Chem 106/112A, Math 132, Physics 191, Chem 261

1.2 Learning Objectives

1. **Applied Python for Chemical Equilibria and Bonding**: Enhance problem-solving skills by applying Python programming to solve complex problems in chemical reaction equilibria, chemical bonding, and balancing chemical equations.

2. **Statistical Analysis in Chemical Research**: Develop proficiency in analyzing reaction orders and calibration data using regression and correlation techniques in statistics.

3. **Bridging Mathematics and Chemistry**: Deepen understanding of chemistry's mathematical principles, including numerical methods that connect abstract mathematical theories with tangible chemical phenomena.

4. **Simulation Techniques in Modern Chemistry**: Gain expertise in modeling chemical phenomena such as chemical bonding, nanoparticle shape, lipid interactions, surface adsorption, and polymer solvation using Monte Carlo and molecular dynamics simulations.

5. **Integration and Exploration in Computational Chemistry**: Foster an environment for exploring special topics of interest in modern chemistry and computation, encouraging students to link their interests with computational methods.

1.3 Transferable Skills

Upon successful completion of this course, students will build a skill set that includes:

1. **Enhanced GitHub Skills for Portfolio Development**: Through effectively using GitHub, students will learn to curate and showcase their computational projects. This skill is crucial for building a professional portfolio reflecting their computational chemistry expertise.

2. **In-Depth Simulation Technique Insights**: The course will enable students to understand and interpret the outcomes of various simulation techniques thoroughly. This knowledge is key to appreciating these techniques' diverse applications and nuances in modeling chemical behavior.

3. **Linking Theory with Practice**: Students will learn to draw parallels between measured chemical properties and their computational models. This skill is vital for comprehensively understanding chemistry's theoretical and practical aspects.

4. **Critical Application of Simulation Methodologies**: The course will cultivate a critical and informed approach toward applying different simulation methods. Students will learn how to effectively employ these methodologies and understand their limitations in solving chemical problems, promoting a well-rounded approach to computational chemistry.

These goals are designed to equip students with robust skills and knowledge, preparing them for advanced studies or professional careers in the evolving field of computational chemistry.

2 Texts, Materials, and Supplies

There will be no required textbook.

2.1 Non-Required Texts

- Introduction to Python Computations in Science and Engineering, Kitchin
- Mathematics for Physical Chemistry: Opening Doors, McQuarrie
- Understanding Molecular Simulation: From Algorithms to Applications, Frenkel and Smit
- Statistical Mechanics: Theory and Molecular Simulation, Tuckerman
- A Guide to Monte Carlo Simulations in Statistical Physics, Landau and Binder
- Computer Simulation of Liquids, Allen and Tildesley

3 Grading

Your grade in this course will reflect a diverse assessment strategy designed to cater to different learning styles and strengths. I am committed to providing a variety of assessment methods to allow you to demonstrate your understanding and skills effectively.

3.1 Final Grade Composition

- **Homework Assignments (40% of final grade, 200 points)**: You will have five homework assignments designed to reinforce the concepts learned in class and through readings. These assignments will test your understanding and ability to apply these concepts in practical scenarios.
- **Projects (40% of final grade, 200 points)**: Two major projects will be a significant part of your grade. These projects will allow you to delve deeper into specific areas of interest,

apply computational methods to solve complex problems and showcase your analytical and coding skills.

- **GitHub Repository (20% of final grade, 100 points)**: Maintaining a GitHub repository will be crucial to your learning journey. This repository will be a portfolio of your work throughout the course, including code from homework and projects. It will be evaluated on organization, documentation, and the demonstration of your computational skills.

The assessment diversity is designed to comprehensively evaluate your skills and knowledge, encompassing theoretical understanding and practical application. Your active engagement and consistent effort in all these components will be key to your success in this course. The grade boundaries will be

%	Grade
≥ 90	A- to A
≥ 80	B- to B+
≥ 70	C- to C+
≥ 60	D- to D+
< 60	F

4 Assignments and Homework

The coursework is designed to blend theoretical understanding with practical application, primarily focusing on Python programming and its application in computational chemistry. **The general expectation is that students will spend six to nine hours outside class studying and doing homework and projects.**

4.1 Homework Assignments

Each homework assignment consists of problems that challenge you to complete and write Python code from scratch. These assignments are crafted to enhance your coding skills, deepen your understanding of course concepts, and apply them to solve real-world chemical problems. Key components of these assignments include:

- **Code Development**: Developing Python code to address specific chemical phenomena or problems.

- **GitHub Integration**: Regularly pushing your code to your GitHub repository will be a dynamic record of your progress and skills.
- **Problem-Solving**: Utilizing your code to analyze and answer questions, linking coding skills with chemical knowledge.

4.2 Projects

Projects in this course are more extensive and in-depth than homework assignments. They are designed to simulate real-world scenarios where you will apply computational methods to conduct chemical research. Each project will involve:

- **Complex Coding Tasks**: Completing and writing multiple Python scripts to address more intricate and comprehensive problems in computational chemistry.
- **GitHub Project Management**: Organizing and maintaining a project directory in your GitHub repository, which will include all your codes, data, and documentation.
- **Computer Experiments**: Using your Python codes to perform computational experiments, analyze data, and derive conclusions.
- **Report Writing**: Compiling your findings, methodologies, and conclusions into a detailed report showcasing your ability to communicate complex scientific concepts effectively.

4.3 GitHub Repository Management

As a crucial component of this course, each student must maintain a GitHub repository that serves as a comprehensive portfolio of their work. This repository will showcase their coding and project work and reflect their ability to professionally organize and document their computational journey.

4.3.1 Final Submission Deadline

All final changes to your GitHub repository must be merged by midnight on December 12, 2024. This deadline ensures ample time to refine your repository and present your work in the best possible light.

4.3.2 Repository Guidelines

- **Adherence to Best Practices**: Your repository should align with GitHub's best practices. This includes effective organization, use of branches for development, and regular commits to track changes.

- **Detailed README File**: A critical aspect of your repository is the README file. This file should:
  - Clearly describe the purpose and contents of your repository.
  - Include instructions on how to navigate your repository and run the codes.
  - Summarize your projects and assignments, providing context and insights into your work.
- **Reflective of Coursework**: The repository should comprehensively cover all your work throughout the course, including codes from homework, projects, and any additional exercises or explorations you have undertaken.

This repository will be a part of your grading criteria and a valuable asset in your professional portfolio, demonstrating your skills and approach to computational chemistry. It is an opportunity to showcase your technical abilities, organizational skills, and commitment to best software development practices.

4.4 Undergraduate vs. Graduate Student Requirements

This course caters to undergraduate and graduate students, with assignments and expectations tailored to each group's expertise level.

4.4.1 Undergraduate Students

- **Focus**: Building a solid foundation in computational chemistry and Python programming.
- **Assignments**: Aimed to develop basic to intermediate coding skills and understand simple chemical phenomena.
- **Projects**: Scoped to ensure achievability, focusing on applying computational methods to model and analyze defined chemical problems.
- **GitHub Portfolio**: Should demonstrate foundational coding skills, comprehension of computational chemistry concepts, and effective documentation.

4.4.2 Graduate Students

- **Focus**: Tackling complex problems and demonstrating advanced proficiency in computational chemistry.
- **Assignments**: Developing sophisticated code for advanced chemical problems and simulations.

- **Projects**: More demanding, integrating multiple computational methods and extensive data analysis to draw conclusions from complex datasets.
- **GitHub Portfolio**: Showcasing advanced coding skills, a deeper understanding of computational chemistry, and critical analysis of results.

5 Attendance, Participation, and Classroom Climate

While class participation and attendance do not factor into course grades, attendance is mandatory as these are vital components of this course. The structure and content of our lectures are designed to impart knowledge and provide a dynamic, interactive learning environment.

5.1 Interactive Lectures with Python Demonstrations

Each lecture will feature live Python demonstrations, offering you a practical view of how theoretical concepts are applied in computational chemistry. These sessions are an excellent opportunity to clarify doubts in real-time.

5.2 Hands-on Sessions

Regular hands-on sessions will be integrated into the lectures. The instructor and AI(s) will assist you with in-class exercises, homework assignments, and projects during these sessions. This is a perfect time to work collaboratively, receive personalized guidance, and enhance your understanding of course material.

5.3 Weekly Office Hours

I, along with the AIs, will host weekly office hours **on Thursdays from 2-4 PM in Jolley 431**. These opportunities allow you to seek additional help, discuss course material in depth, or get feedback on your assignments and projects.

5.4 Hackathons

Twice during the semester, we organize extended evening office hours, termed "hackathons," in a computer lab setting. These sessions provide intensive, focused time to work on your projects, troubleshoot issues, and collaborate with peers and instructors in a supportive environment.

Your regular attendance and active participation in these activities will enrich your learning experience and foster a collaborative and engaging classroom culture. Engaging consistently in

these interactive components of the course will significantly enhance your understanding and proficiency in computational chemistry.

6 Technical Requirements and Support Available

This course is designed to provide students with ample technological support and resources to facilitate a comprehensive learning experience in computational chemistry. Understanding and accessing these resources is essential for maximizing your success in this course. **There will be no additional course fees and all required software will be open-source**.

6.1 Personal Computing Requirements

Ideally, each student should have access to a laptop or personal computer. This will be their main tool for coding, accessing course materials, and participating in hands-on activities. For students who may not have a personal computer, the Department of Chemistry offers access to spare laptops. These resources are available to ensure all students have the necessary technology to participate fully in the course.

6.2 Open-Source Software Installation and Access

Instructions for installing Python will be provided on the course website before the first day of class. Familiarizing yourself with Python installation and setup is crucial for a smooth start to the course. Students are encouraged to gain access to Google Colab, a powerful online platform for Python programming. The university's information technology staff will assist in accessing Google Colab and other Google products.

6.3 Additional Computational Resources

During the semester, you will gain access to high-performance computing resources essential for running complex simulations and analyses. These resources include:

- Research Infrastructure Services (RIS) at Washington University.
- National Science Foundation (NSF)-supported computing facilities.

Access to specialized computer programming courses on DataCamp will be provided. These courses offer additional learning opportunities to enhance your programming skills and understanding of data analysis techniques.

These resources are intended to support your learning journey in this course by providing access to high-quality computational tools and educational materials. Proper utilization of these resources will enable you to engage effectively with the course content and develop your skills in computational chemistry.

7 Course Calendar

1. **Week 1: Introduction to Python Computations**

   Homework 1 assigned on Friday

2. **Week 2: Numerical Methods in Python**

   (a) Chemical Reaction Equilibria and Roots of Equations

   (b) Chemical Bonding and Numerical Integration

   (c) Balancing Chemical Equations and Systems of Linear Algebraic Equations

   Homework 1 due on Friday

   Homework 2 assigned on Friday

3. **Week 3: Statistics – Regression and Correlation**

   (a) Orders of Reaction and Linear Regression Analysis

   (b) Calibration Data, Confidence Intervals, and Correlation Analysis

   Homework 2 due on Friday

   Homework 3 assigned on Friday

4. **Week 4: Introduction to Molecular Simulation**

   (a) Classical Thermodynamics

   (b) Statistical Thermodynamics

   (c) Ensembles

   (d) Ergodicity

   Homework 3 due on Friday

   Homework 4 assigned on Friday

5. **Weeks 5-8: Monte Carlo Simulations**

Week 5

(a) The Monte Carlo Method

(b) Chemical Bonding and Monte Carlo Integration

Homework 4 due on Friday

Homework 5 assigned on Friday

Week 6

(a) A Basic Monte Carlo Algorithm

(b) Nanoparticle Shape and Simulated Annealing

Homework 5 due on Friday

Week 7

(a) Technical Details: Boundary Conditions, Truncation of Interactions, *Etc.*

(b) Lipid Interactions in Membranes and Monte Carlo Simulations

Week 8

(a) Introduction to Project 1: Monte Carlo Simulations of Adsorption on Surfaces

Project 1 assigned on Friday

6. **Weeks 9-12: Molecular Dynamics Simulations**

Week 9

(a) Molecular Dynamics: The Idea

Week 10

(a) Molecular Dynamics: A Program

Project 1 due on Friday

Week 11

(a) Equations of Motion

Week 12

(a) Introduction to Project 2: Molecular Dynamics Simulations of Linear Polymer Melts

Project 2 assigned on Friday

7. **Weeks 13-14: Advanced and Emerging Topics in Computational Chemistry**

Week 13

(a) Grand Canonical Monte Carlo

(b) Kinetic Monte Carlo

(c) Free Energy Computations

Week 14

(a) Machine Learning in Chemistry

(b) Scientific and Molecular Visualization

Project 2 due on Friday

8 University-Wide Policies & Guidelines

8.1 COVID-19 Health and Safety Protocols

Students experiencing symptoms consistent with COVID-19 or concerned about a possible exposure should contact Habif Health and Wellness Center (314 935-6666) to arrange for testing as indicated. If a student tests positive for Covid-19, they will receive a letter with instructions about any necessary isolation that they can share with their instructors. **Update: 9/1/23. Illness activity at the start of the semester is high, and students may not have documentation of their COVID status; instructors should NOT request students provide them with results of PCR tests in order to receive an excused absence. During this time, please extend grace to students who indicate a need to isolate and allow their absence so that we may reduce the likelihood of illnesses being transmitted in our classrooms.** Any accommodation needs for COVID-related absence not covered in an instructor's standard course policies should be discussed between the student and instructor.

While on campus, it is imperative that students follow all public health guidelines established to reduce the risk of COVID-19 transmission within our community. The full set of University protocols can be found on the Health and Safety webpage. This includes:

Masking;

Masking remains a valuable tool in the mitigation of COVID-19, particularly in light of new and emerging variants. Students and instructors are encouraged to treat requests to mask with care and consideration, keeping in mind that some individuals may be at a higher risk, caring for others at a higher risk, or feeling less comfortable in a mask-optional environment. Based on monitoring of regional and campus conditions, a mask requirement may be implemented as needed.

Students with disabilities for whom masked instructors or classmates create a communication barrier are encouraged to contact Disability Resources (www.disability.wustl.edu) or talk to their instructor for assistance in determining reasonable adjustments. Adjustments may involve amplification devices, captioning, or clear masks but will not allow for the disregard of mask policies should a requirement be in place.

8.2 Reporting Sexual Assault and Harassment

If a student discusses or discloses an instance of sexual assault, sex discrimination, sexual harassment, dating violence, domestic violence or stalking, or if a faculty member otherwise observes or becomes aware of such an allegation, the faculty member will keep the information as private as possible, but as a faculty member of Washington University, they are required to immediately report it to the Department Chair or Dean or directly to Ms. Cynthia Copeland, the University's Associate Title IX Coordinator, at (314) 935-3411, cmcopeland@wustl.edu. They will also offer available resources, including confidential support resources through the Relationship and Sexual Violence Prevention (RSVP) at 314-935-3445. Additionally, you can report incidents or complaints to the Office of Student Conduct and Community Standards or by contacting WUPD at (314) 935-5555 or your local law enforcement agency. See: Gender Equity and Title IX Compliance Office

8.3 Disability Resources (DR)

WashU supports the right of all enrolled students to an equitable educational opportunity, and strives to create an inclusive learning environment. In the event the physical or online environment results in barriers to the inclusion of a student due to a disability, they should notify the instructor as soon as possible.

Disabled students requiring adjustments to equitably complete expectations in this course should contact WashU's Disability Resources (DR), and engage in a process for determining and communicating reasonable accommodations. Because accommodations are not applied retroactively, DR recommends initiating requests prior to, or at the beginning of, the academic term to avoid delays in accessing accommodations once classes begin. Once established, responsibility for disability-related accommodations and access is shared by Disability Resources, faculty, and the student.

Disability Resources: www.disability.wustl.edu; 314-935-5970

8.4 Statement on Military Service Leave

Washington University recognizes that students serving in the U.S. Armed Forces and their family members may encounter situations where military service forces them to withdraw from a course of study, sometimes with little notice. Students may contact the Office of Military and Veteran Services at (314) 935-2609 or veterans@wustl.edu and their academic dean for guidance and assistance. See: https://veterans.wustl.edu/policies/policy-for-military-students/.

8.5 Preferred Name and Personal Pronouns

Washington University in St. Louis recognizes that many students prefer to use names other than their legal ones to identify themselves. In addition, in order to affirm each person's gender identity and lived experiences, it is important that we ask and check in with others about pronouns. This simple effort can make a profound difference in a person's experience of safety, respect, and support. See: Pronouns Information and Preferred Name.

8.6 Emergency Preparedness

Before an emergency, familiarize yourself with the building(s) that you frequent. Know the layout, including exit locations, stairwells and the Emergency Assembly Point (EAP). Review the "Quick Guide for Emergencies" that is found near the door in many classrooms and main lobby areas of buildings for specific emergency information and instructions. For additional Information and EAP maps, visit https://emergency.wustl.edu/. To ensure that you receive emergency notifications, make sure your information and cell phone number is updated in SIS, and/or download the WashU Safe app and enable notifications.

To report an emergency:

Danforth Campus: (314) 935-5555

School of Medicine Campus: (314) 362-4357

North/West/South and Off Campus: 911 then (314) 935-5555

8.7 Academic Integrity

Effective learning, teaching and research all depend upon the ability of members of the academic community to trust one another and to trust the integrity of work that is submitted for academic credit or conducted in the wider arena of scholarly research. Such an atmosphere of mutual

trust fosters the free exchange of ideas and enables all members of the community to achieve their highest potential.

In all academic work, the ideas and contributions of others (including generative artificial intelligence) must be appropriately acknowledged and work that is presented as original must be, in fact, original. Faculty, students and administrative staff all share the responsibility of ensuring the honesty and fairness of the intellectual environment at Washington University in St. Louis.

For additional details on the university-wide Undergraduate Academic Integrity policy, please see: https://wustl.edu/about/compliance-policies/academic-policies/undergraduate-student-academic-integrity-policy/

For information specific to the College of Arts & Sciences please refer to the A&S Academic Integrity webpage.

Turnitin

In taking this course, students may be expected to submit papers and assignments through Turnitin for detection of potential plagiarism and other academic integrity concerns. If students do not have an account with Turnitin and/or do not utilize Turnitin when submitting their papers and assignments, the instructor may upload your paper or assignment to Turnitin for processing and review.

9 Resources for Students

9.1 Confidential Resources for Instances of Sexual Assault, Sex Discrimination, Sexual Harassment, Dating Violence, Domestic Violence, or Stalking

The University is committed to offering reasonable academic accommodations (e.g. a no-contact order, course changes) to students who are victims of relationship or sexual violence, regardless of whether they seek a formal investigation or criminal charges. If a student needs to explore options for medical care, other services, or reporting, or would like to receive individual counseling services, there are free, confidential support resources and professional counseling services available through the Relationship and Sexual Violence Prevention (RSVP) Center. If you need to request such accommodations, please contact RSVP to schedule an appointment with a confidential and licensed counselor. Although information shared with counselors is

confidential, requests for accommodations will be coordinated with the appropriate University administrators and faculty. The RSVP Center is located in Seigle Hall, Suite 435, and can be reached at rsvpcenter@wustl.edu or (314) 935-3445. For after-hours emergency response services, call the Sexual Assault and Rape Anonymous Helpline (SARAH) at (314) 935-8080 or call 314-935-6666 or (314) 935-5555 and ask to speak with an RSVP Counselor on call. See: RSVP Center.

9.2 Bias Reporting and Support System (BRSS)

The University has a process through which students, faculty, staff, and community members who have experienced or witnessed incidents of bias, prejudice, or discrimination against a student can report their experiences to the University's Bias Report and Support System (BRSS) team.

9.3 Counseling and Psychological Services

Counseling and Psychological Services' professional staff members work with students to resolve personal and interpersonal difficulties, many of which can affect a student's academic experience. These include conflicts with or worry about friends or family, concerns about eating or drinking patterns, and feelings of anxiety, depression, and thoughts of suicide. Individual, Conjoint, and Group therapy are all provided in addition to referrals for off-campus support. Information can be found on the Mental Health Services webpage.

The Division of Student Affairs also offers a telehealth program to students called TimelyCare. While students are encouraged to visit Counseling and Psychological Services during business hours, this additional service also provides after-hours access to medical care and 24/7 access to mental telehealth care across the United States, with no cost at the time of the visit. 12 counseling visits are provided at no charge as well as a limited number of psychiatry appointments. Students who pay the Health and Wellness fee are eligible for this service.

Additionally, see the mental health services offered through the RSVP Center listed above.

9.4 WashU Cares

WashU Cares specializes providing referrals and resources, both on, and off campus for mental health, medical health, financial and academic resources by using supportive case management. WashU Cares also receives reports on students who may need help connecting to resources or whom a campus partner is concerned about. If you are concerned about a student or yourself, you can file a report here: https://washucares.wustl.edu/.

9.5 The Writing Center

The Writing Center offers free writing support to all Washington University undergraduate and graduate students. Staff members will work with students on any kind of writing project, including essays, writing assignments, personal statements, theses, and dissertations. They can help at any stage of the process, including brainstorming, developing and clarifying an argument, organizing evidence, or improving style. Instead of simply editing or proofreading papers, the tutors will ask questions and have a conversation with the writer about their ideas and reasoning, allowing for a higher order revision of the work. They will also spend some time looking at sentence level patterns to teach students to edit their own work.

The Center is located in Mallinckrodt and open Sunday through Thursday from 11:00 am to 9:00 pm and Friday from 11:00 am to 5:00 pm. Students are seen primarily by appointment, with walk-ins accepted as the schedule allows. They also have dedicated walk-in hours for undergraduates on Tuesday and Wednesday afternoons. Both in-person and online appointments are available. To make an appointment, go to writingcenter.wustl.edu. Email: writing@wustl.edu.

9.6 The Learning Center

The Learning Center provides peer-led support programs, including course-specific mentoring and academic skills coaching (study and test-taking strategies, time management, etc.), that enhance undergraduate students' academic progress. Contact them at learningcenter@wustl.edu or visit ctl.wustl.edu/learningcenter to find out what support they may offer for your classes.

9.7 Center for Diversity and Inclusion (CDI)

The Center for Diversity and Inclusion (CDI) supports and advocates for undergraduate, graduate, and professional school students from underrepresented and/or marginalized populations, collaborates with campus and community partners, and promotes dialogue and social change to cultivate and foster a supportive campus climate for students of all backgrounds, cultures, and identities. Additional Diversity and Inclusion information can be found at https://diversityinclusion.wustl.edu/.

9.8 Gephardt Institute

Students play an essential role in a vibrant and functioning democracy! State and local elections take place throughout the year and have a direct impact on our communities. You can register to vote, request an absentee ballot, confirm your polling location, and get Election Day reminders at http://wustl.turbovote.org for any of the 50 states and Washington D.C. WashU

students are considered Missouri residents, and eligible student voters can register to vote in the state of Missouri or their home state.

If you are ineligible to vote, you can participate by encouraging your friends to register and vote, engaging your peers in local issues, and taking part in other civic and community engagement activities. For more resources on voting and other civic and community engagement opportunities, please visit http://washuvotes.wustl.edu and http://gephardtinstitute.wustl.edu.

9.9 University Libraries

University Libraries include seven unique locations across the Danforth Campus, but they are much more than just beautiful, quiet spaces for studying and group work. The Libraries include librarians for every discipline on campus, with the expertise to work with you to develop research ideas and find the best resources to meet your needs; or you are welcome to explore our research guides, tailored for each subject and available online. The Libraries hold five million items in the collection—print books, journals, electronic resources, databases, and millions more accessible through interlibrary loan—and you can find it all at the search on our home page. Additional resources for students include special collections, data services, citation help, digital publishing, and more. Visit the Libraries website for more details about these and other ways that the Libraries are here to support your academic success. Electronic resources listed on the Libraries' website and catalog are restricted to current students, staff, and faculty for the purposes of research, teaching, and private study. For more information, please visit https://libguides.wustl.edu/RERU

Chemistry Subject Librarian: Rhiannon Iha, (314) 935-4818, rkiha@wustl.edu

10 Additional Considerations

10.1 Religious Holidays & Class Absence Policies

As home to students, faculty, and staff of all the world's major religions and as a non-sectarian institution, Washington University in St. Louis values the rich diversity of spiritual expression and practice found on campus. It is therefore the policy of the university that students who miss class, assignments, or exams to observe a religious holiday should be accommodated as follows:

(i) absences should be counted as excused in any course in which attendance is a measure of academic performance;

(ii) reasonable extensions of time should be given, without academic penalty, for missed assignments;

(iii) exams should be reasonably rescheduled without academic penalty.

To ensure that accommodations may be made, students who plan to miss class for a religious holiday must inform their instructors in writing before the end of the third week of class, or as soon as possible if the holiday occurs during the first three weeks of the semester. Absence for religious reasons does not lessen students' responsibility for course work or material covered during their absence. It is incumbent on the student who misses a class to catch up on any material discussed and assignments given during that class period. If you believe you have not received a reasonable accommodation despite engaging with your instructor on the topic, please follow the course grievance process outlined by your school.

Every effort will be made to avoid scheduling exams on religious holidays, particularly those with work restrictions as noted on the holiday calendar. Where it is not possible to establish a teaching schedule that avoids conflict with the observance of religious holidays, the instructor will make up any missed class in the method most appropriate to student learning in their course; e.g., rescheduling for an alternate time, providing asynchronous material, or engaging a guest lecturer. Appropriate advance notice will be provided to students.

The complete Religious Holiday Class Absence Policy can be found here. The Office of Religious, Spiritual and Ethical Life maintains a calendar of many religious holidays observed by the WashU community.