

ASU Online CHM 343 - Fall 2022 Session-A

Elementary Physical Chemistry Laboratory

August 18, 2022

Overview: This molecular sciences laboratory course will cover topics in modern physical chemistry and biophysical chemistry. Emphasis is placed on molecular thermodynamics, kinetics, and spectroscopy, which parallels the topics covered in Elementary Physical Chemistry (ASU CHM 341) and Physical Chemistry with a Biological Focus (ASU BCH 341).

Virtual Recitations: Online Meetings (Zoom) and Recorded Material (YouTube / Vimeo)
'Cloud' Labs: Computational, Experimental and Data Science components will all be available through online/remote access.

Instructors: Professor: Jeffery L. Yarger, jeff.yarger@asu.edu
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Pchem Email: biopchem@gmail.com
Zoom: <https://asu.zoom.us/my/yarger>

Teaching Assistants: Banashree Gogoi, bgogoi2@asu.edu
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Cloud Lab R&D: Sean Seyler, sseyler@asu.edu
(computational, simulations, physics)
Samrat Amin, samrat.amin@asu.edu
(remote exp., automation, chemistry)

Office hours: Announced on ASU Canvas for TA's and Instructor
or by appointment. All office hours are virtual and will use Zoom.

Web Site: ASU Canvas: <https://canvas.asu.edu/> (2022FallA-X-CHM343)
<https://biopchem.education/> (Prof. Yarger's Open Public Website)

Prerequisites

Concurrent enrollment or completion of ASU CHM 341 (Elementary Physical Chemistry) or ASU BCH 341 (Physical Chemistry with a Biological Focus).

Required Material

- Modern desktop or laptop computer with webcam, audio/mic and good high-speed (> 5 Mbps) internet connection. HTML5 Web Browser (Chrome, Firefox), pdf Reader (Adobe Acrobat), VNC (i.e., AnyDesk, NoMachine), Zoom Video Conferencing, Office Suite (Microsoft, Libre) and analysis software that can be obtained from ASU myApps (<https://myapps.asu.edu>).
- All labs are designed to be performed remotely/online. However, if students are physically in laboratory, or doing optional DIY projects at home, a lab coat, safety goggles and closed toed shoes are required when handling any chemicals.

Recitation

ASU CHM 343 is a remote and/or online course. All recitation material will be online. Recitation will be used for general announcements, laboratory exercise overviews and information, and the general discussion of experimental, computational and data analysis physical chemistry concepts for each laboratory.

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Lab

Students will perform remote computational, experimental and data/error analysis laboratory lab projects. A remote accessibility laboratory experiment schedule will be provided on the official ASU-Online CHM343 Canvas website. Labs are designed to be asynchronous, remotely accessible, and can be independently performed or synchronized online/remote access groups can be organized to perform experiments.

Safety

All labs are online and/or remote. Hence, students will not have to worry about the typical safety concerns of a typical in-person chemical laboratory. However, if students perform any experiments in-person at a chemical laboratory or at their local residence, safety in chemistry labs is critical and lab coats, goggles and close-toed shoes are recommended. If students do attend an in-person laboratory at ASU, no food or drink are allowed in the chemistry laboratory and all. ASU laboratories require that people wear a lab coat, goggles and close-toed shoes.

Learning Outcomes

Upon successful completion of this course students will be able to collect, process, analyze, and disseminate experimental and computational (bio)chemical data. This course is meant to provide experimental and computational laboratory skills to compliment fundamental molecular science concepts taught in physical chemistry (ASU CHM341 and/or Biophysical chemistry courses, e.g., BCH341).

Course Evaluations & Grades

Student's progress and understanding in this online laboratory course will primarily be done through laboratory reports, peer review and active online laboratory participation. This is a letter graded course using the following scale: (100% - 90%) A; (<90% - 80%) B; (<80% - 70%) C; (<70% - 60%) D; (<60% - 0%) E.

To receive a grade in this class you must be registered on Canvas. All grades will be recorded in the ASU Canvas LMS system and each student can view his or her individual laboratory scores.

Laboratory Project Reports	300 pts (50%)
Laboratory Participation	150 pts (25%)
<u>Peer Review</u>	<u>150 pts (25%)</u>
TOTAL	600 pts (100%)

<u>Dates</u>	<u>Scheduled Project</u>
Aug 18-21	Syllabus Overview; Online Pchem Lab Introduction.
Aug 22-28	Project 1 – Properties of Gases – Molecular Thermodynamics (Remote Lab, Data/Error Analysis)
Aug 29-31	Project 1 – Properties of Gases – Molecular Thermodynamics (Reporting, Review, Revision)
Sept 6-11	Project 2 – Thermochemical Processes (Computational, Experimental, Data/Error Analysis)
Sept 12-18	Project 2 – Thermochemical Processes (Reporting, Review, Revision)
Sept 19-25	Project 3 – Chemical Equilibrium & Kinetics (Computational, Experimental, Data/Error Analysis)
Sept 26-30	Project 3 – Chemical Equilibrium & Kinetics (Reporting, Review, Revision)
Oct-1-6	Project X – Argonne APS XRD, Student Independent Research Project and/or Makeup Lab(s)
**	Project X – Substitute Projects Available to Students Aug 22 – Oct 6 (email jeff.yarger@asu.edu)

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Due Date	Project Report #	Due Date	Peer Review
08/30	Project-1 Report	08/31	Project-1 Anonymous Peer Reviews
09/02	Project-1 Report Revised	09/06	Project-1 Revised Report Peer Reviews
09/13	Project-2 Report	09/14	Project-2 Anonymous Peer Reviews
09/16	Project-2 Report Revisions	09/19	Project-2 Revised Report Peer Reviews
09/27	Project-3 Report	09/28	Project-3 Anonymous Peer Reviews
09/29	Project-3 Report Revisions	09/30	Project-3 Revised Report Peer Reviews
10/01 – 10/06	Project-X and/or Makeup Lab Report(s) – Instructor Reviewed and Evaluated.		

Potential Alternative ASU 'Cloud' (Remote / Online) and/or Computational Physical Chemistry Projects

Students can substitute one of the three projects with a proposed remote experimental physical chemistry laboratory and/or computational chemistry exercise. If a student wants to propose a project X, they need to submit a 1-page outline proposal by Sept. 16th (and have it approved by Sept. 23th). Examples of past proposed projects include:

- Project X₁ –Molecular Understanding of Analyte Diffusion in Water using Remote NMR Measurements and Molecular Dynamics Computational Resources.
- Project X₂ – Using Electronic Structure Computational Methods to understand the molecular mechanism and Substituent Effect of Keto-Enol Tautomerism.
- Project X₃ – Molecular Structure and Dynamics of a cyclic peptide - Gramacidin-S.
- Project X₄ – Optical Diffraction using a Remote Laser Optical Setup.

Laboratory Project Reports

To evaluate student's ability to perform computational and/or remote 'experiments', process and analyze associated data, perform error analysis, and put the associated results into context of fundamental molecular physical chemistry concepts, students will be asked to provide a 'report'. This report can be a presentation ([ppt](#), [slides](#)), notebook ([mathematica](#), [jupyter](#), [colab](#)), web blog/dashboard ([kaggle](#)), [poster](#), [memos](#), screencast (video podcast), or written laboratory report. Students are encouraged to collaborate and work in teams or groups for all aspects of computational, experimental, data/error analysis and reporting. To properly acknowledge team or group components, there should be an explicit authorship section with all group members included and an authors' contributions section that specifies the exact contributions of each author in a narrative form. Students should not default to sentences such as 'all authors contributed equally to this report'. It is expected that details of each student's exact contribution are explicitly discussed.

Written lab reports are a traditional way to summarize and convey the results from laboratory or computational experiments in chemistry, biochemistry and physics (biopchem). Report deadlines are given above for each lab project and reports submitted after the due date will not be included in the anonymous peer review process. Instead, late lab reports will have to be evaluated by a teaching assistant or instructor separate from the peer review evaluation process. There is a 5-figure/table and a 5-page limit on all reports (supplemental information does NOT have a page or table/figure limit). Students will be expected to turn in a single electronic file (pdf file) of each lab report. An additional supplemental section is allowed for additional figures and showing detailed calculations for statistical and error analysis (e.g., propagation of error). Lab reports should be in the style and format of a scientific publication (e.g., American Chemical Society (ACS) - *Journal of Physical Chemistry*, *Journal of Chemical Education*).

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Written Lab Report Format (Rubric, 100 pts):

Student lab reports will be modeled after a standard scientific manuscript or journal article. All reports must be electronically generated and submitted. It is recommended that reports follow the standard double column format with embedded figures and tables, as found in a typical ACS scientific journal article. The general report rubric (point distribution) is provided below:

- **Title/Authorship** – The title and authorship should be descriptive and should contain keywords that will allow others to search for your report. Authorship should include your full name, university, department/school, email address and any co-authors, if relevant. (5 pts)
- **Abstract** – This should briefly and clearly describe the purpose of the experiment, the principle results and the major conclusions. The principle results are typically numerical values with the associated errors. (5 pts)
- **Introduction** – The introduction should state the object and provide a concise summary of the relevant background information with appropriate citations. Because most of the labs/projects are well-researched and well-documented, the focus should be to provide the most relevant citations to books, reviews and journal articles that best cover the background material, with only very brief written descriptions (i.e., typically 2-3 paragraphs with 10-20 citations). (5 pts)
- **Materials & Methods** – A description of the chemicals, procedures and equipment used during the investigation. From this section, someone should be able to reproduce the experiments you performed in lab and/or using computational resources. Therefore, the simple evaluation of this section is ‘can you reproduce the computational, experimental and data science (data and error analysis) components performed by the author?’ (10 pts)
- **Results & Discussion (Figures)** – Present the results of the experiments, computation and/or simulations using tables and figures to illustrate all critical components of the project (25 pts, ~5 figures/tables at 5 pts ea). Include detailed figure captions for all tables and figures used in your report (10 pts, ~5 figure/table captions at 2 pts ea). The figures and figure captions should visually ‘storyboard’ the entire report. Discuss the results and compare with your expectations and other known literature results (5 pts). An analysis and discussion of error for the experiment should be included in this section (10 pts), however, often detailed examples of the error analysis statistics and calculations are provided as a supplemental section. All detailed calculations for the data analysis can be put into a supplemental section (10 pts). (60 pts Total)
- **Conclusion** – Briefly summarize your results and interpretation. (5 pts)
- **Acknowledgements** - Acknowledge people who have helped in some way in the preparation of the written report or helped with the computational, experimental or data science components of data collection and/or analysis (for example if data was collected by a group/team). (5 pts)
- **References** – List citations in a corresponding order to their appearance in the text of your lab report. References need to be provided so that someone reading the report could look up all the references and have adequate background material and information. (5 pts)
- **Supplemental Information** – Supplemental information has become a critical component to reporting scientific data and results. Modern digital scientific reporting allows for a more complete set of data, computations, analysis, calculations, analysis, etc to be explicitly shown and reported. This section is commonly overlooked and not emphasized. However, if all associated components are included a supplemental information section can be the most detailed and important component in a scientific report. To emphasize this reporting component, an extra 50 pts will be awarded to reports that provide a complete set of supplemental information for the computational, experimental and data/error analysis. (150 pts total)

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Peer Review

The peer review system exists to validate scientific work and is a widely used tool for scientific communication and evaluation. Single anonymized peer review is the default method. However, double anonymized review is possible upon preparation and request. Using the rubric, peer reviews will be asked to provide both detailed comments as well as peer grading using the point distribution provided in the general lab report rubric. Several points to consider when providing an assessment of a report or presentation:

- Are key results summarized?
- Validity: Does the report have significant flaws? If so, please provide details.
- Data & Methodology: Please comment on the validity of the computational and experimental approach, quality of the data and quality of presentation (figures, plots, visualizations). Please review all data, including any extended data and supplementary information. Is the reporting of data and methodology sufficiently detailed and transparent to enable reproducing the results?
- Appropriate use of statistics and treatment of uncertainties: All error bars should be defined and statistical analyzes explained.
- Conclusions: Do you find that the conclusions and data interpretation are robust, valid and reliable?
- Suggested improvements: Please list additional experimental, computational or data analysis that could help strengthening the work in a revision.
- References: Does the report reference previous literature appropriately? If not, what references should be included or excluded?
- Clarity and context: Is the abstract clear, accessible? Are abstract, introduction and conclusions appropriate?

As part of the peer review of reports, please provide a suggested 'score' or 'points' for each section based on the general lab report rubric. At the end, please provide the overall suggested score/points and a summary of suggestion priorities for a report revision, if applicable. The instructor or teaching assistant will serve the role of editor and will evaluate each student's peer review comments and assessment. The primary criteria for students to receive full peer evaluation points (50 pts per project peer evaluation) is accurate review of the data and methodology. Peer review is one of the most utilized methods scientists use to validate experimental and computational results before public reporting. A good peer reviewer will catch any mistakes in data analysis, computation, calculations and hence prevent incorrect reporting of scientific data and associated analysis.

Laboratory Participation

A critical component to labs is peer-to-peer and peer-instructor interactions and communication. Labs are best when scientific interactions and collaborations are fostered. This online laboratory course will be using YellowDig for fostering questions, collaborations, polling and both peer-to-peer and student-instructor interactions. YellowDig is an active learning community platform designed for virtual classes to foster and reward student engagement. Points are provided in Yellowdig for student engagement and details can be found on the online CHM343 YellowDig site. To emphasize just how important group and peer-to-peer interactions and communication is in laboratory sciences, 25% of students grade will be based on active weekly participation.

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General ASU Policies

Attendance and Participation

Attendance and participation in class activities is an essential part of the learning process, and students are expected to attend class regularly. Some absences are, however, unavoidable. Excused absences for classes will be given without penalty to the grade in the case of (1) a university-sanctioned event [ACD 304-02]; (2) religious holidays [ACD 304-04; a list can be found here <https://eoss.asu.edu/cora/holidays>]; (3) work performed in the line-of-duty according [SSM 201-18]; and (4) illness, quarantine or self-isolation related to illness as documented by a health professional.

Anticipated absences for university-sanctioned events, religious holidays, or line-of-duty activity should be communicated to the instructor by email at least 1 day before the expected absence.

Absences for illness, quarantine or self-isolation related to illness should be documented by a health professional and communicated to the instructor as soon as possible by email.

Excused absences do not relieve students from responsibility for any part of the course work required during the period of absence. Faculty will provide accommodations that may include participation in classes remotely, access to recordings of class activities, and make-up work.

If there is a disagreement as to whether an absence should be accommodated, the instructor and student should contact the academic unit chair immediately for resolution.

Grade Appeals

Grade disputes must first be addressed by discussing the situation with the instructor. If the dispute is not resolved with the instructor, the student may appeal to the department chair per the University Policy for Student Appeal Procedures on Grades.

Student Conduct and Academic Integrity

Academic honesty is expected of all students in all examinations, papers, laboratory work, academic transactions and records. The possible sanctions include, but are not limited to, appropriate grade penalties, course failure (indicated on the transcript as a grade of E), course failure due to academic dishonesty (indicated on the transcript as a grade of XE), loss of registration privileges, disqualification and dismissal. For more information, see <http://provost.asu.edu/academicintegrity>. Additionally, required behavior standards are listed in the Student Code of Conduct and Student Disciplinary Procedures, Computer, Internet, and Electronic Communications policy, and outlined by the Office of Student Rights & Responsibilities. Anyone in violation of these policies is subject to sanctions. Students are entitled to receive instruction free from interference by other members of the class. An instructor may withdraw a student from the course when the student's behavior disrupts the educational process per Instructor Withdrawal of a Student for Disruptive Classroom Behavior. The Office of Student Rights and Responsibilities accepts incident reports from students, faculty, staff, or other persons who believe that a student or a student organization may have violated the Student Code of Conduct.

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Prohibition of Commercial Note Taking Services

In accordance with ACD 304-06 Commercial Note Taking Services, written permission must be secured from the official instructor of the class in order to sell the instructor's oral communication in the form of notes. Notes must have the notetaker's name as well as the instructor's name, the course number, and the date.

Accessibility Statement

In compliance with the Rehabilitation Act of 1973, Section 504, and the Americans with Disabilities Act as amended (ADAAA) of 2008, professional disability specialists and support staff at the Student Accessibility and Inclusive Learning Services (SAILS) center facilitate a comprehensive range of academic support services and accommodations for qualified students with disabilities.

Qualified students with disabilities may be eligible to receive academic support services and accommodations. Eligibility is based on qualifying disability documentation and assessment of individual need. Students who believe they have a current and essential need for disability accommodations are responsible for requesting accommodations and providing qualifying documentation to the SAILS. Every effort is made to provide reasonable accommodations for qualified students with disabilities.

Qualified students who wish to request an accommodation for a disability should contact SAILS by going to <https://eoss.asu.edu/accessibility>, calling (480) 965-1234 or emailing Student.Accessibility@asu.edu. To speak with a specific office, please use the following information:

ASU Online and Downtown Phoenix Campus
University Center Building, Suite 160
602-496-4321 (Voice)

Polytechnic Campus
480-727-1165 (Voice)

West Campus
University Center Building (UCB), Room 130
602-543-8145 (Voice)

Tempe Campus
480-965-1234 (Voice)

Disability Resources

As discussed above, students who feel they will need disability accommodations in this class but have not registered with the Student Accessibility and Inclusive Learning Services (SAILS) should contact them immediately. For additional information, contact SAILS by going to <https://eoss.asu.edu/accessibility>, calling (480) 965-1234 or emailing Student.Accessibility@asu.edu.

Title IX

Title IX is a federal law that provides that no person be excluded on the basis of sex from participation in, be denied benefits of, or be subjected to discrimination under any education program or activity. Both Title IX and university policy make clear that sexual violence and harassment based on sex is prohibited. An individual who believes they have been subjected to sexual violence or harassed on the basis of sex can seek support, including counseling and academic support, from the university. If you or someone you know has been harassed on the basis of sex or sexually assaulted, you can find information and resources at <https://sexualviolenceprevention.asu.edu/faqs>.

As mandated reporters, course instructors (including TAs) are obligated to report any information they become aware of regarding alleged acts of sexual discrimination, including sexual violence and dating violence. ASU Counseling Services, <https://eoss.asu.edu/counseling>, is available if you wish discuss any concerns

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confidentially and privately. ASU online students may access 360 Life Services, <https://goto.asuonline.asu.edu/success/online-resources.html>.

Academic Integrity

Academic honesty is expected of all students in all examinations, papers, and laboratory work, academic transactions and records. The possible sanctions include, but are not limited to, appropriate grade penalties, course failure (indicated on the transcript as a grade of E), course failure due to academic dishonesty (indicated on the transcript as a grade of XE), loss of registration privileges, disqualification and dismissal. For more information, see <http://provost.asu.edu/academicintegrity>

Policy Against Threatening Behavior

All incidents and allegations of violent or threatening conduct by an ASU student (whether on-or off campus) must be reported to the ASU Police Department (ASU PD) and the Office of the Dean of Students. If either office determines that the behavior poses or has posed a serious threat to personal safety or to the welfare of the campus, the student will not be permitted to return to campus or reside in any ASU residence hall until an appropriate threat assessment has been completed and, if necessary, conditions for return are imposed. ASU PD, the Office of the Dean of Students, and other appropriate offices will coordinate the assessment in light of the relevant circumstances. For more information, please visit and <https://eoss.asu.edu/dos/safety/ThreateningBehavior>.

Policy on Sexual Discrimination

Arizona State University is committed to providing an environment free of discrimination, harassment, or retaliation for the entire university community, including all students, faculty members, staff employees, and guests. ASU expressly prohibits discrimination, harassment, and retaliation by employees, students, contractors, or agents of the university based on any protected status: race, color, religion, sex, national origin, age, disability, veteran status, sexual orientation, gender identity, and genetic information. As a mandated reporter, the instructor and TAs are obligated to report any information we become aware of regarding alleged acts of sexual discrimination, including sexual violence and dating violence. ASU Counseling Services, <https://eoss.asu.edu/counseling>, is available if you wish to discuss any concerns confidentially and privately.

Copyrighted Materials

Students must refrain from uploading to any course shell, discussion board, or website used by the course instructor or other course forum, material that is not the student's original work, unless the students first comply with all applicable copyright laws; faculty members reserve the right to delete materials on the grounds of suspected copyright infringement.

Syllabus Disclaimer

The syllabus is a statement of intent and serves as an implicit agreement between the instructor and the student. Every effort will be made to avoid changing the course schedule, but the possibility exists that unforeseen events will make syllabus changes necessary. Please remember to check your ASU email and the course site often.