# CHEM 4521 – Biophysical Chemistry
# Spring 2025
# Course Syllabus

## COURSE MEETING TIME/PLACE

Time: Monday / Wednesday / Friday (MWF) 11:00 am to 11:50 am
Place: Skiles Classroom Building, Room 371
686 Cherry St NW, Atlanta, GA 30332
Dates: Jan 6, 2025 – April 22nd, 2025

## COURSE DESCRIPTION

This is a one-semester course in biophysical chemistry where you will develop knowledge of the theory and application of state-of-the-art techniques that integrate physical chemistry, biophysics, and biochemistry to study macromolecules. When you have completed the course, you should be able to design and interpret experiments for studying biologically interesting problems and applying biophysical concepts to understand how these molecules work. You will earn 3.0 credits from successful completion of this course. Learning objectives will be outlined at the start of each lecture. Lecture slides will be provided for each class (ideally before the lecture so you can take notes as needed).

Biophysical chemistry can be overwhelming since it applies fundamental concepts from several disciplines (chemistry, biochemistry, physics, math). Don't panic! Come to lectures, take notes, study often, complete "practical" assignments, and use supplemental learning sources. You might need to investigate different ways of studying (*i.e.,* flash cards). We are always available to help you and we will provide resources to help you succeed. Make friends and study in groups when possible. We aim to make learning biophysical chemistry interesting, practical, and fun to help hold your attention in the material.

## PREREQUISITES

It is *required* that you have taken college-level Biochemistry I (CHEM 4511) and Physical Chemistry I (CHEM 3411) courses. We will do our best to provide refreshers and summary material related to these subjects, such that everyone is on the same page for learning biophysical biochemistry. However, it impossible to review all required material. If you have concerns about your past experiences or past courses taken in relation to Biochemistry, please talk to us.

## INSTRUCTOR

Andrew McShan, Ph.D.
Pronouns: They/them
Assistant Professor
School of Chemistry and Biochemistry
E-mail: andrew.mcshan@chemistry.gatech.edu
Website: http://mcshanlab.com/
Office Location: Molecular Sciences and Engineering Building (MoSE) G022
901 Atlantic Dr NW, Atlanta, GA 30318
*My office is located on the ground floor of MoSE next to the big lecture hall*
Office Hours: Wednesday 12 pm – 1 pm in MoSE G022
Meetings can be scheduled at different times upon e-mail request.
Virtual meetings may also be scheduled through Zoom upon e-mail request.

How to contact Dr. McShan:
*Recommended contact via e-mail. I try to respond to e-mails within 24 hours of receipt but please be patient with me.*

*When sending an e-mail message, please use the following format in the subject line:*

*CHEM 4521 – Your Name – Subject*

Non-conforming e-mails are likely to be lost in my mailbox and may not receive a reply.

## Teaching Assistants (TAs)

N/A

**COURSE MATERIALS**

- Textbooks:

You will not need to purchase a textbook for this course. We will provide all material needed. However, a textbook might be a helpful supplement for you in which case we recommend:

Biophysical Chemistry ← **this is provided for free on Canvas**
James Allen
ISBN-13 978-1405124362
https://www.amazon.com/Biophysical-Chemistry-James-P-Allen/dp/1405124369

Biophysical Chemistry
Dagmar Klostermeier, Markus G. Rudolph
ISBN-13 978-1482252231
https://www.amazon.com/Biophysical-Chemistry-Dagmar-Klostermeier/dp/1482252236

Physical Chemistry: Principles and Applications in Biological Sciences
Ignacio Tinoco, Kenneth Sauer, James Wang, Joseph Puglisi, Gerard Harbison, David Rovnyak
ISBN-13 978-0136056065
https://www.amazon.com/Physical-Chemistry-Principles-Applications-Biological/dp/0136056067

The Molecules of Life
John Kuriyan, Boyana Konforti, David Wemmer
ISBN-13 978-0815341888
https://www.amazon.com/Molecules-Life-Physical-Chemical-Principles/dp/0815341881

- Required Software:

PyMOL (free educational edition)
https://www.pymol.org/

NMRBox (free account)
https://nmrbox.nmrhub.org/pages/getting-started

Real VNC Viewer (free, no account needed)
https://www.realvnc.com/en/connect/download/viewer/

+ other free webservers mentioned in the practical assignments.

**CANVAS PAGE (COURSE WEBSITE)**
Canvas will include lecture slides, practical assignments, readings, and relevant course updates. Check often!

**FINAL GRADES**
A = 100 - 90%
B = 89.9 - 80%
C = 79.9 - 70%
D = 69.9 - 50%
F = < 50%

Assignments and final grades *will not* be curved.

**EVALUATION CRITERIA**

| Item | Total Number of Points * 100 | Percent of Final Grade (100%) |
|---|---|---|
| Attendance | 42/42 | 35% |
| Practical Assignments | 1200/1200 | 40% |
| Final Exam | 100/100 | 25% |

**I. Attendance – 42/42 points, 35% of final grade**
Lecture attendance is required for this course and will count towards your final grade. Each attended lecture is worth 1 point for a total of 42 points throughout the semester. Attendance will contribute to the final grade with the formula: 42/42 * 100 * 0.35. If you cannot attend class for any reason (for example, illness, conference, research related meeting, etc.), please e-mail Dr. McShan for an excused absence *before* that class. Each student will be allowed two excused absences.

**II. Practical Lab – 1200/1200 points, 40% of final grade**
There will be twelve (12) practical assignments given throughout the semester. You will work in pairs (assigned by Dr. McShan). The purpose of the practical assignments is to work with, analyze, and interpret real world data that you would see in a biophysical chemistry research lab. Practical assignments will include a hands-on activity or worksheet to be completed using freely available software. Detailed descriptions of each practical lab assignments will be uploaded to Canvas, and you will receive guidance in class (and outside of class in office hours, if desired). You will submit completed practical assignment via Canvas. Each practical lab is worth 100 points each for a total of 1200 throughout the semester. Practical assignments will contribute to the final grade with the formula: 1200/1200 * 100 * 0.40. Due dates will be noted on Canvas. Practical assignments will not be accepted late.

**II. Exams – 100/100 points, 25% of final grade**
There will be no exams except for the final exam, which will be given on Wednesday, Apr 30 11:20 AM - 2:10 PM (decided by GaTech's final exam matrix). The final exam will be a mix of multiple-choice questions and short answers that include questions on the biophysical chemistry concepts and techniques learned during the semester. It is worth 100 points. The final exam will contribute to the final grade with the formula: 100/100 * 100 * 0.25.

**COURSE OUTLINE**

| Lecture | Date(s) | Topic(s) | Thing(s) to do (Due dates on Canvas) |
|---|---|---|---|
| **Part I – Introduction** | | | |
| 1 | Jan 6 | Introduction to Biophysical Chemistry | - |
| 2 | Jan 8 | Molecular Interactions | Read: Freitas et al. Medchemcomm. 2017 Sep 26;8(10):1970–1981 |
| 3 | Jan 10 | Molecular Interactions | - |
| 4 | Jan 13 | Biomolecular Structure | Read: Allen, Biophysical Chemistry, Chapter 12, pg 277-289 |
| 5 | Jan 15 | Biomolecular Structure | - |
| 6 | Jan 17 | PyMOL Tutorial | - |
| - | Jan 20 | No Class - Holiday | - |
| **Part II – Computational Methods** | | | |
| 7 | Jan 22 | Forcefields: Rosetta | Read: Alford et al. J Chem Theory Comput. 2017;13(6):3031–3048 |
| 8 | Jan 24 | Practical #1: Forcefields: Rosetta | - |
| 9 | Jan 27 | Structure Prediction: AlphaFold | Read: Abramson et al. Nature. 2024;630(8016):493-500 |
| 10 | Jan 29 | Practical #2: Structure Prediction: AlphaFold | - |
| 11 | Jan 31 | Practical #2: Structure Prediction: AlphaFold | - |
| 12 | Feb 3 | Molecular Docking | Read: Paggi et al. Annu Rev Biochem. 2024;93(1):389-410 |
| 13 | Feb 5 | Practical #3: Molecular Docking | - |
| 14 | Feb 7 | Practical #3: Molecular Docking | - |
| 15 | Feb 10 | Molecular Dynamic Simulations | Read: Rizzuti. Biochim Biophys Acta Proteins Proteom. 2022 Mar 1;1870(3):140757. |
| 16 | Feb 12 | Practical #4: Molecular Dynamic Simulations | - |

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| 17 | Feb 14 | Practical #4:<br>Molecular Dynamic Simulations | - |
| **Part III – Biomolecular Structure** | | | |
| 18 | Feb 17 | Circular Dichroism | Read:<br>Kelly et al. Biochim Biophys Acta. 2005 Aug 10;1751(2):119-39 |
| 19 | Feb 19 | Practical #5:<br>Circular Dichroism | - |
| 20 | Feb 21 | Practical #5:<br>Circular Dichroism | - |
| 21 | Feb 24 | X-ray crystallography | Read:<br>McPherson et al. Acta Crystallogr F Struct Biol Commun. 2013 Dec 24;70(Pt 1):2–20 |
| 22 | Feb 26 | Practical #6:<br>X-ray crystallography | Mid-Course Reflection Survey (Canvas) |
| 23 | Feb 28 | Practical #6:<br>X-ray crystallography | - |
| 24 | Mar 3 | Solution NMR | Read:<br>Marion. Mol Cell Proteomics. 2013 Jul 6;12(11):3006–3025 |
| 25 | Mar 5 | Practical #7:<br>Solution NMR | - |
| 26 | Mar 7 | Practical #7:<br>Solution NMR | - |
| 27 | Mar 10 | Small-Angle X-ray Scattering | Read:<br>Vela et al. Curr Res Struct Biol. 2020 Aug 27:2:164-170 |
| 28 | Mar 12 | Practical #8:<br>Small-Angle X-ray Scattering | - |
| 29 | Mar 14 | Practical #8:<br>Small-Angle X-ray Scattering | - |
| - | Mar 17 | No Class - Holiday | - |
| - | Mar 19 | No Class - Holiday | - |
| - | Mar 21 | No Class - Holiday | - |
| **Part IV – Thermodynamics** | | | |
| 30 | Mar 24 | Isothermal Titration Calorimetry | Read:<br>Bastos et al. Isothermal titration calorimetry. Nat Rev Methods Primers 3, 17 (2023) |
| 31 | Mar 26 | Practical #9:<br>Isothermal Titration Calorimetry | - |
| 32 | Mar 28 | Practical #9:<br>Isothermal Titration Calorimetry | - |
| 33 | Mar 31 | Nano Differential Scanning Fluorimetry | Read:<br>Gao et al. Biophys Rev. 2020 Feb;12(1):85-104 |
| 34 | Apr 2 | Practical #10:<br>Nano Differential Scanning Fluorimetry | - |
| 35 | Apr 4 | Practical #10:<br>Nano Differential Scanning Fluorimetry | - |
| **Part V – Biomolecular Interactions and Kinetics** | | | |
| 36 | Apr 7 | MicroScale Thermophoresis | Read:<br>Jerabek-Willemsen et al. Journal of Molecular Structure 1077 (2014) 101–113 |
| 37 | Apr 9 | Practical #11:<br>MicroScale Thermophoresis | - |
| 38 | Apr 11 | Practical #11:<br>MicroScale Thermophoresis | - |
| 39 | Apr 14 | Surface Plasmon Resonance | Read:<br>Capelli et al. Trends in Analytical Chemistry 163 (2023) 117079 |
| 40 | Apr 16 | Practical #12:<br>Surface Plasmon Resonance | - |

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|---|---|---|---|
| 41 | Apr 18 | Practical #12:<br>Surface Plasmon Resonance | - |
| 42 | Apr 21 | Final Exam Prep | - |
| - | Apr 30 | Final Exam | Wednesday, Apr 30 11:20 AM - 2:10 PM |

**STATEMENT OF INTENT FOR DIVERSITY, EQUITY, AND INCLUSIVITY**

I am committed to creating a learning environment for students that supports a diversity of thoughts, perspectives and experiences that honors your cultural and social identities (including race, gender, class, sexuality, religion, or ability).

To help accomplish this:

- If you have a name and/or set of pronouns that differ from those that appear in your official Georgia Tech records, please let me know. If I pronounce your name wrong, please correct me (I want to do better).
- If you feel like your performance in the class is being impacted by your experiences outside of class, please don't hesitate to talk to me (if you feel comfortable doing so). I will do my best to point you in the direction to get help.
- If something was said by anyone in class (including me) that made you feel uncomfortable, please feel free to bring it up. Anonymous feedback is always an option (see: https://www.gatech.edu/accountability).

Finally, in an ideal world, science would be objective and inclusive. However, much of science is subjective and is historically built on a small subset of privileged voices. I acknowledge that the readings and content for this course were primarily authored in the main by cisgendered white men.

**ACADEMIC INTEGRITY**

All course content is subject to the Georgia Institute of Technology's academic honor code: https://policylibrary.gatech.edu/student-affairs/academic-honor-code. Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. Any student suspected of cheating or plagiarizing an assignment or exam will be reported to the Office of Student Integrity, who will investigate the incident and identify the appropriate penalty for violations.

*The use of AI-powered language models (i.e., ChatGPT or related) is strictly prohibited in this course.*

**ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES**

If you are a student with disabilities that needs that require special accommodation, please contact me to discuss your needs. Also, contact the Office of Disability Services at (404) 894-2563 or http://disabilityservices.gatech.edu/, as soon as possible, to make an appointment to discuss your needs and to obtain an accommodation letter.

**CAMPUS RESOURCES FOR LEARNING**

In your time at Georgia Tech, you may find yourself in need of support academic or emotional support. I am always available to you. However, a summary of additional resources for Georgia Tech students is available at https://catalog.gatech.edu/academics/academic-resources/ and https://grad.gatech.edu/resources.

**CAMPUS RESOURCES FOR MENTAL HEALTH**

The Center for Mental Health Care & Resources (https://mentalhealth.gatech.edu/) is here to offer confidential support and services to students in need of mental health care. During regular business hours, students who are not actively in counseling may **call 404-894-2575** or **walk-in to the office** located on the first floor, Suite 102B Smithgall Student Services Building, 353 Ferst DR NW Atlanta GA 30313 (Flag building next to the Student Center). Any time outside of business hours, students may **call 404-894-2575** and select the option to speak to the after-hours counselor.