University of North Texas

CHEM 3520 – Physical Chemistry II – Spring 2022

Instructor

- Dr. Omar Valsson
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Schedule

- Lecture: 10:00 – 10:50 am, Mon/Wed/Fri in Chemistry Building, Room 352
- Recitation (optional): 2:00 – 2:50 pm, Wed in Business Leadership Building, Room 090
- Both will be given by the instructor, Dr. Omar Valsson

All information given below is subject to change at the discretion of the instructor. All changes will be communicated to students via Canvas or email.

Office Hours

- Mondays, 1:00 – 2:30 pm, or by appointment
- In-person at my office (Chem 205C)
- Or virtually via Zoom:
  - [Meeting and link available in Canvas version]
- A heads-up message if you are planning to come by would be appreciated

Course description and goals

Physical Chemistry II is part of a two-course sequence designed to provide students with the fundamental understanding of fundamental understanding of the principles underlying the behavior of chemical systems. In this course, we will explore the basics of quantum mechanics and spectroscopy. Quantum mechanics provides a mathematical description of the behavior and interactions of very small particles that are not correctly described by classical mechanics.

We will have a detailed discussion of the theoretical fundamentals and chemical applications of quantum mechanics. We will discuss how quantum mechanics determines atomic and molecular structure and spectroscopic transitions in microwave, infrared, electronic, photoelectron, electron spin and NMR.

Familiarity with Calculus I, II and Multivariable Calculus, as well as Mechanics and Electromagnetism will be necessary.
At the conclusion of the course, you will be able to:

- Understand the development and necessity of quantum mechanics
- Define and describe the postulates of quantum mechanics
- Explain atomic/molecular structure and spectroscopy in terms of quantum mechanics.
- Deduce molecular structure from spectroscopic data.

Prerequisite

CHEM 3510 (one of whose prerequisites is two semesters of calculus).

Readings and Material

- Recommend text: *Physical Chemistry*, by Atkins and de Paula (any edition will work, but Chapter references will be based on 11th edition and 10th edition).
- Various online references cover the same material and are useful:
  - Sections 1 to 15 in *Physical Chemistry LibreText*
  - *MIT OCW Physical Chemistry*
- Videos at the TMPchem Channel on YouTube covering the material are very useful and highly recommended – [https://www.youtube.com/user/TMPchem](https://www.youtube.com/user/TMPchem)
- Mathematical background: *Mathematical Methods for Molecular Science*, by Straub (available online [here](https://www.youtube.com/user/TMPchem)) is a good reference for the mathematical background needed.
- Other reading material and handouts, including journal articles, will be made available on Canvas.
- All lecture slides and notes from my lectures will be made available on Canvas.

Course Outline

The schedule of topics listed below is an estimate. Inevitably the pace of the lectures will adjust to the realities of the classroom and we might not cover some of the material.

To make the best usage of the lectures, you should read the relevant readings before each lecture. Throughout the semester, I will inform via Canvas what material will be covered in each lecture beforehand. The readings in Atkins’ *Physical Chemistry* are given below, and I will point to the relevant sections in the online material in the announcements.

Readings in Atkins’ *Physical Chemistry* given in parentheses for 11th / 10th edition

- Introduction, Motivation for Quantum Mechanics (7A / 7A)
- Mathematical background (complex numbers, differential equations, …)
- Introduction to QM (7B-7C / 7B-7C)
- Mathematics for QM and Fundamental Concepts (7B-7C / 7B-7C)
- QM Theory of Motion – Translation (7D / 8A)
- QM Theory of Motion – Vibration (7E / 8B)
- QM Theory of Motion – Rotation (7F / 8C)
- Atomic Structure and Spectra – The H atom (8A / 9A)
- Atomic Structure and Spectra – Many-Electron Atoms (8B / 9B)
• Atomic Structure and Spectra – Atomic Spectra (8C / 9C)
• Molecular Structure – Valence-Bond Theory (9A / 10A)
• Molecular Structure – Molecular Orbital Theory (9B / 10B)
• Molecular Structure – Diatomic Molecules (9C-9D / 10C-10D)
• Molecular Structure – Polyatomic Molecules (9E / 10E)
• Molecular Symmetry (10A-10C / 11A-11C)
• Molecular Spectroscopy – General (11A / 12A)
• Molecular Spectroscopy – Rotational (11B / 12B-12C)
• Molecular Spectroscopy – Vibrational (11C-11E / 12D-12E)
• Molecular Spectroscopy – Electronic Spectra (11F-11G / 13A-13C)
• Magnetic Resonance – General (12A / 14A)
• Magnetic Resonance – NMR Spectra (12B / 14B)
• Magnetic Resonance – Pulse Techniques in NMR (12C / 14C)
• Magnetic Resonance – Electron Paramagnetic Resonance (12D / 14D)

Class Policy
• Connect with me through email and/or by attending office hours. During busy times, my inbox becomes rather full, so if you contact me and do not receive a response within two business days, please send a follow up email. A gentle nudge is always appreciated.
• Research has shown that students who attend class are more likely to be successful. Therefore, attendance to the lectures is, in principle, mandatory and you should attend every class. You will get a part of your grade for attendance of lectures. Acceptable exceptions will be approved on a case-by-case basis. Acceptable university excused absence include active military service, a religious holy day, or an official university function as stated in the Student Attendance and Authorized Absences Policy (PDF). If you cannot attend a class due to an emergency, please let me know. Your safety and well-being are important to me.
• It is important for all of us to be mindful of the health and safety of everyone in our community, especially given concerns about COVID-19. Please contact the instructor if you are unable to attend class because you are ill, or unable to attend class due to a related issue regarding COVID-19. Acceptable exceptions will be approved on a case-by-case basis.
• To be officially excused from attending class for COVID-related reasons, you must receive approval from the Dean of Students or emailed instructions from the UNT Contract Tracing Team, and you must forward these to the instructor. In this case, I will work with you to provide an alternate means of content delivery.
• I encourage everyone to wear a mask in class to reduce the risk of COVID infections. I will have a limited supply of surgical masks available in class.
• I value the many perspectives students bring to our campus. Please work with me to create a classroom culture of open communication, mutual respect, and inclusion. All discussions should be respectful and civil. Although disagreements and debates are encouraged, personal attacks are unacceptable. Together, we can ensure a safe and
welcoming classroom for all. If you ever feel like this is not the case, please stop by my office and let me know. We are all learning together.

- Being punctual indicates our respect for others. Please arrive before class begins to find a seat, prepare your materials, and connect with your peers. The beginning of class is especially critical—just like the beginning of a movie or book. Being late to class is sometimes inevitable. If you are late, know that you are welcome to join the class, but please do so without distracting others. More than two instances of tardiness will result in an absence from class.
- Students are to be prepared for class (read/review assigned chapters prior to lecture) and are expected to participate by answering in-class questions and taking weekly quizzes.
- Silence mobile phones prior to attending class. Put mobile phones away.
- Learning is a two-way street, therefore, I will ask you for feedback throughout the course. I will take your feedback seriously, and work hard to incorporate your ideas on how to improve the course.
- My policy in this class is to not communicate any details regarding your grade through email. I will only discuss these details in private in-person meetings or through private online meetings.

Course Grading
The course grades will be calculated as follows:
- Attendance – 10% (based on lecture attendance only)
- Homework – 30%
- Mid-term project – 25%
- Final exam – 35%

Letter grades will be assigned based on the numerical scores: A = 90-100; B = 80-89; C = 70-79; D = 60-69.

Homework
- There will around 8 homework assignments throughout the semester, depending on the pace at which the material is covered
- All homework assignments will be posted and collected via the internet.
- You must access your assignment online on the course website on Canvas, work the problems, and submit your solutions by the due date indicated online.
- In general, no late assignments will be accepted. Deadline extensions may be given on a case-by-case basis for exceptional cases (e.g., COVID-19 related issues where an official confirmation will be required) or for religious observance. Excused extensions should be arranged prior to the due date.
- Homework will be graded, and the grades returned one week after the due date. All questions concerning the grading of homework assignments must be directed to the instructor in writing within two weeks after the grades are returned to the class.
Homework solutions will be posted after the due date.
The two worst homework assignments will be excluded from the final grade calculation of the homework. All other homework assignments will carry equal weight towards the grade.

Mid-Term Project
- There will be a mid-term project done in group where you will study a research paper applying quantum mechanics to a practical chemistry problem. You will have to write a short report (two pages) and give a short presentation in class. Further information will be given later.

Final Exam
- There will be a comprehensive final exam at the end of the course.
- Final exam will take place Saturday, May 7, 2022, at 8:00 a.m. - 10:00 a.m.
- The final exam questions will be based on lecture material, material contained in the texts and in the homework assignments.
- The final exam will be an open book exam. You will be allowed to bring all lecture notes, textbooks, homework assignments/solutions, and own notes to the final exam.
- Helpful mathematical relations and integral tables needed to solve the problems will be given with the exam.
- A simple scientific calculator will be sufficient for the final exam.
- Any student caught cheating will be given a grade of zero for the final exam.
- All questions concerning the grading of the final exam must be directed to the instructor in writing within two weeks after the grades are returned to the class.

Ancillary Information

Succeed at UNT
UNT endeavors to offer you a high-quality education and to provide a supportive environment to help you learn and grown. And, as a faculty member, I am committed to helping you be successful as a student. Here’s how to succeed at UNT: Show up. Find Support. Get advised. Be prepared. Get involved. Stay focused. To learn more about campus resources and information on how you can achieve success, go to http://success.unt.edu/.

Legal Notice Regarding Lecture Notes
My lectures and notes are protected by state common law and federal copyright law. You are authorized to take notes in class thereby creating a derivative work from my lecture, but the authorization extends only to making one set of notes for your own personal use and no other use. You are not authorized to record my lectures, to provide your notes to anyone else (hard copy or electronic), or to make any other use of those notes without express prior written permission from me.
COVID-19 Impact on Attendance
Students are expected to attend class meetings regularly and to abide by the attendance policy established for the course. It is important that you communicate with the professor and the instructional team prior to being absent, so you, the professor, and the instructional team can discuss and mitigate the impact of the absence on your attainment of course learning goals. Please inform the professor and instructional team if you are unable to attend class meetings because you are ill, in mindfulness of the health and safety of everyone in our community. If you are experiencing any symptoms of COVID (https://www.cdc.gov/coronavirus/2019-ncov/symptoms-testing/symptoms.html) please seek medical attention from the Student Health and Wellness Center (940-565-2333 or askSHWC@unt.edu) or your health care provider PRIOR to coming to campus. UNT also requires you to contact the UNT COVID Team at COVID@unt.edu for guidance on actions to take due to symptoms, pending or positive test results, or potential exposure.

Academic Dishonesty
Students caught cheating or plagiarizing will receive a “0” for that particular assignment or exam. Additionally, the incident will be reported to the Dean of Students, who may impose further penalty. According to the UNT catalog, the term “cheating” includes, but is not limited to: (a) use of any unauthorized assistance in taking quizzes, tests, or examinations; (b) dependence upon the aid of sources beyond those authorized by the instructor in writing papers, preparing reports, solving problems, or carrying out other assignments; (c) the acquisition, without permission, of tests or other academic material belonging to a faculty or staff member of the university; (d) dual submission of a paper or project, or resubmission of a paper or project to a different class without express permission from the instructor(s); or (e) any other act designed to give a student an unfair advantage. The term “plagiarism” includes, but is not limited to: (a) the knowing or negligent use by paraphrase or direct quotation of the published or unpublished work of another person without full and clear acknowledgment; and (b) the knowing or negligent unacknowledged use of materials prepared by another person or agency engaged in the selling of term papers or other academic materials. Further information on UNT’s policy on Academic Dishonesty can be found at: http://www.vpaa.unt.edu/academic-integrity

Acceptable Student Behavior
Student behavior that interferes with an instructor’s ability to conduct a class or other students’ opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UNT. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student’s conduct violated the Code of Student Conduct. The university’s expectations for student conduct apply to all instructional forums, including university and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct can be found at http://deanofstudents.unt.edu.
Withdrawal from Class
The administration of this institution has set deadlines for withdrawal of any college-level courses. These dates and times are published in that semester’s course catalog. Administration procedures must be followed. It is the student’s responsibility to handle withdrawal requirements from any class. In other words, I cannot drop or withdraw any student. You must do the proper paperwork to ensure that you will not receive a final grade of “F” in a course if you choose not to attend the class once you are enrolled.

ADA Policy
UNT makes reasonable academic accommodation for students with disabilities. Students seeking accommodation must first register with the Office of Disability Accommodation (ODA) to verify their eligibility. If a disability is verified, the ODA will provide a student with an accommodation letter to be delivered to faculty to begin a private discussion regarding one’s specific course needs. Students may request accommodations at any time, however, ODA notices of accommodation should be provided as early as possible in the semester to avoid any delay in implementation. Note that students must obtain a new letter of accommodation for every semester and must meet with each faculty member prior to implementation in each class. For additional information see the ODA website (https://disability.unt.edu/).

Canvas
Canvas will be used to post course materials and your grades. To get to this resource, go to https://unt.instructure.com/login/canvas and follow the UNT link to log on. (You will log on using your UNT EUID and password.) Once logged on, select this course.

Course Evaluation - Student Perceptions On Teaching (SPOT)
Student feedback is important and an essential part of participation in this course. The Student Perceptions On Teaching (SPOT) is a requirement for all organized classes at UNT. This short survey will be made available at the end of the semester to provide you with an opportunity to evaluate how this course is taught.

Retention of Student Records
Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Canvas online system, including grading information and comments, is also stored in a safe electronic environment for one year. You have a right to view your individual record; however, information about your records will not be divulged to other individuals without the proper written consent. You are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the university’s policy in accordance with those mandates at the following link: http://essc.unt.edu/registrar/ferpa.html
Emergency Notification and Procedures
UNT uses a system called Eagle Alert to quickly notify you with critical information in the event of an emergency (i.e., severe weather, campus closing, and health and public safety emergencies like chemical spills, fires, or violence). The system sends voice messages (and text messages upon permission) to the phones of all active faculty staff, and students. Please make certain to update your phone numbers at http://www.my.unt.edu. Some helpful emergency preparedness actions include: 1) know the evacuation routes and severe weather shelter areas in the buildings where your classes are held, 2) determine how you will contact family and friends if phones are temporarily unavailable, and 3) identify where you will go if you need to evacuate the Denton area suddenly. In the event of a university closure, please refer to Canvas for contingency plans for covering course materials.

Sexual Assault Prevention
UNT is committed to providing a safe learning environment free of all forms of sexual misconduct, including sexual harassment sexual assault, domestic violence, dating violence, and stalking. Federal laws (Title IX and the Violence Against Women Act) and UNT policies prohibit discrimination on the basis of sex, and therefore prohibit sexual misconduct. If you or someone you know is experiencing sexual harassment, relationship violence, stalking, and/or sexual assault, there are campus resources available to provide support and assistance. UNT’s Survivor Advocates can assist a student who has been impacted by violence by filing protective orders, completing crime victim’s compensation applications, contacting professors for absences related to an assault, working with housing to facilitate a room change where appropriate, and connecting students to other resources available both on and off campus. The Survivor Advocates can be reached at SurvivorAdvocate@unt.edu or by calling the Dean of Students Office at 940-565-2648. Additionally, alleged sexual misconduct can be non-confidentially reported to the Title IX Coordinator at oeo@unt.edu or at (940) 565 2759.