CHM 5210: Advanced Physical Chemistry (MQM)
MW 11:00–12:20 / Env 190

Instructor: G. Andrés Cisneros
Office: 205 C Chemistry
email: andres@unt.edu

Office Hours: W 1:45–3:00
or by appointment

Course Description and Goals

Quantum mechanics provides a mathematical description of the behavior and interactions of very small particles that are not correctly described by classical mechanics. This course is designed to provide students with the knowledge, theoretical background and mathematical tools to understand theoretical aspects of quantum mechanics and how it is applied to quantum chemistry. Familiarity with undergraduate–level physical chemistry and calculus will be necessary. Students are encouraged to bring issues from their own research (or other interest) to my attention that they would like to discuss. The emphasis should be on the principles of quantum chemistry common to all applications of chemistry.
More specifically, at the conclusion of the course you will be able to:

- Define and describe the postulates of quantum mechanics
- Interpret and evaluate literature involving quantum mechanical theory
- Employ analytical or approximate methods to solve the Schrödinger equation for molecular systems and calculate their properties.
- Identify and explain methods employed for quantum chemistry calculations.

However, these goals may be adapted to suit the objectives of the students.

Readings

Strongly Recommended text*: Quantum Chemistry*, I. N. Levine, Pearson Prentice–Hall Inc., New Jersey, 2009.

Other recommended texts include :

Elements of Quantum Mechanics, M.D. Fayer, Oxford University Press.

Molecular Quantum Mechanics, 4th Ed., P. Atkins and R. Friedman, Oxford University Press.

Mathematics for Quantum Chemistry, J.M. Anderson, Dover.

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, A. Szabo and N. S. Ostlund, Dover.

There will be occasional handouts including journal articles. These texts or links to them will be available on the course's Blackboard page.

In addition, there is a very good set of videos on youtube, which cover most of the concepts that will be presented in class:

https://www.youtube.com/user/TMPchem

I **strongly encourage everyone** to look at the video(s) that cover the concepts that will be presented in class **before the corresponding lecture**. This will allow us to do class activities to further your understanding of the material

Course Policies and Evaluation

This course will be interactive in nature; based on this, **attendance** and **participation** will be necessary for you to completely achieve the course goals. Attendance and participation will not be graded directly; however, they are important to the purposes of this course and therefore your active presence in class is expected.

Due to the limited time of the schedule, there will be little time for solving problems in class if you do not read the material prior to the class. In addition, working through problems and examples is absolutely essential for mastering this subject. You will need to do a significant amount of independent studying in this course, including working through examples and homework problems. I will be available for discussion of the problems during office hours or by appointment.

Evaluation of this course will be based on a variety of in–class and take–home assignments. There will be one mid–term and one final exam. Both exams will be take–home. Besides these exams there will be homework assignments, **posted on Blackboard**. Homework will be due on the date specified in the schedule (below). Another course requirement is a project to be completed individually. This project will be due on the final week of class and will involve a class presentation.

Homeworks, exams and the final project with their respective weights are as follows:

Homework	20% (20 pts.)
Project	20% (20 pts.)
Mid-term exam	25% (25 pts.)
Final exam	35% (35 pts.)

Although some of your evaluation will depend on how well you perform in a test–taking situation, the project will focus on learning as a process of trial–and–error, re–reading and re–thinking. Therefore, parts of the project can be submitted for comments, discussed during office hours and revised prior to the due date. The project will be decided by you and can consist of a presentation of a topic from the current literature related to quantum chemistry or computational chemistry, preferably algorithm/method development.

It is expected that you will abide by the academic integrity requirements as stated in the student code of conduct. Turn your cell phone, ipod, etc. off during class time. Use of these devices during class is disrespectful to your classmates and myself. Any person using these devices without explicit request from the instructor during class will have points deducted off her/his final grade.

If you must miss a class, inform me ahead of time. No late assignments will be accepted and no make–up exams will be given. Deadline extensions may be given for exceptional cases or for religious observance. Excused extensions should be arranged prior to the due date. 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.

STUDENT DISABILITY SERVICES: This department has a policy in place to reasonably accommodate individuals with disabilities and complies with the university policy established under Section 504 of the Rehabilitation Act of 1973 and the Americans with Disabilities Act (1990) to provide for equal access and opportunity. Please communicate with your professor as to your specific needs so appropriate arrangements can be made through the department and/or the Office of Disability Accommodation (Room 318A, University Union, (940) 565-4323).

Course Schedule (tentative). Readings key: L=Levine, F=Fayer, AF=Atkins & Friedman

Date	Topics	Readings
1/14	Introduction, Superposition and uncertainty principle	L: 1.1, 1.2; AF: chp. 0
1/16	Mathematical interlude	L: 1.6-1.9, 2.1, 5.2
1/21	Martin Luther King Jr. Observance, No class	
1/23	Mathematical interlude	L: 1.6-1.9, 2.1, 5.2
1/28	Operators, Dirac Notation	L: 3.1–3.3, 7.1–7.4; F: 13.B, chp. 4; AF: 1.3-1.8
1/30	Dirac Notation, Matrix notation	L. 7.10, 8.6; F: chp. 13.C; AF 1.20-1.24
2/4	Postulates of QM, The Schrödinger eq.; **Problem set 1 due**	L: 7.8, 7.9, 1.4; AF 1.0–1.19
2/6	The Schrödinger eq., Free particle in 1D	L: 1.5, 2.3; F: 5.A–5.C; AF: 2.1 2.2
2/11	Particle in a box, Particle in a well; **Problem set 2 due**	L: 2.2–2.5; F: 5.D; AF: 2.3–2.13
2/13	Particle in a well, Harmonic oscillator	L: 2.5, 4.1, 4.2; F: 6.A, 6.B; AF: 2.14-2.18
2/18	Particle on a ring, Angular momentum	L: 5.3, 5.4; AF: chp. 3, 4.1–4.3
2/20	Angular momentum, Rigid rotor	L: 6.1–6.4; F: 15.A–15.E; AF: 3.8
2/25	The Hydrogen atom; **Problem set 3 due**	L: 6.1–6.4; F: 7.A; AF: 3.9, 3.10
2/27	Angular momentum II	L: 11.1–11.8; F: 15.C–15.E; AF: 4.4–4.13
3/4	Variational principle; **Problem set 4 due**	L: 8.1, 8.2; F: 10.B; AF: 6.9–6.10
3/6	Perturbation theory	L: 9.1–9.8 F: 9.A–9.C; AF: 6.1–6.7
3/11	No class, University Holiday	
3/13	No class, University Holiday	
3/18	Electron spin	L: 10.1-10.4; F: 16.A, 16.B
3/20	Pauli exclusion principle, Slater determinants; **Midterm handout**	L: 10.5–10.10; F: 16.C, 16.D, AF: 7.11
3/25	Slater determinants, Molecular structure; **Midterm due**	L: 10.6–10.10, 13.1–13.5; AF: 8.1–8.2
3/27	Electron correlation, Valence Bond	L: 11.3, 16.1, 13.10, 13.11; AF: 9.7–9.9
4/1	Hückel Method and Hartree–Fock ; **Problem set 5 due**	L: 17.2, 11.1–11.2, 14 ; AF: 8.3–8.14, 9.5–9.7
4/3	M$\acute{}$oller–Plesset perturbation theory, CI and CC	L: 16.1–16.3, 13.17; AF: 9.19–9.12
4/8	Density Functional Theory (DFT)	L: 11.3, 16.1–16.3; AF: 9.13–9.14
4/10	Time–dependent QM	L: 1.4, 9.9, 9.10; F: 8, 11; AF: 6.11–6.18
4/15	Rotational and Vibrational spectra; **Problem set 6 due**	AF: 10
4/17	Rotational and Vibrational spectra	AF: 10
4/22	Electronic spectra	F: 12; AF: 11.1–11.12
4/24	**Extra Class Make Up/Presentations**	
4/29	**Extra Class Make Up/Presentations**	
5/1	**Extra Class Make Up/Presentations; Final Handout**	
5/6	presentations; **Final due**	