Syllabus for Chemistry 8541: "Dynamics"
Fall Semester 2023, four credits

11:15–12:30 Mon & Fri (Fri. 9/8/2023 – Mon. 12/11/2023)

Instructor: Donald G. Truhlar
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TA: none

Prerequisite: Undergraduate physical chemistry course

Format of the class:

This course is scheduled as a remote synchronous course. In particular, this class will meet by zoom on Mondays and Fridays from 11:15 am to 12:30 pm, starting Friday Sept. 8 and continuing through Monday December 11.

Holiday: Friday Nov. 24 is a University holiday; there will be no class that day.

Textbooks:

Classical Mechanics
by John R. Taylor
Publisher: University Science Books
required? yes

Mathematical Methods for Scientists and Engineers
by Donald A. McQuarrie
Publisher: University Science Books
required? yes

Description and scope of the course:

Chemistry 8541 is a graduate course in physical chemistry and chemical physics.

The course has two topics. One topic is the mathematics of chemical physics. The other topic is classical mechanics and classical dynamics, including Newtonian, Lagrangian, and Hamiltonian dynamics. We cover mathematics not just because of its importance in classical dynamics, but also because the mathematics covered is the mathematics that every physical Chemistry or Chemical Physics Ph.D. should know. We cover classical dynamics not just because of its importance in its own right, which is considerable, but also because understanding of classical dynamics provides a solid foundation for understanding many parts of quantum mechanics and statistical mechanics. The mathematical topics chosen for coverage are the one most useful for physical chemistry and chemical physics, and much of the math we cover is also useful for quantum mechanics, statistical mechanics, and spectroscopy. The course is focused

on practical mathematics and practical classical mechanics, not on formal developments and proofs.

I have selected two textbooks – one for math and one for dynamics.

Students are also encouraged to broaden their understanding by consulting other books; those on the reading list are especially recommended.

Objective of the course

To give the student the level of understanding of mathematical methods and classical dynamics that is a foundation for large parts of chemical dynamics, quantum mechanics, molecular spectroscopy, chemical kinetics, materials science, and statistical mechanics.

Class participation

The class will be taught in a participatory style emphasizing class discussion (online) and class participation (online). Student should have their cameras on to facilitate communication. Ordinarily I will use my iPad in the same way that one uses white boards in conventional classrooms. However, it will also be useful if student can share their work online as well.

Class preparation

Students should prepare for each class by reading the assigned material *prior* to the class period. Come to class prepared to discuss the material. Have the textbook handy during class so we can refer to it if desired. The material for the next class will be announced at the end of each class. Sometimes there will also be homework.

Class organization

The plan is to spend Mondays on math and Fridays on classical mechanics. However, the class size is small, so we can gear the presentations to student needs, and we may change the schedule to fit the needs of the class if it becomes apparent that that would be advantageous.

I have now taught this course several times, and each time it is different. Most years I have had two textbooks – one for math and one for dynamics, although some years I had a mechanics book with appendices covering some of he needed math. Every year I changed at least one of the textbooks and the order of coverage. The reason I change textbooks every year is to keep the course fresh. Each book covers the topics in a different order, and every year I have developed the lectures fresh in a new order. This year is special. I picked the very best books based on the experience of previous years, and we are reusing them, although lectures will still be fresh. No textbook or even pair of textbooks have everything we need, so we will cover some material, especially mathematical background, that is not in the textbooks.

What is the difference between a graduate class and simply reading a good book on the subject (or checking out a good Web site or tuning in to a set of online asynchronous lectures)? The answer I came up with is real-time, in-person student participation, and current research into learning is coming to the same conclusion. We have always had *a lot* of student participation in this course, and this year we will try for even more. We will try to take full advantage of the interactive nature of zoom. There are many good books and good Web sites

on almost any topic in mathematics or classical dynamics; students are encouraged to learn from all available sources. But in class, I want to do more than present a lecture to a passive audience.

Usually, the material will be covered in class differently than in the reading. I view classes as complementing the reading – this usually means not repeating the same material in the same way. And yet I want class participation, so we will also discuss some of the material in the textbooks that students should come prepared to discuss. We will try to balance discussion of the text material with new perspectives.

Presentations

In addition to active participation in every class, students will assist in presenting the material and in some cases they will be assigned sections of the material to present to the class. Class participation by the whole class is encouraged for every class, no matter who is leading a particular segment.

Grading

For an explanation of the University grading system please see
http://policy.umn.edu/education/gradingtranscripts
The two major grading systems used are A-F and S-N. The present course uses the A–F system.

Different students come in with different backgrounds. Everybody will advance in understanding at a different rate. That's expected in graduate school. Therefore grades will not be based on learning a set amount of material, but rather on full participation in the learning experience.

Grades will be based entirely on class participation, homework, and presentations, with the emphasis being class participation; there will be no written or oral exams, although I will ask questions during classes.

Making up for absences

Absences may occur due to unavoidable or legitimate circumstances. Such circumstances include illness, emergencies, subpoenas, jury duty, military service, bereavement, and religious observances. For complete information, please see:
http://policy.umn.edu/education/makeupwork.
If a class is to be missed, please notify the instructor in advance, when possible. If a class is missed, the makeup assignment is to hand in a three-page PDF summary of the assigned material for that class; this is due one week after the missed class.

Electronic copies of information

Copies of this syllabus, including the reading list at the end, are available at

https://truhlar.chem.umn.edu/courses/chemistry-8541-dynamics

Students with disabilities

Students with disabilities that affect their ability to participate fully in class or to meet all course requirements can arrange reasonable accommodations through the Office of Disability Services (612-626-1333). Students who have concerns about disabilities should notify the lecturer and contact that office within the first week of class.

Student conduct and responsibilities

University policies on student conduct and responsibilities may be found at:

http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf.

http://policy.umn.edu/education/studentresp

https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf

Equity, diversity, equal opportunity, and affirmative action

The University provides equal access to and opportunity in its programs and facilities, without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression. For more information, please consult Board of Regents Policy:

http://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity_Diversity_EO_AA.pdf.

Mental health and stress management

Students may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating, and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance and may reduce a student's ability to participate in daily activities. University of Minnesota services are available to assist with such issues. More information about the broad range of confidential mental health services available on campus may be found on via the Student Mental Health Website:

http://www.mentalhealth.umn.edu