Syllabus for Chemistry 8541: “Dynamics”  
Fall Semester 2020, four credits

11:15–12:30 Mon & Fri (Fri. 9/11/2020 – Mon. 12/14/2020)

Instructor: Donald G. Truhlar  
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TA: none

Prerequisite: Undergraduate physical chemistry course

Format of the class:

This class will be taught as a “Remote-instruction class.” Remote-instruction classes are 100% online and have scheduled times; some people refer to this as a synchronous online class. In particular, this class will meet by zoom on Mondays and Fridays from 11:15 am to 12:30 pm, starting Friday Sept. 11 and continuing through Monday December 14.

Holiday: Friday Nov. 27 is a holiday; there will be no class that day.

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 great importance in its own right, 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. The course is focused on practical mathematics and practical classical mechanics, not on formal developments and proofs.

I have a textbooks that includes a balanced coverage of both the dynamics (pages 1–393 and 487-532) and the mathematics (pages 395–485). Additional mathematical background will be provided in class as needed. Students are also encouraged to broaden their understanding by consulting other books; those on the reading list are especially recommended.

Textbook (available in paperback and as an e-book)

*Lagrangian and Hamiltonian Dynamics* by Peter Mann (Oxford University Press, 2018).  
ISBN 978-0-521-67971-8

Reading list
See separate document for recommendations for other reading.
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). This will be the first time the class is taught by zoom; so it will be experimental. Sometimes experiments don't work out; let's hope for the best.

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. The material for the next class will be announced at the end of each class.

Class organization

I have now taught this course several times, and each time it is different. Most years I have two textbooks – one for math and one for dynamics, and every year I changed at least one of the textbooks and the order of coverage. This year I have a new textbook, and it is a single textbook. This will guide the order or presentation, although we will cover some material out of textbook order. My goal for this constant changing of the course is to keep the presentation fresher.

Furthermore, I have given a lot of thought to the question: 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 an on-line lecture series)? 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, which will be experimental – since the course will be online. 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.

Often 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 the material in the textbook. 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 the later part of the course, they will be assigned sections of the material to present to the class. In particular, the current plan is that students will lead the last few lectures. Class participation by the whole class is encouraged for every class, no matter who is leading.
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; that’s graduate school. So 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; there will be no written exams.

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 the syllabus and reading list are available at

http://truhlar.chem.umn.edu/courses/chemistry-8541-dynamics-fall-2020

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

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

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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:


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: