

Chemistry 395/435: Chemical Dynamics
Department of Chemistry, Loyola University Chicago
Spring 2012

Instructor: Dr. Dan Killelea

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Office Hours: T, 4:00–5:00 and by appointment (FH 103)

Class: MW 7:00 – 8:25 pm, FH-105

Text: Chemical Kinetics and Dynamics, Steinfeld, Francisco, and Hase, 2nd Ed. (1999, Prentice-Hall)

Course Prerequisites: Chemistry 302 or concurrent registration. If you have not completed the course prerequisites, you may be administratively dropped from the class.

Course Overview

The dynamics of molecular collisions lies at the very heart of chemistry. This course will cover several current topics, including the dynamics of gas-surface reactions, unimolecular dynamics, and scattering. This course will also cover some fundamental kinetics and molecular spectroscopy. Students will learn how energy flows through molecules over the course of reaction, techniques for studying quantum state-resolved reactivity and scattering, and how non-equilibrium, dynamical properties may be utilized to guide chemical reactions towards their desired outcomes.

We will begin by looking at kinetics and a bit of statistical mechanics to provide some background. We will then move onto potential energy surfaces, unimolecular dynamics, collision dynamics, and finally, surface dynamics. I will do my best to keep the mathematics down, and keep our focus on the chemistry.

Exams, Homework, and Grading

There will be a single hour exam on the fundamental material, probably on 2 April. Each student will select a current topic in chemical dynamics by 29 Feb and write a short (15 double-spaced pages or so) review of a topic in the field. The paper will be due at the start of class on 2 April. Students will give a 25-30 minute presentation based on their paper. The presentation schedule will be determined in April. There may also be a couple homework assignments before the exam. The homework will not be turned in for a grade.

There will be no make up exams. Late papers lose a letter grade per calendar day. The presentation may not be rescheduled.

Final Exam: It is unlikely that there will be a final exam for this course.

Grading: The grade will be based on the exam, paper, and your presentation, roughly a third each.

Supplementary Texts

Statistical Mechanics, McQuarrie

Physical Chemistry, 2nd Ed., Rice, Ross, and Berry.

Molecular Reaction Dynamics and Chemical Reactivity, Levine and Bernstein

Concepts of Modern Catalysis and Kinetics, Chorkendorff and Niemantsverdriet

These, and some other texts, are on reserve at the library for Chem 435 (Killelea)

Schedule

Note: The instructor reserves the right to make changes to the schedule, and to move things around. S.F.H. is Steinfeld, Francisco, and Hase's textbook (Chemical Kinetics and Dynamics)

<i>Date</i>	<i>Class</i>	<i>Topics</i>	<i>Readings</i>	<i>other</i>
18 Jan	1	Introduction to Dynamics	Handout	
23 Jan	2	Molecular Structure	Handout	
25 Jan	3	Statistical Mechanics	Handout	
30 Jan	4	Kinetics	S.F.H. Ch 1,2	
1 Feb	5	Kinetics	S.F.H. Ch 2,3	
6 Feb	6	Kinetics	S.F.H. Ch 3,4	
8 Feb	7	Potential Energy Surfaces	S.F.H. Ch 6,7	
13 Feb	8	Unimolecular reactions and photochemistry	S.F.H. Ch 10, 11	
15 Feb	9	RRKM / Transition state theory	S.F.H. Ch 10, 11	
20 Feb	10	RRKM / TST in Catalysis	Handout	
22 Feb	11	Collision Dynamics		
27 Feb	12	Surface Structure and Chemistry		
29 Feb	13	Surface Scattering		Select Topic
5, 7 Mar	No classes, Spring break			
12 Mar	14	IVR		
14 Mar	15	IVR		
19 Mar	16	Gas-Surface Dynamics		
21 Mar	17	Gas-Surface Dynamics		
26, 28 Mar		Independent Study Week		
2 Apr	18	Exam		Paper Due
4 Apr	19	Surface Dynamics		
9 Apr	20	Surface Dynamics		
11 Apr	21	Presentations		
16 Apr	22	Presentations		
18 Apr	23	Presentations		
23 Apr	24	Presentations		
25 Apr	25	Presentations		

Teamwork: I also encourage you (the class) to work together to solve assigned and unassigned problems. The assigned problems are a minimum. Work together with your classmates, if you don't understand something, someone else may. You will also find that explaining a solution to your classmate will cement the information in your mind, and make you a better student.

Students with Disabilities

If a student has special needs, please let the instructor know in the first week of classes. The university provides services for students with disabilities. Any student who would like to use any of these university services should contact the Services for Students with Disabilities (SSWD), Sullivan Center, (773) 508-3700. Further information is available at <http://www.luc.edu/sswd/>.

Academic Integrity: Without an open and free exchange of ideas, the university system would fail. All members of the university community must hold themselves, and others, to the highest standards of honesty in their scholarly work. The university has strict policies regarding academic dishonesty. Please see the Academic Standards and Regulations page for the full details (<http://www.luc.edu/academics/catalog/undergrad/reg.shtml>), and in particular the policy on Academic Integrity (http://www.luc.edu/academics/catalog/undergrad/reg_academicintegrity.shtml) for more information. Some important points from the website above are:

Plagiarism is a serious form of violation of this standard. Plagiarism is the appropriation for gain of ideas, language, or work of another without sufficient public acknowledgement and appropriate citation that the material is not one's own. It is true that every thought probably has been influenced to some degree by the thoughts and actions of others. Such influences can be thought of as affecting the ways we see things and express all thoughts. **Plagiarism, however, involves the deliberate taking and use of specific words and ideas of others without proper acknowledgement of the sources.**

The faculty and administration of Loyola University Chicago wish to make it clear that the following acts are regarded as serious violations of personal honesty and the academic ideal that binds the university into a learning community:

Submitting as one's own:

1. Material copied from a published source: print, internet, CD-ROM, audio, video, etc.
2. Another person's unpublished work or examination material.
3. Allowing another or paying another to write or research a paper for one's own benefit.
4. Purchasing, acquiring, and using for course credit a pre-written paper.

The critical issue is to give proper recognition to other sources. To do so is both an act of personal, professional courtesy and of intellectual honesty.

Plagiarism on the part of a student in academic work or dishonest examination behavior will result minimally in the instructor assigning the grade of "F" for the assignment or examination. In addition, all instances of academic dishonesty must be reported to the chairperson of the department involved. The chairperson may constitute a hearing board to consider the imposition of sanctions in addition to those imposed by the instructor, including a recommendation of expulsion, depending upon the seriousness of the misconduct.

Academic cheating is another serious act that violates academic integrity. Obtaining, distributing, or communicating examination materials prior to the scheduled examination without the consent of the teacher; providing information to or obtaining information from another student during the examination; attempting to change answers after the examination has been submitted; and falsifying medical or other documents to petition for excused absences all are violations of the integrity and honesty standards of the examination process.

Any instance of dishonesty as detailed on the websites provided above will result in a grade of zero for that particular item, be it homework or an exam. The Dean and Chair of The Department of Chemistry will also be notified. I truly hope to never have to invoke these processes. Please be honest with your work.

When working as a group, if each member contributes to the discussion, and you each hand in very similar work, that is perfectly acceptable given the nature of the assignments. On the other hand, if someone simply copies an assignment from someone else, that is plagiarism, and will be treated as such.