**CHEM 854  CHEMICAL KINETICS AND DYNAMICS**

**Spring 2017**

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B031 Malott  
*Available drop-in or by appointment*

**Meets:**  
3059 Malott  
Tuesday & Thursday, 11:00am-12:15pm

**Description:**  
This course provides an advanced overview of chemical kinetics, statistical theories of reaction rates, and the microscopic aspects of chemical reaction dynamics with an emphasis on modern theoretical and experimental methods.

**Material:**  
Lectures will cover material from multiple texts and from the primary literature. Although I will provide references throughout the semester, you are responsible for finding supplementary reading material as needed in order to understand the material I cover in class. Several recommended books are available on reserve in Anschutz Library:

- QD502.S74 Chemical Kinetics and Dynamics by Steinfeld, Francisco and Hase. (Prentice Hall, 1999)
- QD461.L66 Molecular Reaction Dynamics by R.D. Levine (Cambridge, 2005)

You are not required to purchase a textbook. However, if you would like to own a book for future reference, I recommend any of the following (all three are available on reserve):

- Molecular Reaction Dynamics by R.D. Levine (Cambridge, 2005)  
  - Excellent advanced text, with emphasis on microscopic reaction dynamics
- Chemical Kinetics and Dynamics by Steinfeld, Francisco and Hase. (Prentice Hall, 1999)  
  - Comprehensive graduate-level text covering kinetics and dynamics
- Chemical Kinetics and Reaction Dynamics by P.L. Houston (McGraw-Hill, 2001)  
  - Very good introductory text, written for advanced undergrad/beginning grad

**Grading:**  
Your active participation is expected. Homework sets will be assigned approximately every 1-2 weeks, in which you will be asked to work through assigned problems, refer to the current literature, and/or prepare a short presentation for the class on a relevant topic. (Note: Some problems may require use of Maple mathematical software, which is available free of charge to KU students.)

*Each assignment will carry roughly equal weight, except for the final assignment, which may be worth up to twice that value at the instructor’s option. You must complete all assignments to receive a passing grade.*

**Conduct:**  
Plagiarism, cheating, and all other forms of academic misconduct will not be tolerated. All incidents will be reported, and students found in violation will be punished severely. You are encouraged to discuss assignments with your classmates, but any work you submit must be entirely your own.
I. Classical kinetics
   - Differential and integrated rate laws
   - Temperature-dependence and the Arrhenius equation
   - Determining mechanisms from the rate law
   - Controlled and uncontrolled chain reactions
   - Catalysis and enzyme kinetics

II. Bimolecular collisions
   - Kinetic theory of gases
   - Interaction potentials
   - Virial expansion
   - Molecular scattering
   - Differential cross-sections
   - Molecular beams (experimental)
   - Newton diagrams

III. Reactive collisions and the potential energy surface
   - Simple collision theory
   - Polyatomic molecules and the potential energy surface
   - Reaction dynamics and the Polanyi rules
   - Skewed and scaled coordinates and trajectories
   - State-to-state reactions and microscopic reversibility
   - Differential reaction cross-sections
   - Beyond triatomic molecules

IV. Statistical reaction theories and vibrational dynamics
   - Transition state theory
   - Microcanonical TST
   - Vibrational dynamics and energy flow

V. Photodissociation reactions
   - Wavepackets
   - Non-adiabatic dynamics
   - Controlling the reaction dynamics

VI. Reactions in solution
   - Potentials of mean force
   - Diffusion and transport
   - Friction and Kramers’ theory
   - Electron transfer reactions

A calendar with the approximate class schedule will be provided, and updated regularly.

Topics and schedule are subject to change at any time. I am open to suggestions if there are any topics of special interest (i.e. related to your research) that you would like to cover in class.