

Syllabus for Chemistry 8565: "Chemical Reaction Dynamics"  
Spring Semester 2018, two credits

11:15–12:30, Mondays and Fridays (1/19/2018 – 3/5/2018), 283 Kolthoff

Instructor:

Donald G. Truhlar

Office: 247 Smith Hall

Preferred method of contact: in person, usually available after lectures

TA: none

Prerequisite:

Undergraduate physical chemistry course

Description of the course: The course covers fundamentals of chemical reaction dynamics including topics such as potential energy surfaces, collision theory, statistical mechanical background and transition state theory, variational transition state theory, activation energy, tunneling, unimolecular reactions, energy transfer, reactions in solution, solvation free energy, potential of mean force, quasithermodynamic treatment, diffusion control, Kramers' theory, and photochemistry.

The course is literature based, without a textbook. At every lecture, one or more readings will be specified for reading before the following lecture. Many of the recommended readings are identified on a reading list handed out at the first class (Jan. 18) and many of the readings assigned later in the course will be taken from this list.

Grading: The plan is to grade the course on class participation, with no written examination. There might be a few written homeworks as well. If class participation is insufficient, the plans may have to be changed. Students should study the assigned reading before the next class and be prepared for class discussion of the literature assigned. Different students come in with different backgrounds. Everybody will advance in understanding at a different rate; so grades will not be based on learning a set amount of material. Final grades will be based mainly or entirely on class participation and on students advancing their knowledge from whatever point they start it.

Objectives of the course: To give the student the level of understanding of reaction dynamics that is a foundation for molecular simulations and the interpretation of dynamics and kinetics experiments. This includes chemical kinetics, chemical dynamics, and statistical thermodynamics.

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 a massive open on-line course)? The answer I came up with is class participation. I am prepared to go faster or slower to meet the needs of the individuals in the class. In addition, the collection of topics covered in this course is unique, based on my experience of what is good foundational knowledge for physical chemists.

Lecture schedule: This is given on the reading list.

**Incompletes:**

Registered students who do not complete the course will ordinarily receive a failing grade unless they officially withdraw from the course. Incompletes will be given only when discussed with and approved by the instructor before the end of the semester.

**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 contact that office within the first week of class.

**Academic Dishonesty:**

Scholastic dishonesty is discussed under the College of Science and Engineering scholastic policies. According to the CLA Classroom Grading and Examination Procedures, scholastic dishonesty is defined as “any act by a student which misrepresents the student’s own academic work or that compromises the academic work of another. Scholastic dishonesty includes (but is not necessarily limited to) cheating on assignments or examinations; plagiarizing, i.e., misrepresenting as one’s own work any work done by another; submitting the same paper, or substantially similar papers, to meet the requirements of more than one course without the approval and consent of all instructors concerned; depriving another of necessary course materials; or sabotaging another’s work.”