Syllabus for Chemistry 8565: "Chemical Reaction Dynamics"

Spring Semester 2023, two credits

1:00–2:15 PM, Tuesdays and Thursdays (1/17/2023 – 3/2/2023), zoom course
[zoom URL, meeting ID, and password sent by email]

Instructor: Donald G. Truhlar
TA: none

Prerequisite:
Undergraduate physical chemistry course

Description of the course: The course covers fundamentals of chemical reaction dynamics. Based on time available and class interest, it will include such topics as collision theory, conventional and variational transition state theory, activation energy, tunneling, unimolecular reactions, photochemistry, reactions in solution, solvation free energy, potential of mean force, diffusion control, and catalysis. A key aspect of the course is coverage of the background necessary to appreciate the material, especially potential energy surfaces and the statistical thermodynamical background.

Textbook
There is no textbook. Assigned reading will be from the literature and online resources.

Grading: The course will be graded on class participation (including readings and/or homework, where applicable) with no written examinations. Students should study the provided reading topics or homework questions before each class and be prepared for class. 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, but rather on class participation and on students advancing their knowledge from whatever point they start at. Class participation will include some student presentations.

Objectives of the course: To give the student the level of understanding of the concepts of chemical reaction kinetics and dynamics that are a foundation for the interpretation of dynamics and kinetics experiments in all areas of chemistry and for molecular simulation and theoretical predictions. This includes chemical kinetics, chemical dynamics, and the relevant statistical thermodynamics. A special focus will be transition state theory and associated concepts.

activated complex theory ≡ transition state theory

> "The overall picture is that the validity of the transition state theory has not yet been really proved and its success seems to be mysterious."
>
> Raymond Daudel et al., *Quantum Chemistry* (1983).

One of the goals of the course is that by end of the course you will agree with me that this is not true.

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 watching an on-line course)? Answer: class

participation. I am prepared to go faster or slower to meet the needs of the individuals in the class. The collection of topics covered in this course is unique, based on my experience of what is good foundational knowledge of chemical dynamics for physical chemists. Please ask questions to help me cover the material that will help you the most.

Class participation: Please log in on time. Please participate by video and audio. If possible, be prepared to share your screen.

Class absence: Because the class is graded on class participation, absence is discouraged. If for some reason an absence is unavoidable, please make up the missing lecture by handing in a three-page summary and discussion (pdf file format submitted by email) of the assigned reading or readings for that lecture. This is due no later than one week after the missed lecture. If a class is to be missed, an advance email to the instructor will be appreciated when possible so that we do not wait for you.

Auditors: Auditors are allowed only if they commit to full class participation.

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.

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."

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 inform the lecturer and contact that office within the first week of class.

Equity, Diversity, Equal Opportunity, and Inclusion
We welcome individuals of all ages, backgrounds, beliefs, ethnicities, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability, and other visible and nonvisible differences. Collaboration among people of all cultures and backgrounds enhances our experiences and contributes to excellence in teaching, learning, and research. We strive for a climate that celebrates our differences and strengthens our department by embracing and working to increase diversity, equity, and inclusion. For more information about our departmental efforts and upcoming activities:
http://z.umn.edu/ChemDiversity.
For a list of diversity related resources:
http://z.umn.edu/DiversityandInclusionResources.

Sexual Harassment and related topics
In this course, we strive to provide a safe and positive environment for everyone. Please review policy regarding sexual harassment and related topics:

http://regents.umn.edu/sites/default/files/policies/SexHarassment.pdf
For support and help, please contact the Aurora Center:
http://aurora.umn.edu

A PDF of this syllabus is available at
http://truhlar.chem.umn.edu/courses/chemistry-8565-chemical-reaction-dynamics

Readings for Thursday, January 19:

1. "Potential Energy Surfaces," D. G. Truhlar, in *The Encyclopedia of Physical Science and Technology,* edited by R. A. Meyers (Academic Press, New York, 1987), 3rd ed. (2001), Vol. 13, pp. 9-17.

   Available online at https://comp.chem.umn.edu/Truhlar/docs/C27.pdf
2. "Potential Energy Surfaces for Atom Transfer Reactions Involving Hydrogens and Halogens," C. A. Parr and D. G. Truhlar, Journal of Physical Chemistry **75**, 1844-1860 (1971). doi.org/10.1021/j100681a015