Syllabus for **Chemistry 8565: "Chemical Reaction Dynamics"**
Spring Semester 2020, two credits

11:15–12:30, Mondays and Fridays (1/24/2020 – 3/6/2020), 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, photochemistry, reactions in solution, solvation free energy, potential of mean force, and quasithermodynamic treatment and – if time permits and if there is interest — diffusion control, Kramers' theory, energy transfer, catalysis, ….

Textbook:
"Chemical Kinetics and Reaction Dynamics," Paul L. Houston (Dover Publications, 2001).

Grading: The plan is to grade the course on class participation, with no written examination. (If class participation is insufficient, the plans may have to be changed.) Students should study the assigned reading before each 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, but rather on class participation, on homework, and on students advancing their knowledge from whatever point they start at. There will sometimes be homework problems. Class participation may include some student presentations in the final few lectures.

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 the relevant statistical thermodynamics.

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)? Answer: 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 will be updated as we go along _ to meet the needs of the class.

Auditors: Auditors are invited, but if you audit the course, please do all the readings and homework, come to every class, and participate fully in class discussion.

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

### Department of Chemistry Diversity and Inclusion Committee
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.

### Equity, Diversity, Equal Opportunity, and Affirmative Action
We welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability – and other visible and nonvisible differences to this course.

### 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