

Syllabus for Chemistry 8561
"Thermodynamics, Statistical Mechanics, and Kinetics I"
Fall Semester 2007, four credits

1:25-2:15, Mon, Wed, Fri (09/05/2007 - 12/12/2007)
121 Smith Hall / 283 Kolthoff

<http://comp.chem.umn.edu/truhlar/index.htm#courses>

Instructor: Donald G. Truhlar

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Office hours: anytime on Monday, Wednesday, or Friday

Preferred method of contact: in person, except when directed otherwise

TA: to be announced

Prerequisite - Undergrad physical chemistry course

Description: Chemistry 8561-8562 is a two-part sequence. Thermodynamics, equilibrium statistical mechanics, ensemble theory, partition functions. Applications, including ideal gases/crystals. Theories of simple liquids, Monte Carlo, and molecular dynamics simulations. Reaction dynamics from microscopic viewpoint. The first semester, Chemistry 8561, will cover selected topics in statistical mechanics and statistical thermodynamics. The second part, Chemistry 8562, will focus on molecular simulations of strongly interacting systems and an introduction to kinetics and chemical dynamics.

Textbook:

"Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology" by Ken A. Dill and Sarina Bromberg, Garland Science (Taylor & Francis Group), 2003. Paperback. Required.

Class participation: The class will be taught in an experimental style emphasizing class discussion. Students should prepare for each class accordingly. The material to be prepared for each class will be announced at the

previous class; usually it will be the next chapter in the textbook. Homework primarily consists of preparing for class discussion and problems worked in class, but there will be occasional exceptions.

Presentations: Every student will present at least one lecture, on a topic to be determined approximately half way through the course.

Written examinations: There may be occasional written quizzes at the beginning of class on random dates. A longer written examination in October and/or a final written examination in December may be scheduled if class participation is insufficient to gauge the progress of the class.

Written homework: Occasional written homework assignments may be worked in groups.

Grading: Final grades will be based on the instructor's evaluation of the level of active class participation (60%), presentations (20%), written quizzes (10%), and written homework (10%). The percentages are tentative at this time. Preliminary feedback on class progress will be provided by the instructor in October. If class participation is insufficient to gauge the progress of the registered students, there may be one or two written examinations (see above); if such examinations are scheduled, their percentage contribution to the grade will be announced when they are scheduled.

Incompletes: Registered students who do not complete the course will receive an F 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.

Schedule: The lecture schedule is flexible; we may cover more or less material depending on the needs and desires of the class.

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 this office within the first week of class.

Academic Dishonesty: Scholastic dishonesty is discussed under the Institute of Technology's 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."

Additional information: Additional information is available at

<http://comp.chem.umn.edu/truhlar/index.htm#courses>