

CHM 6720: Chemical Dynamics

Instructors: Dr. T. Lam Nguyen and Prof. John F. Stanton

Office hours: 9 am to 5 pm, NPB 2348 (in person or by appointment):

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Suggested textbooks: Chemical kinetics and dynamics (by Jeffrey Steinfeld et al.),
Chemical kinetics (by Keith J. Laidler)

Course Schedule

Week	Dates	Material
I		Introduction of chemical kinetics and dynamics; (Small) class project (a few pages);
II		Basic kinetic concepts: Rate, Order, Elementary, Composite, Rate-determining step, thermal equilibrium, so on... Distribute 1 st homework
III		Analysis of kinetic results: basic math techniques (deterministic and stochastic methods), steady-state approach
IV		Potential energy surface: activation energy, mechanism, Arrhenius's equation Distribute 2 nd homework
V		Theories of reaction rates: theory of collisions,
VI		Transition state theory, Lindemann's theory, RRKM theory,
VII		Variational transition state theory,
VIII		Semi-classical transition state theory (SCTST) Distribute 3 rd homework
IX		Partition functions, quantum states, direct count method, Wang-Landau method
X		Master-equation techniques: deterministic and stochastic approaches to compute $k(T,p)$: part 1
XI		Master-equation techniques: deterministic and stochastic approaches to compute $k(T,p)$: part 2 Distribute 4 th homework
XII		Applications: elementary gas-phase reactions in combustion, atmosphere, and interstellar medium
XIII		Isotopic effects, quantum effects, so on
IVX		Trajectory (dynamic) calculations
XV		Wrap-up of projects and others
XVI		Report final grades to students

Small class project (20 points):

A topic may be selected by student. Anything (including a research work, a mini review, and a novel idea / theoretical or experimental method) relevant to dynamics and kinetics is always welcome.

Homework (80 points):

There are four homework assignments: 20 points for each.

Grading: The grade will be determined by project (20%) and homework (80%).

Grading scale:

A > 90

A- 87.5 to 89.99

B+ 82.5 to 87.49

B 77.5 to 82.49

B- 75 to 77.49

C+ 72.5 to 74.99

C 67.5 to 72.49

C- 65 to 67.49

D+ 62.5 to 64.99

D 57.5 to 62.49

D- 55 to 57.49

E < 55

Disabilities

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter, which must be presented to the instructor when requesting accommodations. Students with disabilities should follow this procedure as early as possible in the semester.

Counseling

The University of Florida provides counseling services for students, sta_, and faculty. See <http://www.counsel.ufl.edu/> or call (352) 392-1575 during regular service hours (8am 5pm). For other hours or on weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352) 392-1171.

Honor Code

This class will operate under the policies of the student honor code, which can be found at:

<http://www.registrar.ufl.edu/catalog/policies/students.html>. The students, instructor, and TAs are honor-bound to comply with the Honors Pledge: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

Evaluations

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be noticed when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.