CHEM 7540
Chemical Dynamics (MWF 10:20-11:15 am)

Objective: This course is an introduction to advanced molecular dynamics. We will cover chemical reactions and dynamics both in gas phase and in condensed phase and address the fundamental motions of atoms and molecules during chemical transformation using time-dependent quantum mechanical descriptions (theory) and ultrafast laser spectroscopy (experiment). The content is tightly connected with frontier research topics, facilitating students to quickly enter the modern chemical dynamics field and to master the basic knowledge underlying the frontier studies of molecular dynamics.

Prerequisites: At least have taken one quantum chemistry/mechanics or have the instructor approval.

Course topics:

Week	Topics
1	*Potential energy surface*: *Ab initio* calculations, semi-empirical methods, intermolecular potentials
2	*Dynamics of bimolecular collision*: Elastic scattering, complex scattering processes
3,4	*Theory and experiment on reactive collisions:* Thermal rate data, angular and translational-energy distributions, state-resolved methods
5,6	*Basics of light-matter interactions:* Dynamics in two-level systems, *Rabi* oscillations, photochemical kinetics and photophysics
7,8	*Dynamics in quantum mechanics:* Time-dependence and -independence pictures, state preparation and quantum decoherence, time-dependence perturbation theory, Fermi's golden rule
9,10	*Dynamics in the presence of dissipation:* Coherence and decoherence, Markovian and non-Markovian dynamics, Fluctuation-dissipation theorem, phase space and the Liouville equation
11,12	*Energy-transfer Dynamics:* Vibrational and rotational energy transfer, Forster and Dexter theories of electronic energy transfer, electronic coupling in molecular dimers, electronic energy transfer in nultichromophoric molecules
13,14	*Charge-transfer dynamics:* Surface hopping, nonadiabatic dynamics, semiclassic and quantum theories of charge transfer, tunneling dynamics, Marcus theory, adiabatic and nonadiabatic limits

Exams

There are two midterm exams and one final exam. If you become sufficiently ill on the day of the exam to the point where it will affect your performance, do not take the exam, see a doctor, obtain a medical excuse, have no discussions with students who did take the exam, and you will be allowed to make up the exam without penalty. Do not take an exam if a medical condition will affect your performance.

Homework

There are 8-10 sets of homework. A penalty of 10% per day will be assessed for late homework. Each set of homework could have different points. Students are encouraged to work together on problem sets, but each student must turn in his or her own solutions. The submitted work should properly reflect the student's level of understanding.

Grading

The homework, 2-midterm and final exams will be scaled to 30%, 20%, 20% and 30%. The final total points are 100.

Students with Disabilities

Students with documented disabilities should see the instructor privately as early in the quarter as possible to arrange suitable accommodations. If your disability requires materials in alternative format, please contact the Office for Disability Services at 292-3307, Room 150 Pomerene Hall.

Course Web Page

Students will have access to lecture notes, assignments, answer keys and announcements via the course website.

Recommended Textbooks

1. David J. Tannor, ***Introduction to Quantum Mechanics (A Time-Dependent Perspective)***
2. Abraham Nitzan, ***Chemical Dynamics in Condensed Phases***
3. R.D. Levine, *Molecular Reaction Dynamics*
4. J. I. Steinfeld, J.S. Francisco and W.H. Hase, *Chemical Kinetics and Dynamics*
5. Rodney Loudon, *The Quantum Theory of Light*
6. S. Mukamel, *Principle of Nonlinear Optical Spectroscopy*
7. Biman Bagchi, *Molecular Relaxation in Liquids*

Other recommended readings will be announced in class.

Learning outcomes

- Understand chemical reactions at the most fundamental level. For isolated systems, understand quantum state-resolved reaction dynamics with potential surface and collision theory.
- Understand the light-matter interactions and the fundamental photophysics and photochemistry of molecules.
- Learn time-dependent quantum methods to describe chemical dynamics, especially introducing wavepacket concept.
- Learn theoretical methods to describe the chemical dynamics in dissipation systems such as in solution phase.
- Understand important energy transfer dynamics in molecular systems including rotational, vibrational and electronic.
- Understand important modern electron transfer dynamics with various theories and models, especially on quantum effects and in biological systems.