January 2009

Chemistry 3490: *Chemical Rate Process Theory*

This course will survey fundamentals of Rate Process Theory applied to both Classical and Quantal processes of interest in chemical dynamics (broadly defined!).

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Course webpage: http://mercury.chem.pitt.edu/~rob/chem3490_spring09/

Lectures: Tues., Thurs. 1:30-2:45 p.m.; 307 Eberly Hall

Required Textbook: "Nonequilibrium Statistical Mechanics", Robert Zwanzig [Oxford Univ. Press, 2001; **ISBN-10:** 0195140184 ; **ISBN-13:** 978-0195140187].

Prerequisites: Knowledge at the level of a good 1st year graduate course (in Chemistry or Physics) in i) Quantum Mechanics and ii) Statistical Mechanics.

Grading: Weekly problems sets, plus a term project. The term project topic will be determined by the student (with instructor's consent). It will consist of a ca. 10 page written report and an oral presentation to the class at the end of the semester.

Office Hours: anytime (day, night, weekend …)

Tentative Syllabus:

Part I: Classical Rate Process Theory

Jan. 6 Brownian Motion (BM) Theory: The Problem of Random Flights (Markov)

Jan. 8 BM Theory: Langevin Equation

Jan. 13 BM Theory: Fokker-Planck and Smoluchowski Eqs.

Jan. 15 Kramer's Theory of Activated Processes

Jan. 20 Kramer's Theory (cont.)

Jan. 22 Generalized Langevin Eq.

Jan. 27 Drift-Diffusion Processes: Basic Concepts

Jan. 29 Drift-Diffusion Processes: Mean-First Passage Times

Feb. 3 Drift-Diffusion Eqs.: Application to Ion Permeation through Protein Channels

Feb. 5 Drift-Diffusion Eqs.: Mean-field theories of Ion Permeation and Ionic Solvation

Feb. 10 Kinetic Master Eqs.: Basic Principles

Feb. 12 Kinetic Master Eqs.: Basic Principles

Feb. 17 Kinetic Master Eqs.: Applications to Ion Channel Permeation and Gating

Feb. 19 Kinetic Master Eqs.: Applications to Protein Conformational Kinetics

Part II: Quantum Rate Process Theory

Feb. 24: Fermi Golden Rule (GR) for Quantum Transition Rates

Feb. 26 Fermi Golden Rule: Application to Linear Vibronic Spectroscopy (Electronic Absorption and Resonance Raman)

Mar. 3 Fermi Golden Rule: Stochastic Lineshape Theory

Mar. 5 Pauli Master Equations

Mar. 17 Redfield Theory and 2nd Order Quantum Relaxation Theories (QRTs)

Mar. 19 Redfield Theory and 2nd Order QRTs (cont.)

Mar. 24 The Spin-Boson (S-B) Model of Multi-dimensional Tunneling

Mar. 26 Condensed Phase Electron Transfer (ET): Marcus Theory

Mar. 31 Condensed Phase ET in the Nonadiabatic Regime (S-B model again)

Apr. 2 Externally Driven Quantum Dynamics: Isolated N-level Systems

Apr. 7 Externally Driven Quantum Dynamics: Condensed Phase Systems

Part III: Student Project Presentations:

Apr. 9, 14, 16