Syllabus for Chem 541
Special Topics in Physical Chemistry: Thermodynamics & Kinetics

Textbooks:
Molecular Driving Forces by Dill & Bromberg (Garland Sciene, 2011, 2nd ed) – primary [recommended] (MDF)
Chemical Kinetics and Reaction Dynamics by Houston (Dover 2006) – secondary
Physical Chemistry by Atkins (OUP, 2009, 9th ed) – secondary

Section 1. Statistical Approach to Chemistry – The Basics

Week 1: Sept 1,2
1) Intro. to probability, statistics of particles (MDF 1,2)
2) Entropy and energy as driving forces (MDF 2,3)
3) Optimizing thermodynamic functions (MDF 4)

Week 2: (Sept 8,9)
4) Maximum Entropy & the Boltzmann principle (MDF 5)
5) Energies, enthalpies, thermodynamic states (MDF 6)
6) Free energies, chemical potentials (MDF 8,9)

Section 2. Statistical Thermodynamics of Physical and Chemical equilibria

Week 3: Sept 15,16
7) Microscopic Modeling & Boltzmann's Law (MDF 10)
8) Equilibrium constants, binding affinities (MDF 13)
9) Liquids, phase equilibria (MDF 14)

Week 4: Sept 22,23
10) Solvation, free energies of transfer, colligative properties (MDF 16)
11) Coulomb's Law & Electrostatics: how charges interact (MDF 20)
12) Electrostatic potentials (MDF 21)

Week 5: Sept 29,30
13) Electrochemical equilibria, Nernst equation, Batteries and Cells (MDF 22)
14) Salts shield charges (Poisson-Boltzmann) (MDF 23)
15) Intermolecular interactions (MDF 24)

Week 6: Oct 6,7
16) Adsorption & binding (MDF 27)
17) Conformational equilibria of organic molecules (MPOC)
18) Acid-base equilibria, pH (MPOC)

MIDTERM EXAM Oct 12 (TBD)

Week 7: Oct 13,14
19) Molecular recognition, supramolecular chemistry (MPOC)
20) Experimental methods to measure equilibria, including estimation of errors and uncertainty

Section 3. Macromolecular equilibria

Week 8: Oct 20,21
21) Polymers 1: conformations & random flights (MDF 33,34)
22) Polymers 2: polymer solutions, Flory-Huggins (MDF 32,33)
23) Water: pure and as a solvent, the hydrophobic effect (MDF 32,33)
Section 4. Chemical Kinetics and Dynamics

Week 9: Oct 27, 28
24) Diffusion, Fick's Law, Physical Dynamics (MDF 17,18)
26) Transition states & activation processes (MDF 19)

Week 10: Nov 3,4
27) Energy surfaces & chemical dynamics
28) Reactions in liquid solutions
29) Reactions at solid surfaces

Week 11: Nov 10, 11
30) Dynamics modeling methods - MD, QM, QM/MM (Guest Lecture by Dave/Darrin/TaiSung?)
31) Catalysis – heterogeneous, homogeneous, enzymatic

Week 12: Nov 17, 18
32) Experimental methods and data interpretation (fitting, errors etc.)
33) Photochemistry/atmospheric chemistry

Week 13: Nov 24 (No class Wed Nov 25)
Section 5. Guest Lectures
34) Drug discovery in industry: guest lecture by Wendy Cornell from Merck.

Week 14 & 15 (Dec 1,2,8,9):
Research case study presentations