# CHM 6461: Statistical Thermodynamics

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# Books

We will not use a main book, but I will be following some sections of "Statistical Mechanics: Theory and Practice through Molecular Simulation", Oxford University press M. E. Tuckerman.

Some of the content will be taken from
D.A. McQuarrie, Statistical Thermodynamics
D. Chandler, Introduction to Modern Statistical Mechanics
Often, material will be drawn from current literature in statistical mechanics.

I strongly recommend you being familiar with the level of basic statistical thermodynamics shown in the McQuarrie book.

# Course Outline

I. Review of Classical Statistical Mechanics
1. Microscopic equations of motion
2. Phase space, phase space vectors, and Liouville's Theorem
3. The Liouville equation and equilibrium solutions
4. Review of the basic ensembles
A. Microcanonical ensemble B. Canonical ensemble C. Isothermal-isobaric ensemble D. Grand canonical ensemble

II. Molecular Dynamics
1. Algorithms
2. Numerical implementations

III. MonteCarlo
1. Algorithms
2. Numerical implementations

IV. Distribution functions and liquid structure
1. Spatial distribution functions and the radial distribution function
2. Virial equation of state
73. Perturbation theory and the Van der Waals equation

V. Calculating the free energy
1. Free-energy perturbation theory
2. Adiabatic switching and thermodynamic integration
3. Jensen's inequality and Jarzynski's equality: Nonequilibrium methods
4. Reaction coordinates and rare events

5. The “blue moon” ensemble 6. Transforming the partition function
7. Driving variables: Adiabatic dynamics and metadynamics

VI. Time-dependent processes (Classical case)
1. Perturbative solution of the Liouville equation
2. Linear response and Green-Kubo theory
3. Classical time-correlation functions
4. Examples of transport properties
5. Reaction rates and transition state theory

Homework:.......... 30%
Midterm:...............35%
Final:.................... 35%