Chemistry 7960 **Syllabus** **Fall 2024**

I. **Fundamentals & big ideas of quantum statistical mechanics** C3, McQ2, 3
- -Ensemble averages
- -Distributions of quantum microstates
- -Fluctuations: why thermodynamics works (mostly)

II. **Molecular gases** C4, McQ4-6,8-9
- - Boltzmann statistics
- -Gases of polyatomic molecules
- -Chemical equilibrium

III. **Fundamentals & big ideas of classical statistical mechanics** C7.1, McQ7
- -Distributions of classical microstates
- -Entropy in classical mechanics

IV. **Structure and thermodynamics of liquids** C7, McQ13,14
- -Liquid structure, distributions, and correlation functions
- -Connection between structure and thermodynamics
- -Free energy calculations and thermodynamic perturbation theory

V. **Phase transitions and critical phenomena** C5
- -Phenomenology
- -Lattice models
- -Mean field theory and beyond

VI. **Simulation techniques** C6
- -Monte Carlo methods: Metropolis method, sampling rare events, free energy calculations
- -Molecular dynamics: integrators for classical dynamical equations

VII. **Nonequilibrium statistical mechanics** C8, McQ20, 21
- -Nonequilibrium ensemble average
- -Dynamical fluctuations and correlations
- -Linear response theory & fluctuation-dissipation theorem with applications to:
  - -molecular transport
  - -molecular spectroscopy
  - -chemical reaction kinetics
- -Stochastic dynamics: Langevin and Fokker-Planck equations, microscopic origin of dissipation

At the level of *Statistical Mechanics* by McQuarrie or *Introduction to Modern Statistical Mechanics* by Chandler