

CHM 8309 G00
Introduction to Statistical Mechanics
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Course Website: <https://mysite.science.uottawa.ca/salavish/content/teaching>

Study materials: -Lecture presentations are posted on-line;
-Extended discussions for some sections of the course are in my book:
Molecular Simulations: Fundamentals and Practice (see UOttawa Library)
-Please note list of typos on my website.
-Older versions of the slides with voice recording are on my website

Useful textbooks:

- Donald A. McQuarrie, *Statistical Mechanics or Statistical Thermodynamics*
- Terrell Hill, *Introduction to Statistical Thermodynamics*
- Mark Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation*

Background material used:

- Undergraduate physics (mechanics) and calculus
- Familiarity with probability theory
- Thermodynamics at the level of undergraduate physical chemistry
- Quantum mechanics of simple systems (particle in a box, harmonic oscillator, rigid rotor, Pauli exclusion principle)

Topics covered

- Introduction to classical mechanics / the Lagrangian and Hamiltonian approaches / phase space
- Review of some simple quantum mechanical systems
- Introduction to probability theory: Discrete variable distributions / continuous variable distributions / the Central Limit Theorem
- The Maxwell-Boltzmann distribution
- The method of Lagrange multipliers
- The concept of ensemble
- Derivation of the quantum mechanical partition function: Canonical ensemble / isothermal – isobaric ensemble / grand canonical ensemble
- The partition function for ideal gas systems: Translation / rotational / vibrational partition functions
- Statistical mechanics of solids, adsorption, ...
- Classical statistical mechanics and MD simulations