

Basic Statistical Mechanics CHM 8309

Each talk will be 25-30 minutes. With 10-15 minutes for questions

End-of-term presentation topics

More theoretical topics

- The Nosé-Hoover algorithm for Canonical Ensemble distribution in MD simulations.
- The principle of detailed balance and Monte Carlo simulations
- The Gibbs Ensemble Monte Carlo method.
- Generating the Maxwell-Boltzmann distribution for molecular simulations
- Information theory and entropy
- The classical equipartition principle and its failures

More applied topics

- The Langmuir adsorption isotherm for 1 and 2 dimensions. Introduction to Ising Model
- The Saha equation and temperature determination and classification of stars and use in atomic absorption spectroscopy.
- The shape of the HCl rotational-vibrational spectrum
- Calculating equilibrium constants of gas phase reactions with statistical mechanics
- The absolute rate (Eyring) theory for the rate of chemical reactions
- Ideal gas in electric and magnetic fields

Marking

- Instructor (80 %)
- Audience gives constructive / critical feedback (marked) on talk which will be returned to speaker in anonymous form (15 %)
- The quality of the feedback you provide on other talks (5 %)