

CHM 6461: Statistical Thermodynamics

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Professor Adrian Roitberg

Office: LEI 440

Phone: 392-6972

E-mail: roitberg@ufl.edu

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. MonteCarlo

1. Algorithms
2. Numerical implementations

III. Molecular Dynamics

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
3. 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
6. 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%

Homework:

Homework due date is posted on the class calendar. Late homework (if it is turned in on the same day, but after deadline) will have a 20% deduction on the grade. No more homework will be accepted for grading after that. Each homework problem has to show the full derivation. The homework answers should be present in a professional manner, with all steps explained. No points will be given for a final result without justification.

Exams and quizzes:

There will be 2 progress exams with dates to be announced soon.

There will be no make-up exams.

Cheating on an exam will result in a grade of zero for that case. If any homework or quiz assignment is suspect, a grade of zero will also be given for that assignment. If cheating is suspected, it will be reported to the university as such.

Honor Code:

The student honor code can be found at www.dso.ufl.edu/sccr/honorcodes/honorcode.php

The students and instructor are honor bound to comply with the Honors Pledge: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.