

**Chemistry 540:**

**STATISTICAL MECHANICS IN CHEMISTRY**

**Spring 2021**

**Instructor:** Prof. Oleg Prezhdo

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**Required Textbooks**

“Statistical Mechanics” by Donald McQuarrie (chapters 1-11)

“Statistical Mechanics” by David Chandler (chapters 5, 8)

**Lecture**

TTh 11:00am to 12:20pm over Zoom, will be adjusted based on student time-zones

**Goal**

The goal of this course is to introduce the basic concepts of Statistical Mechanics and to consider its applications to atomic and molecular systems, as they are encountered in chemistry. The course starts with a brief review of quantum and classical mechanics, thermodynamics, and statistics, considers in detail the canonical ensemble, and moves onto other ensembles and a variety of simple applications. Several deeper and more complex topics and applications of statistical mechanics in chemistry will be covered towards the end of the class.

**Other Recommended Textbooks**

Norman Davidson “Statistical Mechanics”

Linda Reichl “A Modern Course in Statistical Physics”

Abraham Nitzan “Chemical Dynamics in Condensed Phases”  
(chapter 11)

**Your Favorite Undergrad Text**

McQuarrie&Simon “Physical Chemistry: A Molecular Approach”

Peter Atkins “Physical Chemistry”

Thomas Engel, Phil Reid “Physical Chemistry”

**Topics:**

- I. Chapters 1-5 of McQuarrie, including Introduction & Review; Canonical, Grand-canonical, Micro-canonical Ensembles and Fluctuations; Ideal Monoatomic Gas.

The first half of the class will be followed by the Midterm Exam.

- II. Chapters 6-9, 10.5, 11 of McQuarrie, including Diatomic and Many-atomic Ideal Gases, Crystals, Chemical Equilibrium, Black-body Radiation and Classical Statistical Mechanics. Chapters 5 and 8 of Chandler (Phase Transitions, Ising Model, Mean-Field Model, Correlation Functions)

The second half of the class will be followed by the Final Exam.

**Assessment**

Homework (one problem set per week, due Tuesday before class)

40%

1<sup>st</sup> Exam, take home

30%

2<sup>nd</sup> Exam, take home (to include 2nd half of class only)

30%