Statistical Mechanics for Chemistry

CHM 8309-B00 – 1.5 units

Instructor: Dr. Saman Alavi
Department of Chemistry and Biomolecular Sciences
University of Ottawa
Contact: salavish@uottawa.ca
Website: https://mysite.science.uottawa.ca/salavish/

Course schedule

Sept. 7 to Oct. 21, 2022.
Lectures: Tuesdays & Thursdays 5:30 – 6:50
Room: VNR 4084
Office hours / Tutorials: Wednesdays: 4:30 – 5:20 (online / in-person)

Background knowledge required

-Physical chemistry (in particular, classical thermodynamics)
-Quantum mechanics of the particle in a box, harmonic oscillator, and rigid rotor system
-Knowledge of classical mechanics, Newton's equations of motion in differential equation form

Teaching methods

- In-person lectures
- Recorded lectures from a previous year are available to help review
- A textbook by the instructor covering much of the material covered in the course is available

Assessment method

-One problem set: 10% of mark. Problem set due at end of week 5.
-Mid-term exam: 50% of mark. End of week 4 (after completing Canonical Ensemble lecture)
-End-of-term presentations: 40% of mark. Last week of course / First week after the end of the course.

Important Dates

- Problem set: Due at end of week 5.
- Mid-term exam: End of week 4 (after completing Canonical Ensemble lecture)
- End-of-term presentations: Last week of course / First week after the end of the course.

Syllabus

- Overview of classical and quantum mechanics of simple systems (MSFP, Chapter 2, Secs. 2.1 - 2.3, 2.8. Appendix)
- Overview of probability theory (MSFP, Chapter 5)
- Review of probability concepts; The central limit theorem

- Maxwell-Boltzmann probability distribution for ideal gases
- Statistical mechanics: Ensembles and method of most probable distribution (MSFP, Chapter 6)
- Application of statistical mechanics
- Ideal monatomic gases
- Ideal diatomic and polyatomic gases
- Chemical equilibrium in the gas phase
- Solids
- Introduction to classical statistical mechanics

List of readings

Parts of the course are from my book:
- Saman Alavi, Molecular Simulations: Fundamentals and Practice, Wiley-VCH, 2020.
This book is available to U Ottawa students in electronic form from the University of Ottawa library.

Other books for reference:
- Donald McQuarrie, Statistical Mechanics, Harper-Row.
- Terrell Hill, An Introduction to Statistical Thermodynamics, Dover.
- Mark Tuckerman, Statistical Mechanics, Theory and Molecular Simulation, Cambridge University Press.
- Gregory Wannier, Statistical Physics, Dover.

Papers to give insight into some of the topics discussed.
John P. Lowe. Entropy: Conceptual Disorder. J. Chem. Ed. 1988, 65, 403.
Robert L. Scott. The Heat Capacity of Ideal Gases. J. Chem. Ed. 2006, 83, 1071.

Learning outcomes

-Understand the concept of ensemble and to be able to reproduce the flow of statistical mechanical reasoning which extracts macroscopic information from the microscopic description of a system.

Link to University Regulation on Plagiarism and Academic Fraud

Library information on plagiarism
University regulations

Language of Instruction:

- English

- Please note (Academic regulation I-2 on bilingualism): All students have the right to produce their written work and to answer examination questions in the official language of their choice, regardless of the course's language of instruction.