

STATISTICAL MECHANICS, CHEM 563

Spring 2021

Instructor: Davit Potoyan	Time: MW at 1:40pm – 3:00pm
Email: potoyan@iastate.edu	Place: Hach 1221.

Course Pages:

1. <https://canvas.iastate.edu/courses/77227>
2. <https://github.com/DPotoyan/Chem563>

Office Hours (Webex): Scheduled on individual basis. Slack is used as means for quick communication and discussions outside of lecture hours.

Format of Lectures (In-person): Lectures will be done in person. Video tutorials dedicated to numerical aspects will be pre-recorded and placed in Canvas.

Objectives: The objective of this course is to provide a gentle introduction to theoretical ideas and computational tools of statistical mechanics with a particular emphasis placed on computer simulations. Completion of the course will arm students basic skills to take advantage of computer simulating techniques for solving problems in chemistry, physics, biophysics and material science. The lectures consist of discussions of theoretical ideas, hands on paper and pencil problem solving and building computer simulations of toy model systems. All the coding is done mostly in Python3 which has become a universal language used by both computational experimental researchers from diverse fields. No programming experience is assumed. A brief introduction to python and scientific computing will be given at the beginning of the class which would be followed up by regular lab sessions/office hours. All of the computations can be done using a personal laptop or in the cloud via *GoogleCollab* using any on campus computer connected to fast internet.

Main References: The main textbook(s) which we will be following are.

- Casquilho and Teixeira *Introduction to Statistical Physics* 2014.
(Succinct exposition combining the fundamental theory with practical simulation concepts)
- Dill and Bromberg *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics and nanoscience*, 2010 2nd edition.
(Fairly detailed text with great visuals focusing on applications to chemical and biochemical problems.)

Recommended texts: For a good undergraduate refresher on thermodynamics and probability theory see the following texts

- SJ Blundell KM Blundell, *Concepts in Thermal Physics*, 2009.
- A Lawrence, *Probability in Physics*, 2019

Tentative Course Outline:**A. Physics, complexity and probability****A1** Math refresher: probabilities, calculus and linear algebra**A2** Intro to Statistical mechanics: Molecular diffusion and random walks**A3** Intro to the Monte Carlo and sampling ideas**A4** Intro to simulation, numerical stats and machine learning**B. Statistical Mechanics of non-interacting systems****B1** Thermodynamics: 2nd law, free energies and legendre transforms.**B2** Equilibrium, ergodicity and entropy.**B3** Canonical and grand-canonical ensembles.**B4** Quantum gases: Fermi and Bose statistics**C. Theory of phase transitions****C1** Ising models and lattice gas**C2** Computer simulations of ising models**C3** Critical phenomena, scaling and renormalization group ideas**C4** Enhanced sampling ideas for modeling rare events**D. Statistical Mechanics of interacting systems****D1** Liquid state theory: distribution functions, virial coefficients**D2** Perturbation methods and free energy calculations**D3** Computer Simulations of simple fluids: MD and MC**D4** Computer Simulations of complex fluids, biopolymers and colloids**Grading Policy:** Homework (30%), Midterm (30%), Final (40%)**Important Dates:**

Midterm March 22

Final Exam May 4, 12:00 PM

Prerequisites: Chem 325 and an undergraduate-level understanding of thermodynamics and multi-variate calculus.**Disabilities:** If you have a documented disability that requires assistance, you will need to go to the Disability Resource (DR) Office for coordination of your academic accommodations. The DR Office is located in the Student Services Building, Room 1076. The DR office phone number is 515-294-7220, TDD 5152946335.**Statement:** Iowa State University supports and upholds the First Amendment protection of freedom of speech and the principle of academic freedom in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.