

STATISTICAL MECHANICS, CHEM 563

Spring 2024

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

Course Pages:

1. Canvas page
2. Online lecture notes: <https://dpotoyan.github.io/Statmech4ChemBio>

Office Hours Scheduled on individual basis. Slack and Canvas will be used for quick communication and discussions outside lecture hours.

Objectives: The main objective of the course is to introduce the fundamental theory and computational techniques of statistical mechanics. The course is specifically designed for students with research interests in chemistry, physics, biophysics and material science. The lectures consist of group discussions, hands on paper and pencil problem solving and building computer simulations. All the coding is done in python. No programming experience is assumed. A brief introduction to python and scientific computing will be given at the beginning of the class. All of the computations will be in the cloud via *GoogleCollab*. Hence any working laptop connected to internet should suffice.

Main References:

- Malcolm P. Kennett *Essential Statistical Physics* 2020.
(Main required text)

Recommended texts:

- Dill and Bromberg *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and nanoscience*, 2010 2nd edition.
(Slow-paced text with plenty of examples, graphical illustrations, and solved problems. More focused on applications to chemical and biochemical problems.)
- SJ Blundell KM Blundell, *Concepts in Thermal Physics*, 2009. (A rather comprehensive and lucid exposition of fundamentals of thermodynamics, thermal physics and statistical thermodynamics)

Tentative Course Outline:**A. Probability, statistics and sampling****A1** Math and python refresher**A2** Statistical mechanics of random walks and diffusion**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 transform.**B2** Micro-canonical ensemble**B3** Canonical and grand-canonical ensembles.**B4** Molecular applications of equilibrium statistics**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** Monte Carlo simulations of fluids**D4** Molecular Dynamics simulations of fluids**Grading Policy:** Homework and participation (70%), Final project (30%)**Important Dates:**

HW due every Tuesday in class

Final Exam TBD

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.**Free Expression:** 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 appropriately.**Face masks encouraged:** Because of the continuing COVID-19 pandemic, all students are encouraged but not required to wear face masks, consistent with current Centers for Disease Control and Prevention recommendations. Further information on the proper use of face masks is available [here](#).

Vaccinations encouraged: All students are encouraged to receive a vaccination against COVID-19. Multiple locations are available on campus for free, convenient vaccination. Vaccinations may also be obtained from health care providers and pharmacies. Further information is available [here](#).

Physical distancing encouraged for unvaccinated individuals: Classrooms and other campus spaces are operating at normal capacities, and physical distancing by faculty, staff, students, and visitors to campus is not required. However, unvaccinated individuals are encouraged to continue to distance themselves from others when possible physically.