

STATISTICAL MECHANICS IN CHEMISTRY

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February 23, 2026

General information of the course

- **Time and place:** Summer semester, Tuesdays, 10:15 AM – 12:00 AM, room F7.
- **Consultation time:** Thursdays, 1:00 PM – 3:00 PM, room B325 or online.
- **Method:** Classroom lectures
- **Assessment & scoring:** Problem sets.
- **Lecture slides and problem sets:**
<https://liwo.strony.ug.edu.pl/DigitChem/index.html>

Course scope

- 1 Introduction: molecular geometry, energy surfaces of molecular systems.
- 2 Basic concepts of probability calculus: probability, random variables, probability distribution, moments of probability distribution.
- 3 The Boltzmann law.
- 4 Ensembles: microcanonical, canonical, and grand canonical ensemble. The Boltzmann cell method.
- 5 Basic concepts of chemical thermodynamics: variables of state, functions of state, Guggenheim diagram.
- 6 Statistical sums and their connections to system properties.
- 7 Entropy, heat, and work in statistical mechanics. Relationship of entropy and information theory.
- 8 Simple applications of statistical mechanics: photon gas, crystals.

Course scope

- 9 Bose-Einstein and Fermi-Dirac statistics. The λ transition in liquid helium.
- 10 Statistical mechanics of an ideal monoatomic gas. Atomic terms.
- 11 Statistical mechanics of an ideal diatomic and polyatomic gas. Normal modes, rotational and vibrational levels and symmetry numbers of molecules.
- 12 Energies and equilibrium constants of chemical reactions in the gas phase.
- 13 Statistical mechanics of non-ideal gases and liquids. Meyer's diagrams and correlation functions.
- 14 Potentials of mean force and coarse graining.
- 15 Statistical mechanics and molecular simulations.

Literature

- 1 P. Atkins, R. Friedman: Molecular Quantum Mechanics, Fourth Edition (<https://web.stanford.edu/oas/SI/QM/Atkins05.pdf>)
- 2 D. McQuarrie: Statistical Mechanics.
- 3 A. R. Leach: Molecular Modeling: Principles and Applications.
- 4 F. Reif: Statistical Mechanics (part of Berkeley Physics Course).
- 5 K. Huang: Statistical Mechanics.
- 6 R.P. Feynman: Statistical Mechanics. A Set of Lectures.