STATISTICAL MECHANICS IN CHEMISTRY

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General information of the course

- **Time and place:** Summer semester, Thursdays, 10:15 AM – 12:00 noon, room C209.
- **Consultation time:** Wednesdays, 10:00 AM – 12:00 noon, room B325 or online.
- **Method:** Classroom lectures
- **Assessment & scoring:** Problem sets, final test.

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 distributon.
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. D. McQuarrie: Statistical Mechanics.
2. A. R. Leach: Molecular Modeling: Principles and Applications.
3. F. Reif: Statistical Mechanics (part of Berkeley Physics Course).
4. K. Huang: Statistical Mechanics.
5. R.P. Feynman: Statistical Mechanics. A Set of Lectures.