CHAPTER OVERVIEW

7: Statistical Mechanics

Learning Objectives

In this Chapter, you will be introduced to many of the main concepts and methods of statistical mechanics. You will be familiar with the following topics:

a. Microcanonical, canonical, and grandcanonical ensembles and their partition functions.
b. Ensemble averages being equal to long-time averages; the equal a priori postulate.
c. Fluctuations
d. Expressions for thermodynamic properties in terms of partition functions.
e. Monte Carlo methods including Metropolis sampling and umbrella sampling.
f. Molecular dynamics simulations, including molecular mechanics force fields.
g. Coarse graining methods.
h. Time correlation functions.
i. Einstein and Debye models for solids' phonons.
j. Lattice theories of adsorption, liquids, and phase transitions.
k. Virial expansions of thermodynamic properties.

When one is faced with a system containing many molecules at or near thermal equilibrium, it is not necessary or even wise to try to describe it in terms of quantum wave functions or even classical trajectories following the positions and momenta of all of the constituent particles. Instead, the powerful tools of statistical mechanics allow one to focus on quantities that describe the many-molecule system in terms of the behavior it displays most of the time. In this Chapter, you will learn about these tools and see some important examples of their application.

Contributors and Attributions

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