CBE 310
Molecular Concepts and Applications

Quantum Chemistry Review

Introduction to Statistical Mechanics

2014 10 06

Statistical Mechanics

Defining statistical mechanics:

Statistical Mechanics provides the bridging connection between microscopic world governed by the laws of quantum mechanics and the macroscopically observable world that is described by thermodynamics.

The macroscopically observable quantities such as temperature, pressure, entropy, free energy, heat capacity, chemical potential, viscosity, spectra, reaction rates, etc. can be derived and /or explained as the average properties of large collection of individual molecules with particular quantum mechanically allowed behaviors.

Why do we need Statistical Mechanics?:

1. Why not just solve everything using quantum mechanics?

   The problem is that real systems are much to large and complex to be solved. Statistical Mechanics provides a way of bridging this divide based on the statistical properties of very large assemblies. The microscopic behavior of atoms can be transformed into thermodynamics. Without this description based on a physical model of the world thermodynamics is just a phenomenological theory.

2. Statistical mechanics offers a way to go beyond thermodynamics and examine non-equilibrium situations as well as properties that depend on a detailed molecular view of matter

3. Ultimately statistical mechanics is the molecular theory of thermodynamics, it offers a window into the microscopic details that give rise to macroscopically observable phenomena.