The main objective of this course will be to show the relationship between energy levels characteristic of individual atoms and molecules and the properties of macroscopic bulk samples. The course will be taught with the assumption that students have had a solid exposure to basic chemical thermodynamics (Chem 351 level) and quantum mechanics (Chem 352 level). The course will follow and cover Chapters 1 through 9 of McQuarrie’s book Statistical Thermodynamics and include:

- A review of chemical thermodynamics, including the 1st and 2nd laws, Legendre transforms, and conditions for equilibrium and stability.
- An introduction to statistical mechanics with descriptions of different types of ensembles and how they can be used to connect quantum mechanics to thermodynamics.
- Discussion of Boltzmann, Fermi-Dirac and Bose-Einstein statistics.
- Application of statistical mechanical methods to determining the equation of state for gases.
- Discussion of how one can calculate thermodynamic quantities such as $\Delta H$, $\Delta S$ and $\Delta G$ at 298 K for a molecule starting from an ab initio calculation on the molecule.
- In the last part of the semester, once Chapters 1 through 9 have been covered, we will discuss how statistical mechanical ideas are used in either the basic principles of performing molecular simulations on materials or describing the properties of nanomaterials.

**Grading**

The final grade will be determined through extensive problem sets (30%), two Midterms (40%) and a Final Exam (30%)

**Recommended Texts:**

“Statistical Mechanics” or “Statistical Thermodynamics”, Donald A. McQuarrie, University Science (2000).

Some useful background reading:

“Physical Chemistry”, Peter Atkins and Julio de Paula.