CME 572: Advanced Thermodynamics of Materials (Spring 2019)

Meetings: Wednesdays 5-7:30 PM, Lecture Center Building A, Room A005
Instructor: Sara Kadkhodaei (Email: `sarakad@uic.edu`)

Understanding the equilibrium properties of materials throughout the laws of thermodynamics is essential in a wide range of disciplines, e.g., physics, chemistry, materials science, chemical engineering, mechanical engineering, etc. In this course, we review the theory of statistical thermodynamics, a probabilistic approach that describes the equilibrium properties of materials in terms of the microscopic variables of their constituents (atoms, molecules, etc). Moreover, we study the application of laws of thermodynamics to equilibrium and properties of materials, which lays out the foundation to treat general phenomena in materials, including phase transformations, chemical reactions, magnetism, elasticity, etc.

In the first half of the course meetings, we explore the fundamental concepts and techniques of statistical mechanics which provides us with the theoretical tool to study many-particle systems. In the second part of the course, we will study the application of the thermodynamic concepts to the analysis of phase equilibria, phase transformations, and phase diagrams starting from one-component until multicomponent systems. Finally, we will combine the theoretical tools discussed throughout the course to examine the thermodynamics properties of a real physical system via computational techniques, including i) state of the art quantum mechanical computer programs (eg., abinit) to explore the microscopic actions of atoms, and ii) computer programs for thermodynamic modeling to obtain macroscopic equilibrium states and build phase diagrams (eg., FactSage, Pandat).