Applications of quantum chemistry to (1) the interaction of electromagnetic radiation with matter for spectroscopy and strategic bond breaking and (2) the behavior of electrons in solids – insulators, conductors, and semiconductors. Quantum and statistical mechanics for classical thermodynamics – 1st and 2nd laws, phase equilibrium, chemical equilibrium, and heat pumps. Devising rate equations for chemical reactor design from experiment and theory – kinetic theory of gases and transition state theory.

Learning Outcomes:

- Predict the outcome of electromagnetic radiation interacting with a substance – heating, chemical dissociation, or ionization.
- Predict if a solid is an insulator, conductor, or semiconductor.
- Understand the effects of doping a semiconductor for electronic devices – conduction paths, diodes, and transistors.
- Analyze experimental data to obtain a rate equation.
- Analyze a rate equation, an overall reaction, and chemical intuition to devise a mechanism of elementary chemical reactions for homogeneous and heterogeneous (solid-catalyzed) reactions.
- Predict the spontaneity of a chemical process.
- Devise a heat engine or heat pump and calculate the efficiency.
- Analyze the phase behavior of a pure substance.
- Predict the spontaneity of a chemical process; design a chemical reactor with recycle.