THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING

Computational Catalysis

CBE 5710

Credit Hours:
3.00 - 3.00

Course Components:
Lecture

Course Description:
Methods used to model catalyst reactivity at the atomic-scale; application of quantum methods, primarily density functional theory (DFT); kinetic Monte Carlo and microkinetic modeling; using DFT to simulate surface science and catalysis spectroscopy methods.

Prerequisites and Co-requisites:
Prereq: 3610 and Chem 4300; or Grad standing; or permission of instructor.

Course Goals / Objectives:
- Understand basic catalyst kinetic and surface science experiments with the goal of trying to model this output from computational modeling
- Run practical DFT calculations for surface reactions
- Use statistical mechanics with DFT to evaluate the free energy and rates of surface processes (diffusion, adsorption/desorption, reaction).
- Use kinetic Monte Carlo (kMC) or microkinetic modeling to study catalyst kinetics.
- Become aware of advantages and limitations of molecular modeling in catalysis
- Synthesize modeling results and interpret in relation to catalyst experiments
- Understand and evaluate literature involving computational catalysis