

Dr. Stacey Wetmore

Advanced Computational Chemistry

This course will extend upon the ideas presented in Chemistry 3730 (Advanced Physical Chemistry) related to using computers to model the structure and properties of molecules. The theory behind techniques based on *ab initio* and density functional theory will be covered in depth. Techniques based on classical mechanics (molecular mechanics, molecular dynamics), as well as hybrid methods, will also be discussed. Other topics that may be presented include how to calculate charge distributions, spectroscopic properties and thermodynamic properties, as well as how to model condensed phases and excited states. An emphasis will be placed on understanding the computational techniques and routines used to model molecules that extend beyond simple calculations in the gas phase. Laboratory assignments will use sophisticated computational chemistry software packages, such as Gaussian 03, and high-performance computing resources to apply techniques discussed in class.

Prerequisites: Chemistry 2600 and Chemistry 3730