

Dr. Stacey Wetmore

Introduction to Molecular Modeling

This course will provide an introduction to the use of computer simulations to study chemical systems. Basic background of the theory behind techniques commonly used to model chemical structures, properties and reactions will be presented. Emphasis will be placed on understanding the benefits and disadvantages of different computational models and how to use these techniques in conjunction with experimental data to gain a greater understanding of chemical processes. The laboratory component will use common chemistry software packages to apply techniques discussed in class, and recent chemical literature will be reviewed and critiqued.

Prerequisites: Chemistry 2600 and Chemistry 2740