

## Chemistry 477: Computational Chemistry

*Course description:* The course aims to develop an understanding of the benefits and limitations of applying different computational models to chemical phenomena, accounting for the relevant length and time scales and including the appropriate molecular behaviours.

### Course Goals

Develop an understanding of the different types of interactions between molecules

Develop the ability to apply quantitatively the formalism of quantum mechanics to standard systems

Develop the ability to apply qualitatively the concepts of quantum mechanics to chemical bonding and standard chemical systems.

Develop an understanding of how computational methods are applied to chemistry

Develop the ability to use computational chemistry/molecular modeling software

Develop an understanding of the relationship between the accuracy of a calculation and the assumptions of a model

Develop the ability to use theoretical frameworks in chemistry to rationalise or predict experimental observations

Develop an understanding of the different theoretical frameworks for bonding and structure

Develop the ability to quantify macroscopic properties based on molecular energy levels

Develop an understanding of the mathematical description of molecular bonding

### Program Goals

Develop the ability to represent chemical information.

Develop the ability to apply mathematics to chemistry.

Develop an understanding of the use of models, their premises, advantages and limitations.

Develop competence in problem solving.

Develop the ability to use the chemical literature in a critical manner.