

## **CBC 733 - Advanced Computational Chemistry**

### **Aims and objectives**

To introduce various simulation programs and demonstrate their applications in selected research areas. To educate students to use these software to assist in their experimental research.

### **Syllabus**

Student attending the course will learn how to choose and how to use appropriate computer programs to study reaction mechanisms, catalysis, transport phenomena, organic and bioorganic binding, device simulations and molecular conformation. Students will be required to complete a computational project in discussion with the module lecturer and their research advisor to obtain hands-on experience.

### **Assessment**

Lab report: 20 %

Course project: 80 %

### **Prerequisites**

PhD Advisor and Division approval.