

School of Chemistry

Aims and Objectives: Session 2023-2024, Semester 1

Module CH4716: Electrochemistry and Computational Chemistry

Course Title: Computational Chemistry

Duration: 10 hours

Lecturer: Professor M. Buehl

Aims: This part of the course will build on the foundations laid in module CH2701 and introduce further aspects of modern computational chemistry related to the electronic structures of atoms and molecules. The goal is to achieve a basic understanding of the underlying approximations made in practical calculations and to appreciate the strengths and weaknesses of the resulting "model chemistries".

Objectives:

1. To provide an introduction into the Hartree-Fock method and basis sets used with it.
2. To provide an introduction into electron correlation and its approximation through *ab initio* and density functional methods.
3. To consider applications of computed structures and energies in chemistry.