

Advanced Computational Chemistry

School of Chemistry

College of Engineering and Physical Sciences

Details

Code 10861

Level of study Third/Final year

Credit value 10

Semester 1

Module description

This course is designed to provide an introduction to the role that computers play in modern chemistry. Students will obtain an understanding of how computation relates to a number of areas of chemistry, and how it can help as an investigative tool complementary to experiment. The course is divided into four parts to illustrate different aspects of computational chemistry covering simulation methods, genetic algorithms and swarm intelligence for search and optimisation, computer programming, and the use of computer simulations to study biochemical problems.